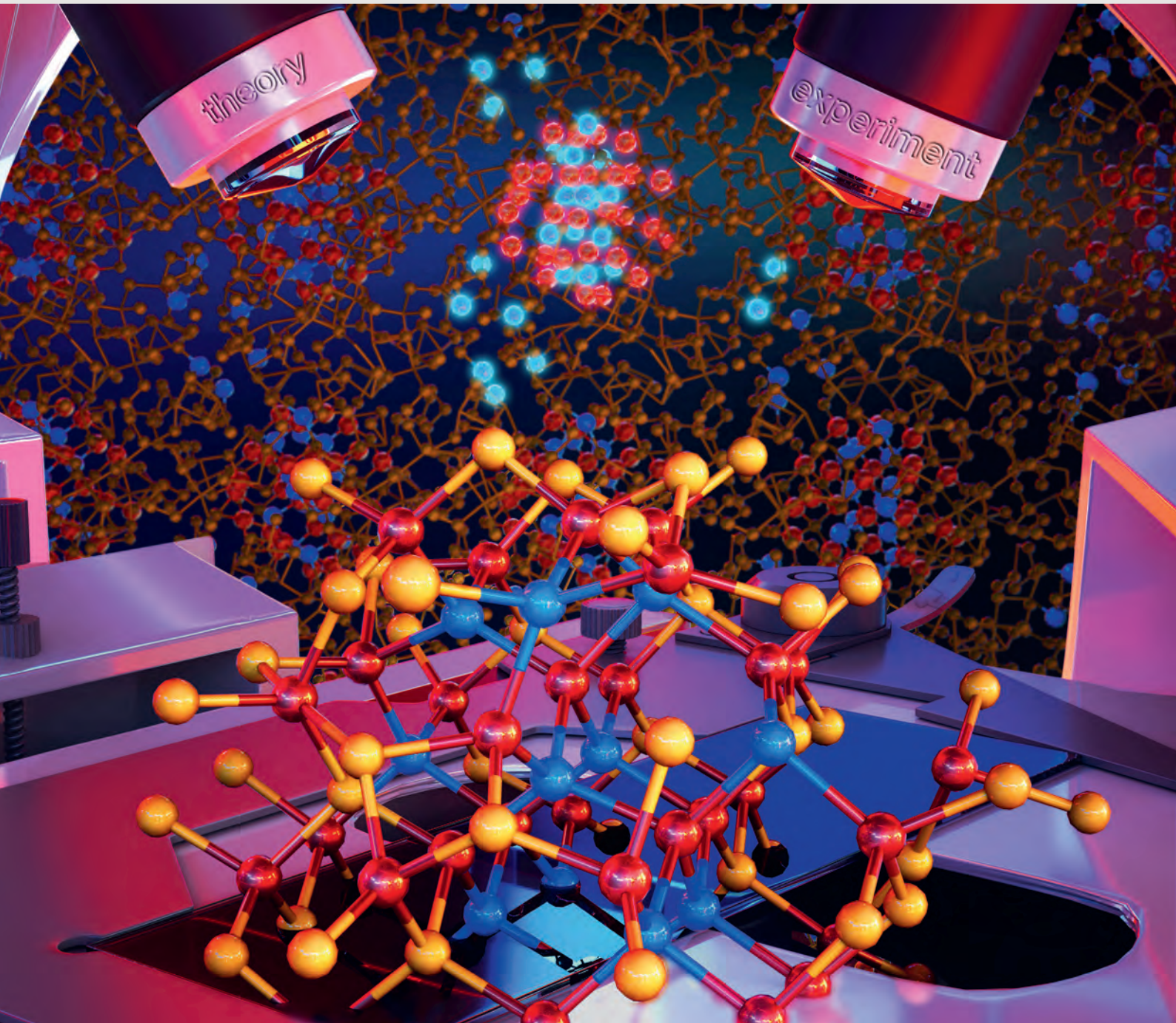
MAX-PLANCK-GESELLSCHAFT

# Scientific Report 2016 - 2018

Max-Planck-Institut
für Eisenforschung GmbH



Max-Planck-Institut für Eisenforschung GmbH

# Scientific Report 2016 - 2018

December 2018
Max-Planck-Institut für Eisenforschung GmbH
Max-Planck-Str. 1 · 40237 Düsseldorf
Germany

*Front cover*

A joint theoretical and experimental approach, represented by the dual microscopes, allows to isolate individual nanoparticles within nanoparticle-in-glass systems (background). The interfaces between nanoparticles and their surrounding matrix can be characterized with atomistic resolution.

Scalise, E.; Srivastava, V.; Janke, E.; Talapin, D.; Galli, G.; and Wippermann, S. M.: *Surface chemistry and buried interfaces in all-inorganic nanocrystalline solids.* Nat. Nanotechnol. 13 (2018) 841

Picture: S. Wippermann, P. Allen

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Max-Planck-Str. 1, 40237 Düsseldorf, Germany
Phone: +49-211-6792-0
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Homepage: http://www.mpie.de

*Editorship, Layout and Typesetting*
Yasmin Ahmed Salem
Katja Hübel
Brigitte Kohlhaas
Frank Stein

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# *PREFACE*

This report documents the scientific activities and achievements of the Max-Planck-Institut für Eisenforschung GmbH (MPIE) focussing on the years 2016 to 2018. For evaluation purposes, some main trends are described over the past 6 years. Also, selected long-term methodological and large collaborative projects are presented.

Our mission is to understand and design nanostructured materials down to atomic and electronic scales. In this spirit, we conduct basic research on structural and functional materials, mostly metallic alloys, embracing synthesis and processing, characterization and properties, as well as their response in engineering components exposed to harsh environmental conditions.

We work interdisciplinary, with intense mutual stimulation among experimentalists and theoreticians as well as among different groups and departments. Fields of particularly intense interaction are:

- Stability of Surfaces and Interfaces
- Microstructure-related Materials Properties
- Development of Advanced Materials
- Scale-bridging Simulation and Materials Informatics

Along these topics we enable progress in key fields of highest relevance for manufacturing and society:

- Mobility (e.g., ductile magnesium, steels and magnets for light weight hybrid vehicles)
- Energy (e.g., hydrogen-tolerant structural alloys, catalysis materials, high temperature alloys, semiconducting materials for photovoltaics and photo-electrochemistry, fuel cell components)
- Infrastructure (e.g., steels for infrastructures, such as wind turbines and chemical plants)
- Medicine (e.g., biomedical tribology, compliant implant alloys)
- Safety (e.g., high toughness alloys, cryogenic alloys, coatings and thin film materials, hydrogen tolerant materials).

Our projects rest on pre-competitive fundamental research, yet, we also consider applications and system challenges. With this agenda and our institutional co-sponsoring by industry, the MPIE is a unique example of more than 100 years public private partnership both for the Max Planck Society and for the European industry. We took this last year's anniversary also as an opportunity to celebrate with a scientific colloquium, a public outreach program and a scientific project about the history of the Institute. We pursue strategic collaborations with several academic partners, namely, R. Kirchheim (materials physics; University of Göttingen) who is an external scientific member of the Max Planck Society, J. Schneider (combinatorial and self-reporting materials; RWTH Aachen University) who is a fellow of the Max Planck Society and with G. Eggeler (high temperature alloys; Ruhr-Universität Bochum) who is an external group leader at the MPIE. These and other collaborations have helped to intensify our scientific network with participation in large projects funded by Deutsche Forschungsgemeinschaft, e.g., the collaborative research centers SFB 761 (TWIP steels), TR 103 (novel superalloys), TR 188 (damage controlled forming), and SFB 1232 (combinatorial alloys design).

Out of the 372 people working at the MPIE the majority (266) are scientists. 130 scientists are funded from the basic budget and about 136 additional scientists are supported by external sources, such as the European Research Council (ERC), German Research Foundation (DFG), Alexander von Humboldt Foundation (AvH), Research Fund for Coal and Steel (RFCS), German Academic Exchange Service (DAAD), Bundesministerium für Bildung und Forschung (BMBF), the Max Planck Graduate School IMPRS-SurMat, Chinese Scholarship Council (CSC), and Bundesministerium für Wirtschaft und Energie (BMWi) to name but a few.

Numerous strategically selected industry partners provide further momentum to the dynamic growth of the MPIE. Besides well-established links to the steel industry regarding medium manganese steels, advanced characterization, surface functionalization, and computational materials science, several new collaborations were established also in non-ferrous materials research fields. Examples are additive manufacturing

and design of aerospace alloys, through process and texture simulation in the aluminium industry, fuel cell and hydrogen-systems related materials for the automotive industry, superalloys for airplane turbines and hydrogen tolerant Nickel alloys. This mixture of third-party funds from fundamental and applied science places the MPIE into a singular position within the Max Planck Society.

The MPIE researchers have achieved several scientific breakthroughs in the past years, e.g., on the interplay of lattice defects and local composition, machine learning and quantitative simulation in materials science, nanostructured steels and high entropy alloys, self-healing coating systems, structure-chemistry imaging of catalyst nanoparticles, ductile Magnesium alloys, and new methods on joint atomic scale imaging of structure and chemistry.

These breakthroughs were enabled by several long-term methodological projects which led to the development of novel experimental and simulation tools. Examples are the combinatorial corrosion and catalysis probing cell, the scanning Kelvin probe, the correlative atom probe tomography (APT) - transmission electron microscopy (TEM) analysis conducted on the same specimens, the field ion microscopy time of flight methods, the simulation toolbox DAMASK, the wet chemical cell for *in situ* reaction analysis in TEM, the computational framework *pyiron* that provides automated tools for high-throughput calculations using high precision *ab initio* simulation methods and the site specific mechanical testing strategies under harsh environmental conditions.

This report is structured into four parts:

- *Part I* presents the organization of the Institute including a short section on recent scientific developments, new scientific groups, large network activities, and new scientific laboratories.
- *Parts II* and *III* cover the research activities of the Institute. Part II provides a description of the scientific activities in the departments and Part III contains selected short papers which summarize major recent scientific achievements in several topical areas of common interest at the MPIE.
- *Part IV* summarizes statistically relevant information about the Institute.

The Directors of the MPIE

Düsseldorf, December 2018

# CONTENTS

# PART I.

# THE INSTITUTE

# Management of the Institute

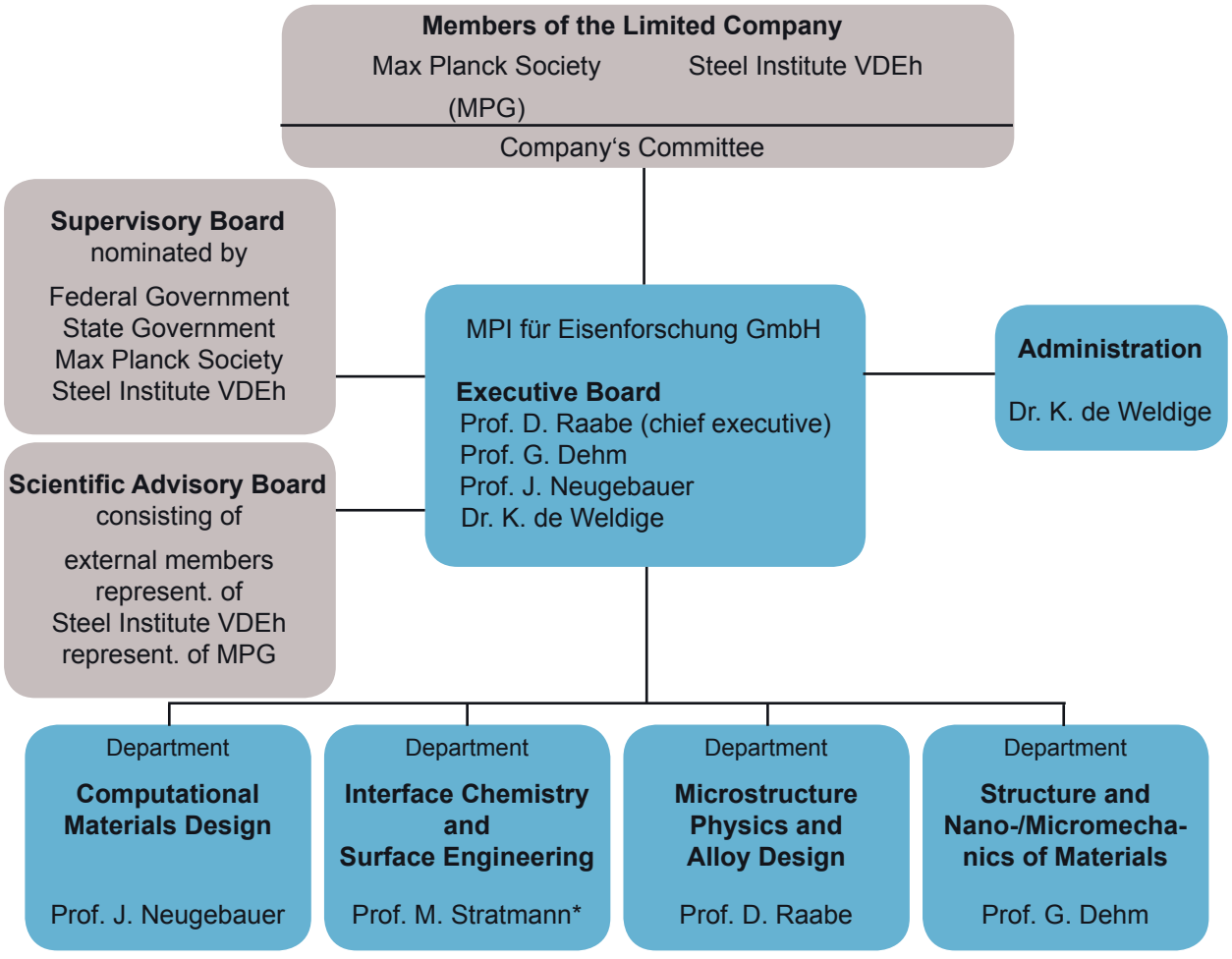
The Max-Planck-Institut für Eisenforschung GmbH (MPIE) is a joint venture between the Max Planck Society and the Steel Institute VDEh. As the Institute's budget is supplied indirectly through industry, this Institute is unique within the Max Planck Society.

The Institute was founded in 1917 by the Verein Deutscher Eisenhüttenleute (VDEh) and incorporated into the Kaiser-Wilhelm-Gesellschaft, the predecessor of the Max Planck Society. The MPIE was first located in Aachen and was associated with the Technical University of Aachen. Later, in 1934/35, the Institute moved to its present location on a site donated by the city of Düsseldorf.

In 1946, the Institute's heavily damaged buildings were reconstructed, work resumed and the MPIE was integrated into the newly formed Max Planck Society in 1948. The Institute rapidly expanded and new laboratory buildings were built in the early 1960s. Following the appointment of H.J. Engell as director in 1971, a complete reorganization of the Institute was carried out. Since then it has operated on the legal basis of a limited liability company (GmbH) and its budget is covered by the Steel Institute VDEh and the Max Planck Society.

Until 2002, the Institute was headed by a chief executive director (1971-1990: Prof. Engell, 1990-2002: Prof. Neumann) and an associated administrative director. Since June 2002, all scientific members and the administrative head of the Institute form an executive board of directors. The position of a managing director is filled, in rotation, by one of the board members. A board, the Supervisory Board, reflects and debates with the MPIE management and shareholders on strategic questions regarding fundamental scientific research related to corporate purpose; it consists of representatives from the federal government, the state of North Rhine-Westphalia, the Max Planck Society and the Steel Institute VDEh. A Scientific Advisory Board comprised of prominent scientists assists the Institute in balancing fundamental research and technological relevance.

MAX-PLANCK-INSTITUT FÜR EISENFORSCHUNG GMBH
Management and Organization (Nov. 2018)




* Prof. M. Stratmann is on leave. Provisional head of the department is Prof. J. Neugebauer.

# Scientific Organization

The Institute conducts fundamental research on metallic alloys and related materials. It pursues a holistic approach where material systems are studied under consideration of their complex compositions and nanostructures on the one hand and their exposure to extreme environmental conditions on the other hand.

The Institute has four departments:

- Computational Materials Design (Prof. J. Neugebauer): exploration of materials properties and processing based on *ab initio* (parameter free) multiscale simulation techniques
- Interface Chemistry and Surface Engineering (Prof. M. Stratmann; on leave, provisional head: Prof. J. Neugebauer): environmentally accelerated degradation of surfaces and interfaces by corrosion and de-adhesion. Engineering of new and stable surfaces and interfaces
- Microstructure Physics and Alloy Design (Prof. D. Raabe): Development of novel metallic materials and microstructures with improved mechanical and functional properties using simulation, microscopy, atom probe tomography and diffraction methods
- Structure and Nano-/Micromechanics of Materials (Prof. G. Dehm): Understanding the structure and imperfections of metals, alloys and intermetallics by advanced electron microscopy and exploring their interplay with mechanical and tribological properties at small length scales by *in situ* nano-/micromechanical approaches

Each department consists of several research groups, which are managed by group leaders. In addition to the departments an Independent Max Planck Research Group, headed by Prof. C. Scheu on Nanoanalytics and Interfaces has been established in 2014. The figure on page 12 shows the organization of the groups and their scientific aims. Part II of this report reviews the scientific concepts and achievements of the departments and the research conducted in the individual groups.

In addition to the individual scientific goals of the departments, many research topics are highly interdisciplinary and require the experimental and theoretical expertise of several departments, enabling breakthroughs in highly competitive research areas. Part III describes selected scientific highlights including such interdepartmental research activities. It is divided into the four topics:

- Stability of Surfaces and Interfaces
- Microstructure-related Materials Properties
- Development of Advanced Materials
- Scale-bridging Simulation and Materials Informatics

Several short papers on selected scientific topics provide an overview of results obtained during the last years for each of these central research areas.

The organisation of research within the MPIE, both vertically in departments and research groups with highly specialized expertise as well as horizontally in the form of interdepartmental research activities, combines a high level of individual scientific skills available within each department and group with a highly ambitious cross-disciplinary spirit among them. It is the basis for the development of advanced materials with useful properties, combining, e.g., high mechanical strength with high surface functionality. This approach unleashes very high scientific synergy effects, which have enabled several exciting discoveries, more efficient use of scientific equipment, a homogeneous research profile and intense interdepartmental collaborations.

Service groups support the scientific departments with valuable expertise. These include the production, processing and testing of materials, chemical analysis of metallic substrates, metallography and a mechanical workshop equipped for handling hard and brittle materials, facilities to design and build scientific equipment, an electronic workshop, a library, a computer network centre and a research coordination office.

## Scientific Scopes of the Departments

| Department **Computational Materials Design** Prof. J. Neugebauer | Department **Interface Chemistry and Surface Engineering** Prof. M. Stratmann* | Department **Microstructure Physics and Alloy Design** Prof. D. Raabe | Department **Structure and Nano-/ Micromechanics of Materials** Prof. G. Dehm |
|---|---|---|---|
| Ab Initio Calculation of Thermodynamic and Kinetic Data | Electrochemical Surface Science | Alloy Design and Synthesis | Micro-/Nanomechanics and -tribology of Materials and Interfaces |
| Theoretical Studies on Microstructure Properties and Dynamics | Catalysis and Corrosion | Micromechanics | In situ Methods Interlinking Mechanics and Microstructure |
| Computer Aided Alloy Design | Adhesion and Functional Coatings, Surfaces and Interfaces | Correlative Atom Probe Tomography | Advanced Transmission Electron Microscopy |
| Multiscale Modelling | Fundamental Research on Surface and Coating Related Process Technology | Segregation Engineering and Interface Manipulation | Thin Films, Nanostructured Materials and Intermetallics |

## Interdepartmental Research Activities

| Department **Computational Materials Design** Prof. J. Neugebauer | Department **Interface Chemistry and Surface Engineering** Prof. M. Stratmann* | Department **Microstructure Physics and Alloy Design** Prof. D. Raabe | Department **Structure and Nano-/ Micromechanics of Materials** Prof. G. Dehm |
|---|---|---|---|
| **Stability of Surfaces and Interfaces** | | | |
| **Microstructure-related Materials Properties** | | | |
| **Development of Advanced Materials** | | | |
| **Scale-bridging Simulation and Materials Informatics** | | | |

* Prof. M. Stratmann is on leave. Provisional head of the department is Prof. J. Neugebauer.

# Scientific Groups and Departments (2018)

## Computational Materials Design
Prof. J. Neugebauer

- **Adaptive Structural Materials** — Dr. B. Grabowski
- **Computational Phase Studies** — Dr. T. Hickel
- **Computer Centre** — Dr. C. Freysoldt
- **Defect Chemistry and Spectroscopy** — Dr. C. Freysoldt
- **Electrochemistry and Corrosion** — Dr. M. Todorova
- ERC Starting Grant **Bridging Length and Time with Atomistic Simulation** — Dr. B. Grabowski
- Fund. by The Netherlands Organisation for Scientific Research **Complex Concentrated Alloys** — Dr. F. Körmann (since Mar. 2017)

## Interface Chemistry and Surface Engineering
Prof. M. Stratmann*

- **Atomistic Modelling** — Dr. S. Wippermann
- **Corrosion** — Dr. M. Rohwerder
- Guest Group **Electrocatalysis** — Dr. K. J. J. Mayrhofer
- Guest Group **Interaction Forces and Functional Materials** — Dr. M. Valtiner
- Guest Group **Interface Spectroscopy** — Dr. A. Erbe

## Microstructure Physics and Alloy Design
Prof. D. Raabe

- **Adaptive Structural Materials** — Dr. C. Tasan (until Dec. 2015)
- **Alloys for Additive Manufacturing** — Dr. E. Jägle
- **Atom Probe Tomography** — Dr. B. Gault (since Jan. 2016)
- **Biological Composites** — Dr. H. Fabritius (until Dec. 2017)
- **Combinatorial Metallurgy and Processing** — Dr. H. Springer
- **Microscopy and Diffraction** — Dr. S. Zaefferer
- **Mechanism-based Alloy Design** — Dr. D. Ponge
- **Theory and Simulation** — Dr. F. Roters
- ERC Consol.Grant **Hydrogen in Energy Materials** — Dr. B. Gault (since Jan. 2018)
- Funded by German Research Foundation **High-Entropy Alloys** — Dr. Z. Li (since Jan. 2017)
- Funded by BMBF **Materials Science of Mechanical Contacts** — Dr. M. Herbig (since Oct. 2016)
- Joint group with RWTH Aachen **Interface Design in Solar Cells** — Dr. O. Cojocaru-Mirédin

## Structure and Nano-/ Micromechanics of Materials
Prof. G. Dehm

- **Advanced Transmission Electron Microscopy** — Dr. C. Liebscher
- **Intermetallic Materials** — Dr. M. Palm, Dr. F. Stein
- **Nano-/ Micromechanics of Materials** — Dr. C. Kirchlechner
- **Nanotribology** — Dr. S. Brinckmann
- **Thin Films and Nanostructured Materials** — Dr. M. Ghidelli (since Nov. 2018)
- Max Planck Research Group **High Temperature Materials** — Prof. G. Eggeler

## Independent Max Planck Research Groups

- **Nanoanalytics and Interfaces** — Prof. C. Scheu
- **External Members and Fellows**
- Max Planck Fellow **Self-Reporting Materials** — Prof. J. Schneider
- External Scientific Members — Prof. M. Hillert, Prof. R. Kirchheim

## Scientific Service Groups

- **Synthesis and Processing** — Alloy production, Annealing & welding, Thermom. treatments — Dr. H. Springer
- **Metallography** — Light microscopy, Metallographic sample preparation, SEM — Dr. S. Zaefferer
- **Materials Testing** — Mechanical properties, Physical properties, Varying environments — Dr. H. Springer
- **Research Coordination Office** — Doctoral Programme, International Office, Public Relations, Research Funding — Dr. K. Hübel

* Prof. M. Stratmann is on leave. Provisional head of the department is Prof. J. Neugebauer.

# Recent Developments

Here we reflect some of the recent changes at the MPIE between 2016 and 2018 which have helped us to strengthen the Institute's scientific profile and administrative efficiency. For evaluation purposes some trends are described over the past 6 years.

Constructions on G. Dehm's advanced electron microscopy laboratory which is a key facility of his department on "Structure and Nano-/ Micromechanics of Materials" have been finished and a scientific opening workshop was held in November 2018. The microscopy group is a key asset in many cross-departmental research projects including interfacial interaction phenomena of structure and composition effects, precipitation and transformation phenomena and high entropy alloys as well as in essential methodological projects related particularly to the correlative use of electron microscopy and atom probe tomography. Activities by the department are further boosted by the ERC Advanced Grant that has been awarded to G. Dehm in 2018.

Likewise the independent research group on "Nanoanalytics and Interfaces" which was opened by C. Scheu in 2014 is fully operative, pursuing multiple interdisciplinary collaborations in the fields of hydrogen generation and fuel cell related materials problems, materials for catalysis and nanostructured thermoelectrics.

Permanent scientific stimulation among in-house groups and departments but also with external partners takes place through a bi-weekly inter-departmental workshop series where topics of high mutual interest are identified and discussed. In these discussion rounds often younger scientists take the lead and initiate new collaborations or identify new promising joint research topics of high scientific risk, gain and synergy. Examples for topics discussed in recent months are high throughput experiments, complexions, big data and machine learning in microscopy and atom probe tomography, simulation-enhanced analytical field ion microscopy, grain boundary segregation and ordering effects, high strength aluminium alloys, defect phase diagrams, medium and high entropy alloys, magnetic high entropy alloys, thermodynamics of high entropy alloys, nanostructures in tribological interfaces, lattice defects in thermoelectric materials to name a few.

Over the past 6 years several new research groups have been initiated, namely, the group on "Nanotribology" by S. Brinckmann, the group for "Nano-/Micromechanics of Materials" by C. Kirchlechner, the group for "Advanced Microstructure Characterization" by C. Liebscher, the group on "Electrochemistry and Corrosion" by M.Todorova and the group of "Synthesis of Thin Films and Nanostructured Materials" by M. Ghidelli (since November 2018). Further groups have been set up with the support of third-party funding, namely, the BMBF-funded group on "Interface Design in Solar Cells" by O. Cojocaru-Mirédin who is now a group leader at RWTH Aachen and co-operates the group under the new designation "Advanced Functional Materials", a BMBF NanoMatFutur funded group on "Semiconducting nanocomposites with tailored electronic and optical properties for solar energy conversion" by S. Wippermann, a BMBF funded group by M. Herbig on "Materials Science of Mechanical Contacts", a DFG supported initiative on "High-Entropy Alloys" headed by Z. Li, a group funded by the joint Max-Planck-Fraunhofer initiative on "Alloys for Additive Manufacturing" by E. Jägle, an ERC Starting Grant group by B. Grabowski on "Bridging Length and Time with Atomistic Simulation", a group on "Hydrogen in Energy Materials" which is funded by an ERC Consolidator Grant awarded in 2018 to B. Gault, and a group funded by the Netherlands Organisation for Scientific Research on "Complex concentrated Alloys" headed by F. Körmann. Guest groups have been set up in cooperation with our former group leaders: a guest group on "Electrocatalysis" by K.J.J. Mayrhofer (now at Helmholtz Institute Erlangen-Nürnberg for Renewable Energy), a guest group on "Interaction Forces and Functional Materials" by M. Valtiner (now at TU Vienna) and a guest group on "Interface Spectroscopy" by A. Erbe (now at NTNU Trondheim).

Also, several large-scale and networking projects were initiated or prolonged during the last years. Examples are European research networks like "AccMet - Accelerated Metallurgy - the accelerated discovery of alloy formulations using combinatorial principles", „ADVANCE: Sophisticated experiments and optimisation to advance an existing CALPHAD database for next generation TiAl alloys", "EPPL - Enhanced Power Pilot Line", „HERCULES-2 - Fuel flexible, near-zero emissions, adaptive performance marine engine", "MECANO - Mechanics of Nano-Objects", "PowerBase - Enhanced substrates and GaN pilot lines enabling compact power applications" as well as currently 6 RFCS projects. Another important collaboration is the cooperation with the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) at the Ruhr-Universität Bochum. ICAMS focuses on the development and application of a new generation of simulation tools for multi-scale materials modelling. Other initiatives included the joint group on "Adaptive Structural Materials" which was funded through an ERC Advanced Grant that was jointly awarded to J. Neugebauer and D. Raabe for the development of novel experimental and theoretical tools to

understand mechanisms associated with metastable phases in structural alloys. A newly established Max-Planck network project entitled BigMax is concerned with Big Data and Machine Learning in materials science and engineering (https://www.bigmax.mpg.de). It is an initiative where 10 Max Planck institutes collaborate on big data, machine learning, software science, applied mathematics and materials science. The MPIE is also participating in the MaxNet Energy, a research cooperation that aims at obtaining a deeper understanding of fundamental processes in chemical energy conversion and the rational design of novel catalysts, materials and techniques. Further funded networks include RESOLV (DFG Excellence Cluster), Initial Wear (Max-Planck-Fraunhofer initiative), CarMon (Leibniz-Max-Planck initiative) and the "Knowledge and Technology Platform for Prediction of Durability and Lifetime of Organic Coated Metals under Long-Term Environmental Corrosion" (joint project with the Free University of Brussels (VUB), within the framework of the Research Foundation - Flanders (FWO).

The Institute pursues also several large joint initiatives with its neighbour universities RWTH Aachen (SFB 761: Steel *ab initio*, 3rd funding period granted by DFG; newly founded Max Planck Fellow Group on Self-Reporting Materials by J. Schneider) and Ruhr-Universität Bochum (SFB/TR 103: Next Generation Single Crystalline Superalloys, 2nd funding period granted by DFG; International Max Planck Research School (IMPRS SurMat) which is managed by E. Gattermann and S. Wippermann; Center for Electrochemical Sciences; external research group of the MPIE on High Temperature Materials by G. Eggeler). The IMPRS SurMat has been recently successfully evaluated and prolonged, extending the number of members to now also including colleagues from the University Essen-Duisburg. Further joint collaborative research centers funded by Deutsche Forschungsgemeinschaft are the SFB TR 188 (damage controlled forming) with University Dortmund and SFB 1232 (combinatorial alloys design) with Bremen University.

Over the past years several group leaders from the MPIE received professorship offers from prestigious universities such as Ohio State University, Delft University, University Bern, Trondheim University, Erlangen University, University of Vienna, RWTH Aachen, University of Stuttgart, Massachusetts Institute of Technology (MIT), Shanghai Jia Tong University, Xian University, Indian Institute of Technology Bombay, Postech and the Korea Institute of Science and Technology KIST.

MPIE members were and are also involved in several science community und service activities such as serving as vice-president and president of the Max Planck Society (M. Stratmann), as member of the reviewer panel (Fachkollegiat) of the German Research Foundation DFG (J. Neugebauer), as head of the division Metals and Materials of the German Physical Society DPG (J. Neugebauer), member of the selection committee for the allocation of Humboldt Research Fellowships (G. Dehm), member of the selection committee for Max Planck Research Groups and the Lise Meitner Excellence Program (G. Dehm), panel member for the strategic evaluation of the research field "Matter" of the Helmholtz Association of German Research Centres (C. Scheu), member of the evaluation board of the state North Rhine Westphalia "EFRE NRW 2014 – 2020 "Neue Werkstoffe NRW" (C. Scheu), as a member of the German Council of Science and Humanities (Wissenschaftsrat) (D. Raabe), the Joint Strategy Commission (Strategiekommission) for the German Excellence Initiative (D. Raabe) and the Senat of the Helmholtz Association of German Research Centres (D. Raabe).

Several highly visible awards were won by MPIE members in the past years, among them an ERC Advanced Grant, an ERC Co-Investigator Grant, an ERC Consolidator Grant and two ERC Starting Grants, 6 Alexander von Humboldt Awards for Senior Professors, one Otto-Hahn Medal, the NRW Innovation Award, the DECHEMA-Award and 3 BMBF Junior Research Group Awards to name a few important recognitions. In 2017 the MPIE reached the 3rd best position in the Humboldt-Ranking among all non-university research organizations in Germany with 30 scholarships won between 2012 and 2016.

In order to stay connected to graduates and former scientists of the Institute and to benefit from their experience MPIE established a very active alumni network. A website launched in 2015 presents the Institute's research and achievements to different target groups ranging from scientists over students, journalists, politicians, industry representatives and pupils to the wider public. Measures to increase the Institute's visibility and to attract the next generation of junior scientists are: a new series of lectures named "KopfSalat", regular Kids' Labs, Kids' Universities and participation in the Girls' Day.

In the last years several measures to reconcile the demands of family and career have been taken. Since 2017 we have four reserved places in a day-care facility for children, in 2018 a Gender Equality Officer was elected and the Institute appointed a "MPIE Female Science Career Mentor".

With all these recent achievements we look now upon a period of more than 100 years of successful and sustainable public private partnership between the Max Planck Society and the European industry. We celebrated this anniversary in 2017 with a scientific colloquium, a public outreach program and a scientific project reviewing the history of the Institute.

# Max Planck Research Groups

## Independent Max Planck Research Group on Nanoanalytics and Interfaces

*Group Head: C. Scheu*

### Research Mission and Scientific Concepts

The scientific mission of the independent research group Nanoanalytics and Interfaces (NG) is to explore materials in all aspects of renewable energy applications by in-depth analyses of their nano-/microstructure. Material science concepts are less frequently applied in this field despite of their importance to design materials with better performance. The NG group correlates the findings of the nano-/microstructural analysis to the growth conditions and functionality, and uses them to improve synthesis and processing strategies. A strong focus is laid to understand the stability of nanostructured materials in harsh environments such as elevated temperatures.

**Fig. 1:** *The NG group in summer 2018.*

The core expertise of the NG group are *ex situ* and *in situ* electron microscopy-based techniques including aberration-corrected (scanning) transmission electron microscopy ((S)TEM), electron energy-loss spectroscopy (EELS), energy-dispersive X-ray spectroscopy (EDX), *in situ* heating experiments and electron tomography [1-25].

The NG group was founded in April 2014 by C. Scheu, who is at the same time a full professor at the RWTH Aachen University. The group has bachelor and master students, PhD candidates, and postdocs (Fig. 1), and a strong commitment in training and scientific education of young professionals. The group is also actively involved in supervising summer students and pupils of the Girl's day. Seven PhD students, two master students, and one bachelor student have graduated from the NG group with great success since 2014, some of them with distinction. Besides teaching at the RWTH Aachen University, C. Scheu also actively participates as a committee member in several university boards. She is also active as a co-supervisor of PhD students from RWTH Aachen University, Ruhr-University Bochum (RUB) and Ludwig-Maximilians-University (LMU Munich). Since October 2018 C. Scheu is the mentor at the MPIE for female postdocs and group leaders to support their career in science, in a similar way as she has done during her time at the LMU where she was the mentor for the faculty Chemistry and Pharmacy.

The close connection to several universities is also demonstrated in joint projects funded by the German Science Foundation (DFG) via individual grants with A. Ludwig (Prof. at RUB) and L. Schmidt-Mende (Prof. at University of Konstanz) or within DFG Priority Programmes such as the SPP 1613 and SFB 761/3 "Steel ab initio". Research funding is also received from the Federal Ministry of Economic Affairs and Energy (BMWi) and the Leibniz Association (see p. 57). The research activities of some of these projects will be described in more detail below. The NG group is also very well integrated within the MPIE and strong collaborations have been established in the last years with the other MPIE departments and the Max Planck Fellow Group on Self-Reporting Materials. This is reflected in a large number of jointly supervised PhD students, collaborative research work, and a large number of joint publications in the field of correlative aberration-corrected STEM and atom probe investigations partly coupled with atomistic simulations [26-32], dewetting of Al thin films on $Al_2O_3$ [9,10], electrochemistry [1,6,7,33,34] and on $Mo_2BC$ coatings [11-13,35,36] (see p. 183). Furthermore, the NG group has also an established network with international partners from Czech Republic, France, Israel, Sri Lanka and the USA.

C. Scheu is actively involved in the organization of national and international meetings and conferences. Recent examples are the co-organization of "Experimental and Theoretical insights on Interfaces of Ceramics" at the Conference on Electronic and Advanced Materials in Orlando, USA (2018) or "PS12 - Materials for Energy Production, Storage and Catalysis" at the 19th International Microscopy Congress (IMC19) in Sydney, Australia (2018). At the MPIE, she co-organized two workshops on "Challenges in Characterisation of Interfaces for Electrochemical Applications part I and part II" (2016/2017). In addition,

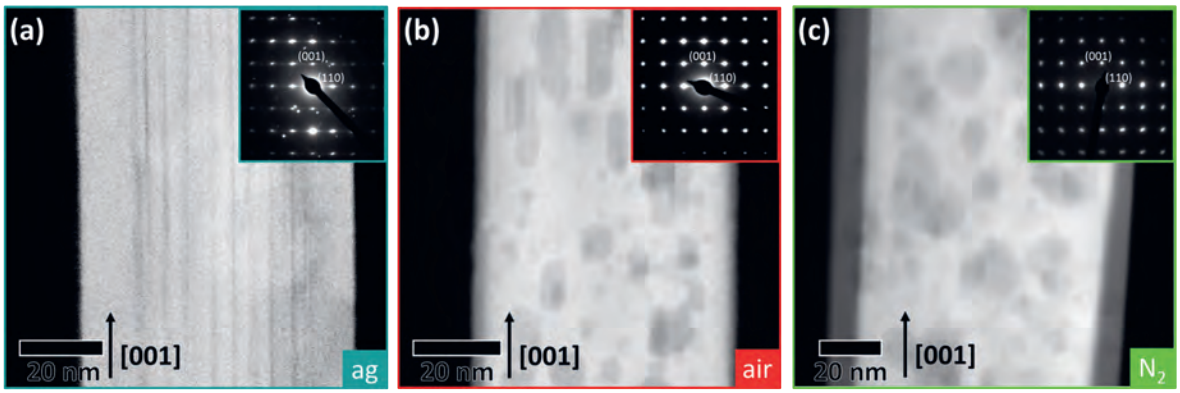



**Fig. 2:** *STEM images and corresponding diffraction patterns of rutile $TiO_2$ nanowires (a) as grown at 150°C, (b) after annealing at 500°C in air and (c) after annealing at 500°C in nitrogen. The nanowires show different defects depending on the heat treatment. Figure taken from [2].*

she organized the scientific colloquium dedicated to the 100 years anniversary of the MPIE (2017) and a meeting on "Hydrogen Technology" (2017). C. Scheu is also a co-organiser of the joint retreats "Mechanics meets Energy" between the department of Structure and Nano-/Micromechanics of Materials (SN) and the NG group.

The NG group is visible in the scientific community as shown by the number of invited and keynote talks at conferences and colloquia in universities and research institutions as follows. C. Scheu had keynote lectures at the EMRS Fall Meeting in Warsaw, Poland (2016) and at the MST conference in Salt Lake City, USA (2016). Her invited talks include the International Conference on Functional Nanomaterials and Nanodevices in Budapest, Hungary (2017), the 13th Multinational Congress on Microscopy, Rovinj, Croatia (2017), the Second Sino-German Symposium on Advanced Electron Microscopy and Spectroscopy of Materials, Xi'an China (2017) and the Grand Opening of UC Irvine Materials Research Institute, Irvine, USA (2018). All group members regularly attend national and international conferences and present their work in oral presentations or posters. Some notable achievements include S. Hieke receiving a travel award from the European Microscopy Society (EMS) to participate at the IMC19 in Sydney, Australia, and his nomination for the Young Scientist Assembly which was held prior to the IMC19 (2018), and L. Abdellaoui receiving the best oral communication award at the "1st International Meeting on Alternative and Green Energies" in Mohammedia, Morocco (2018).

Further awards to the NG group are the Alexander von Humboldt postdoc fellowship of J. Lim in the field of synthesis and advanced characterization of catalytic active, low-dimensional materials, and the nomination of C. Scheu to serve as a panel member for the strategic evaluation of the research field Matter of the Helmholtz Association. C. Scheu has also been elected and serves as a member for the evaluation board of the state North Rhine Westphalia "EFRE NRW 2014 – 2020 "NeueWerkstoffe. NRW".

The material portfolio studied within the NG group ranges from oxides [1-7,17-22], semiconductors [14-16,23], carbides [11-13] to metallic compounds [6-10] for applications such as photovoltaics, water splitting, fuel cells, conduction lines and functional coatings. Advanced characterisation methods, in particular, *ex situ* and *in situ* (S)TEM techniques are the link of the group members. In the following, the progress on three selected research examples in the field of materials for renewable energy applications is

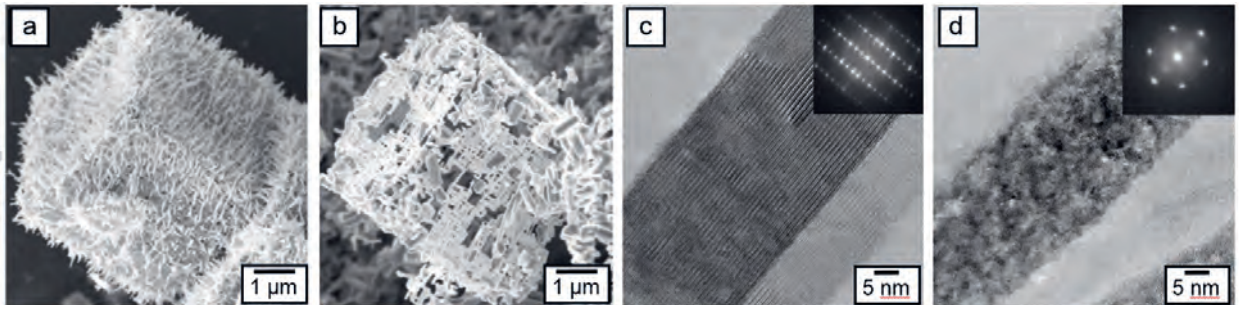



**Fig. 3:** *SEM images of (a) as grown $Nb_3O_7(OH)$ nanoarrays and (b) after ex situ annealing at 850°C. The ex situ annealing induced a phase transformation to H-$Nb_2O_5$. High resolution TEM images of an identical nanowire at (c) room temperature and (d) during in situ annealing at 800°C. Images and video frames taken from [5].*

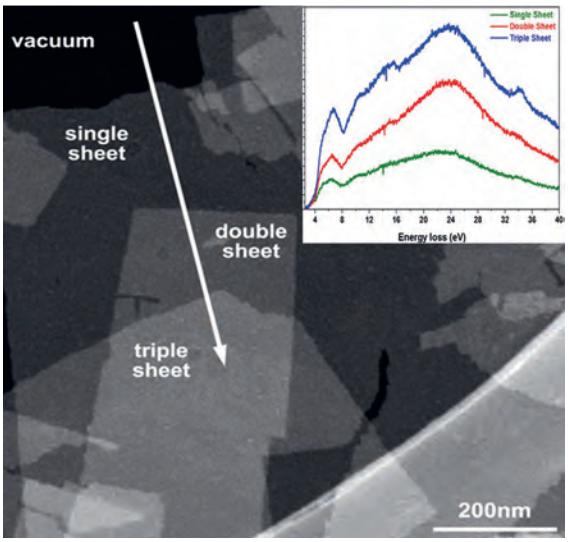



**Fig. 4:** *Low loss EELS data and STEM image of single, double and triple $Ca_2Nb_3O_{10}$ 2D nanosheets. Image reproduced from [40].*

described in detail, namely nanostructured transition metal oxides for photocatalytic application, materials for polymer-based fuel cells and thermoelectric materials for electricity generation.

**Nanostructured Transition Metal Oxides for Photocatalytic Application**

Transition metal oxides can be used as electrode material in energy storage devices, as support material in electrocatalysis or as photocatalyst. Large surface areas from nanostructuring introduce more reactive sites on their surface and shorter diffusion paths for charge carriers to reach the surface. The research activities, supported by the DFG, are based on $TiO_2$ and $Nb_3O_7(OH)$ nanostructures which are grown by NG members using facile hydrothermal-synthesis approaches.

The properties of $TiO_2$ nanoarrays were modified in the PhD thesis of A. Folger by using various heat treatments in different atmospheres [1-3]. These studies were done in close collaboration with Prof. L. Schmidt-Mende's group (University of Konstanz). Hydrothermally grown rutile $TiO_2$ nanoarrays possess a large number of defects (Fig. 2a) such as oxygen vacancies and tiny nanofingers on top, which act as recombination sites and limit the performance of functional devices [37]. Annealing in air eliminates these defects, but voids were formed in the interior of the nanowires [37]. As the involved mechanism remained open, *in situ* STEM heating experiments were performed which allowed to observe "live" the formation of the voids above 500 °C [1]. As shown by electron tomography and aberration-corrected STEM images, these voids are faceted and possess a Wulff-shape (Fig. 2b). They form via oxygen vacancy condensation. Moreover, above 250 °C, the hydroxide groups on the surface of the nanofingers are removed and a zipper-like condensation reaction closes the space between the nanofingers resulting in a single crystal [1].

The oxygen vacancy condensation has consequences on the electrical behaviour. In contrast to the as-grown nanowires, which are n-type semiconductors, the nanowires annealed in air are insulating [2]. By changing the annealing treatment from air to a slightly reducing $N_2$ atmosphere, the nanowires display a metal-like conductivity due to the formation of a 10 nm thin, sub-stoichiometric $TiO_{2-x}$ shell (Fig. 2c). Within this shell, the oxidation state of Ti is mainly $Ti^{3+}$ as found by energy loss near edge structure (ELNES) analysis, different from the $Ti^{4+}$ state of the core. The rutile core still contains facetted voids [2].

An elegant way to introduce a different shell material on $TiO_2$ nanowires is the use of Si substrates and subsequent annealing treatments [3]. A 3-4 nm thin, amorphous $SiO_x$ shell forms at 1050 °C, and homogenously covers the individual nanowires. In contrast to the nanowires heat-treated at lower temperatures, the core is free of lattice defects except for oxygen vacancies/$Ti^{3+}$ ions at the area adjacent to the shell [3]. The shell is expected to increase the performance of photochemical devices and photovoltaic cells by minimizing carrier recombination. The presence of rutile seed layers on the morphology of hydrothermally grown rutile $TiO_2$ nanostructures was also studied [38]. Current activities include chemical etching of $TiO_2$ nanowires to increase the surface area further. Onto these hollow nanowires a Pt catalyst is deposited. The stability of these nanostructure is analyzed by J. Lim and R. Aymerich Armengol in close collaboration with O. Kasian and M. Ledendecker from the department of Interface Chemistry and Surface Engineering (GO).

Research activities on a blue $TiO_2$ photocatalyst deposited on an Al foil were initiated during a 3-month visit of J. Bandara (Prof. at the National Institute of Fundamental Studies, Sri Lanka) who was granted a renewed research stay from the Alexander von Humboldt Foundation. The joint research unravelled the mechanism responsible for the observed superior hydrogen production during UV illumination [39]. Detailed microstructural characterization of A. Folger and S. Zhang showed that $Ti^{3+}$ and $Ti^{2+}$ states are present at the surface of $TiO_2$ nanoparticles. They are stabilized by an aluminium hydroxide oxide layer surrounding them. These reduced states are continuously self-generated via absorption of UV light and deliver the electrons required for the hydrogen generation [39].

The functional properties of a $Nb_3O_7(OH)$ photocatalyst and its modifications by doping and phase transformation were investigated by S. Betzler (now at: Lawrence Berkeley National Laboratory, USA) in her PhD thesis [4,5,40] together with B. Lotsch (Di-

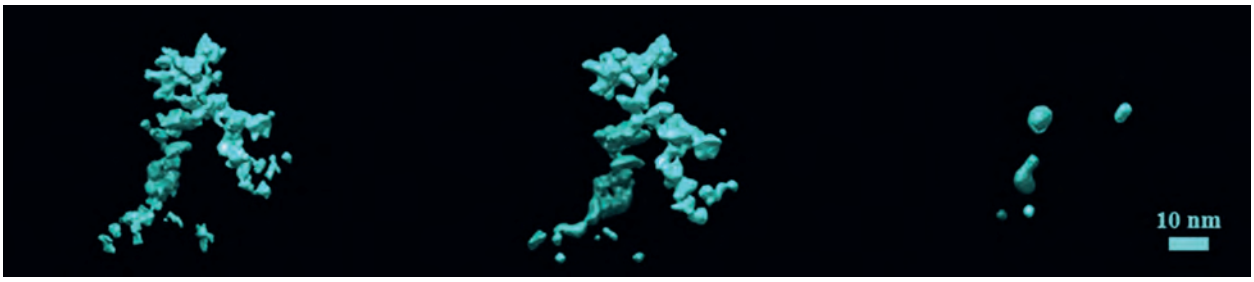



**Fig. 5:** *Electron tomography reconstructions of an identical Pt/Ru catalyst network before (left) and after 2000 cycles (middle) and 7000 cycles (right) of a cyclic voltammetry experiment performed at [0-1.2]$V_{RHE}$ in saturated $HClO_4$. Strong dissolution is observed. Modified image from [8].*

rector at the MPI for Solid State Research, Stuttgart) and L. Schmidt-Mende. 3D nanoarrays consisting of nanowires with a width of few tens of nanometres and a length of micrometres which are arranged perpendicular to each other can be grown with the developed hydrothermal synthesis strategy [40]. Incorporation of Ti within the orthorhombic crystal structure leads to a higher hydrogen production rate in UV light [4]. Up to 12 at.% Ti can be homogeneously incorporated in the crystal lattice as proven by EDX and EELS measurements in the STEM. Ti not only lowers the number of surface defects at the nanowires, but also leads to changes in the aspect ratio resulting in a morphology with a larger surface area [4]. The $Nb_3O_7(OH)$ morphology can be also modified by the type of precursor used as observed in the master thesis of T. Gänsler. He will continue working in this field during his PhD at the MPIE. In general, other factors such as temperature and time are also important for the growth of nanostructures via hydro/solvothermal synthesis strategies as demonstrated by A. Frank in her PhD thesis [14-16].

A different approach to modify the functional properties of the $Nb_3O_7(OH)$ nanoarrays is the thermally induced phase transformation to $Nb_2O_5$ [5]. The structural changes of the 3D networks were investigated both *ex situ* in air and *in situ* under reducing atmosphere in the TEM (Fig. 3). The *in situ* TEM studies reveal the release of water from the crystal structure and the formation of an oxygen-deficient niobium oxide phase. Thereby, stacking faults play an important role, which are mainly located at the interior of the nanowires. At these defective regions, dislocations form at ~450 °C, which move towards the surface. This initiates the phase transformation which is completed at temperatures >750 °C. To compensate for the volume differences of the original $Nb_3O_7(OH)$ crystal and the oxygen-deficient niobium oxide, pores are formed (Fig. 3) [5]. The *in situ* TEM also reveals an extremely high thermal stability of the nanowire network, as confirmed by *ex situ* heating studies. The 3D morphology remains up to 850°C where merging of nanowires occurs (Fig. 3). Due to the constant supply of oxygen, the *ex situ* annealing in air leads to a different niobium oxide phase. Stoichiometric $Nb_2O_5$ possessing a monoclinic crystal structure is formed [5]. The *in situ* TEM studies were performed in close collaboration with T. Harzer and G. Dehm from the Department of Structure and Nano-/Micromechanics of Materials (SN).

The differences in electronic structure and properties between $Nb_3O_7(OH)$ and H-$Nb_2O_5$ have been evaluated by comparing experimental data with density functional theory (DFT) calculations performed by the group of J. Minar (Prof. University of West Bohemia, Plzen, Czech Republic) [41]. The band gap calculated by the modified Becke-Johnson (mBJ) potential is in good agreement with both UV-VIS measurements and low loss EELS. Also the calculated low loss EELS region and O-K, and Nb-$M_{2,3}$ ELNES agree well with the experiment. The DFT calculations reveal that both compounds are n-type semiconductors with a similar electron mobility but higher hole mobility of $Nb_3O_7(OH)$ [41].

Further promising UV active photocatalysts are 2D nanosheets based on niobates obtained via exfoliation of different perovskite parent phases [19,42,43]. These studies are done in collaboration with the group of B. Lotsch who synthesized the material and explored the functional properties while the NG contributes to atomic scale characterization (Fig. 4). Monochromated EELS measurements were used to determine the band gap of 2D $Ca_2Nb_3O_{10}$ nanosheets with a high spatial resolution of <10 nm [19]. In contrast to most nanostructures where the band gap increases due to quantum size effect, the value of the $Ca_2Nb_3O_{10}$ nanosheets was similar to that of the bulk parent phase $KCa_2Nb_3O_{10}$. This unexpected result can be explained with the help of DFT calculations, which show that the partial density of states related to the K atoms is not affecting the band gap value. Currently, S. Zhang performs *in situ* heating experiments to understand the growth mechanism of $NiO_x$ nanoparticles on the 2D $Ca_2Nb_3O_{10}$ nanosheets. These sheets are also interesting for lighting application, when doped with lanthanides. R. Changizi investigated in her master thesis successfully the doped bulk parent phase with cathodoluminescence experiments and she will continue to conduct such measurements at the nanosheets in her PhD thesis.

Exploring materials for solar hydrogen production is also conducted by the NG group within the DFG priority programme 1613 “Fuels Produced

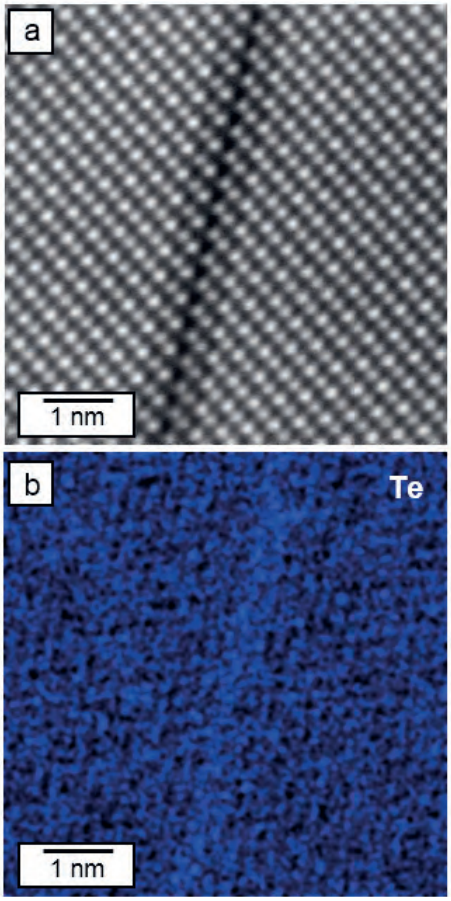



**Fig. 6:** *STEM image and corresponding tellurium map of an as-quenched $AgSbTe_2$ thermoelectric material. The figure is adapted from [50].*

Regeneratively Through Light-Driven Water Splitting: Clarification of the Elemental Processes Involved and Prospects for Implementation in Technological Concepts". After a positive evaluation, the NG group continued in the second funding period to carry out scale bridging microstructural characterisation of novel materials synthesized by project partners within the SPP 1613/2. The activities of A. Müller during his PhD thesis [17,18] and S. Zhang in collaboration with the groups of T. Bein (Prof. at LMU Munich), D. Fattakhova-Rohlfing (Prof. at FZ Jülich), R. Pentcheva (Prof. at University of Duisburg-Essen), A. Ludwig and W. Schuhmann (both Prof. at RUB) and A. Fischer (Prof. at University of Freiburg) have led to several joint publications in the field of photoabsorbers (Sn-doped $Fe_2O_3$ [21,20], $Fe_2O_3/WO_3$ [17]), photoanodes (zinc ferrite [44], Sn doped $Fe_2O_3$ [20], Mo-doped $BiVO_4$ [45]), photocathodes (FeCrAl oxide [46]) and various catalyst [47,48]. Only new publications since the last scientific report 2013-2015 are included.

In line with this activities, the NG group studied together with T. Li (Jun.-Prof. RUB), O. Kasian and K. Mayrhofer (both GO), B. Gault and D. Raabe (both department of Microstructure Physics and Alloy Design (MA)) Iridium-oxide based catalyst for the oxygen evolution reaction (OER) for water electrolysis [34] (see p. 163). Another interesting approach is the use of multinary noble metal free catalyst which are explored together with A. Ludwig and W. Schuhmann [49]. They are fabricated by co-sputtering several elements into an ionic liquid and A. Garzón-Manjón performs *ex situ* and *in situ* STEM experiments to unravel their crystal structure and phase transformation [50].

**Materials for Polymer-based Fuel Cells**

The hydrogen produced by solar-driven water splitting or water electrolysis can be used in fuel cells to generate electricity for households or driving vehicles without the release of harmful by-products during operation. C. Scheu and her team members are working on polymer-based fuel cells since 2010, together with industry partners. The centrepiece of the polymer-based fuel cells is the membrane electrode assembly with the electrode consisting of a high surface area support material on which a catalyst is deposited. This assembly is prone to degradation and the aim of the studies is to discover the underlying mechanism. The goal is to develop guidelines for material selection with improved lifetime and reliability. For example, C. Scheu and her team have successfully determined how the polymer membrane type and molecular weight distribution of the polymer chains affect the degradation leading to poisoning of the cathode layer [24]. A narrow molecular weight distribution is optimal as long chains block the catalyst surface while short chains are able to move very far into the microporous layer hindering efficient mass transport. They also discovered that cross-linkers and the addition of inorganic particles can be successfully used to minimize degradation [24].

The electrode materials are also affected by operation related degradation effects. In the PhD thesis of K. Hengge [6-8], the commonly used Pt catalyst in the anode was replaced by a Pt/Ru catalyst and its behaviour during various fuel cell operating conditions was analysed in detail [7,8]. These studies were done in close collaboration with the group of K. Mayrhofer (GO). Cyclic voltammetry and STEM experiments were performed on identical catalyst nanoparticles located on their carbon support. The change in chemical composition was studied with EDX and electron tomography was used to monitor the surface and volume changes of the individual nanoparticles (Fig. 5). Dissolution and agglomeration are the dominant degradation mechanisms occurring in the dynamic fuel cell operation mode [7]. Both depend strongly on the applied voltage with dissolution and agglomeration increasing when the upper potential increased. The catalyst dissolution has a strong effect on the real stack performance and the formation of a catalyst band within the polymer membrane after continuous fuel cell operation was observed [8]. The position of the band depends on the ratio of the molar flux of $H_2$ and $O_2$.

In an earlier work, the carbon support had been replaced by non-stoichiometric tungsten oxide $WO_{3-x}$ where novel platinum networks grow instead of nanoparticles [51]. The assembled fuel cells possessed a long-term stability related to the stability of the Pt networks [51], however, its growth mechanism remained unknown. K. Hengge was able to close this knowledge gap in her PhD by performing systematic studies to understand the formation process [6]. In the first step of the synthesis, the liquid precursor is deposited on the $WO_{3-x}$ and is thermally reduced in the second step. The reduction begins at the surface of the initially formed Pt and $Cl^-$-containing truncated bulk octahedral solid [6]. It progresses with time into the interior which consists of an amorphous matrix in which Pt nanocrystals are embedded while the exterior is already the network of interconnected Pt nanocrystals. After a reduction time of only 20 minutes, the $Cl^-$ is completely removed and a Pt network with pores of different sizes remains. With a further increase in the reaction time, networks with a higher surface area can be produced [6].

As degradation is a major problem not only in fuel cells but also battery materials, similar experiments are planned for novel electrode materials. First experiments are done by R. Sahu, K. Hengge and J. Lim on a copper hexacyanoferrate electrode prepared by F. La Mantia (Prof. at Bremen University) in cooperation with K. Schweinar and D. Raabe (MA).

**Thermoelectric Materials for Electricity Generation**

Thermoelectric materials can be used to generate electricity from waste heat through the Seebeck effect. The conversion efficiency can be increased by introducing defects that efficiently scatter phonons, but not electrons to keep a good electrical conductivity. In the ongoing PhD thesis of L. Abdellaoui and the bachelor thesis of R. Bueno Villoro several promising thermoelectric materials are explored together with the project partners O. Cojocaru-Mirédin (RWTH Aachen), Y. Amouyal (Prof. at Technion, Israel), and the MA department [29-31].

In particular, electron channeling contrast imaging in a scanning electron microscope is used together with S. Zafferer (MA) to analyse the density of stacking faults in a quantitative manner. Stacking faults in as-quenched $AgSbTe_2$ act as scattering sites for phonons leading to a strong reduction of the lattice thermal conductivity. A much higher density of stacking faults is observed at small-angle grain boundaries. They are further characterized at the atomic scale using Z-contrast imaging in STEM and EDX mapping (Fig. 6). These results are complemented with 3D atom probe tomography studies of the groups of O. Cojocaru-Mirédin and B. Gault (MA) to determine the chemistry of the stacking faults with high accuracy. The results show that Ag is depleted, and Sb/Te are enriched at the stacking faults [52]. The phase stability of the $AgSbTe_2$ compound will be investigated by *ex situ* and *in situ* annealing experiments. Such studies have been very successfully conducted in the NG group in the PhD theses of S. Gleich on $Mo_2BC$ coatings [13] and by S. Hieke on thin Al films on $Al_2O_3$ substrates [9,10] (see p.183).

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# Research Projects in Progress

*Abdellaoui, Bueno Villoro, Scheu (with S. Zaefferer*, B. Gault*, D. Raabe*, O. Cojocaru-Miredin**, Y. Amouyal*** (*MA Department, **RWTH Aachen, ***Technion, Israel))*: Microstructural and spectroscopic analysis of thermoelectrics

*Changizi, Scheu (with T. Schwarz, *MA Department):* Combining cathodoluminescence studies of functional materials with structural investigations

*Frank, Scheu* (*with A. Kruth*, V. Presser**, *Leibniz Institute for Plasma Science and Technology, Greifswald, ** Leibniz Institute for New Materials in Saarbrücken):* Characterisation of nanohybrids for renewable energy applications *(Leibniz Project)*

*Gänsler, Scheu (with S. Betzler*, B. Lotsch**, L. Schmidt-Mende*** (*Lawrence Berkeley National Laboratory, USA, **LMU Munich and MPI for Solid State Research, ***University of Konstanz))*: Tailoring functional properties of niobium hydroxide *(DFG Project)*

*Garzón-Manjón, Scheu (with A. Ludwig, RUB University)*: *Ex situ* and *in situ* studies of binary and multinary nanoparticles grown in ionic liquids *(DFG Project)*

*Hieke, Scheu (with G. Dehm, SN Department)*: Stability of thin films under harsh environments

*Lim, Aymerich Armengol, Scheu (with O. Kasian, M. Ledendecker, GO Department)*: Synthesis and characterization of catalytic active, low-dimensional materials (J. Lim supported by AvH)

*Hengge, Obermaier, Scheu:* Investigation of degradation mechanism in polymer based fuel cells

*Sahu, Scheu (with J. Schneider* (*RWTH Aachen))*: Characterization of nanolaminated and 2D materials by electron microscopy and spectroscopy

*Scheu (with M. Lipinska-Chwalek and J. Mayer, RWTH Aachen)):* Microstructure characterization – local structure, defect and chemical analysis (SFB 761/3 partial project C01)

*Zhang, Scheu (with T. Bein*, D. Fattakhova-Rohlfing***, R. Pentcheva** (*LMU Munich, **Forschungszentrum Jülich, ***University of Duisburg)*: Investigation of photo-electrochemical water splitting-active nanostructures

# Max Planck Fellow Group on Self-Reporting Materials

*Group Head: J. M. Schneider*

MATERIALS CHEMISTRY | RWTH AACHEN UNIVERSITY

**A: Self-Reporting Materials:**

Future technology challenges will no longer be simply addressed by today's material and processing solutions, which are often based on trial and error. Instead guidance will be attained from correlative experimental and theoretical research bridging all length scales. It is e.g. conceivable that future engineering components will be made of materials that are self-reporting. Self-reporting materials "communicate" damage of the material via changes of properties that can be measured in service as a consequence of chemical changes on the atomic length scale and/or phase transformations. Harnessing this would provide invaluable functionality for damage assessment and control and would constitute a major leap forward as the "health" of any material component exposed to mechanical loads could be monitored in service. This fascinating basic materials science with tremendous technological implications is the focus of Schneider's Max Planck Fellow Group.

One material property that can be measured in service is the electrical resistivity which is a measure for how strongly a material opposes the flow of an electric current. The measurement is non-destructive. Within the Max Planck Fellow Group the resistivity changes of magnetron sputtered, amorphous $Cr_2AlC$ thin films were measured during heating in vacuum for the first time. For this Pt electrodes were deposited onto the as deposited $Cr_2AlC$ thin films. Our previous work has established that annealing amorphous $Cr_2AlC$ triggers the transformation into a disordered, hexagonal solid solution phase [1]. Subsequently, upon further heating the disordered solid solution phase transforms into the (ordered) hexagonal MAX phase [1]. Hence, amorphous $Cr_2AlC$ was selected for this proof of concept study.

Fig. 1 shows the results of in situ resistivity measurements during heating as well as the structural changes of samples (monitored by ex situ X-ray diffraction (XRD)) and previously published differential scanning calorimetry (DSC) data [1]. In Fig. 2 bright field images and selected area electron diffraction (SAED) patterns of focused ion beam (FIB) lamellas extracted from $Cr_2AlC$ coatings after annealing to temperatures from 500 to 800 °C in vacuum are shown.

Based on the correlative XRD data from Fig.1, the SAED from Fig.2, and the DSC data from Fig.1 it is evident that the resistivity changes at approx. 552 °C indicate the phase transitions from amorphous to a disordered hexagonal solid solution and that the resistivity changes at approx. 585 °C signal the phase transition from disordered hexagonal solid solution to the ordered MAX phase. Hence, we have shown that

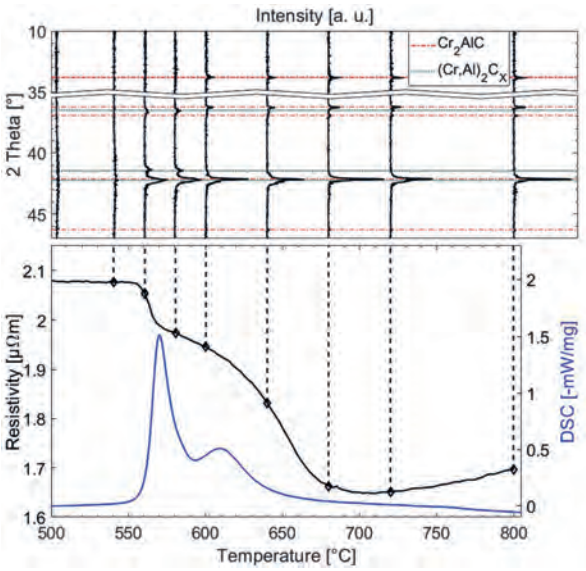


**Fig. 1:** *X-ray diffraction data of $Cr_2AlC$ samples annealed to various temperatures up to 800 °C and resistivity measured while annealing (black) [unpublished] compared to DSC results (blue) [1].*

thermally stimulated phase changes in $Cr_2AlC$ thin films can be revealed by in situ resistivity measurements. These results underline the potential of in situ resistivity measurements for monitoring structural change in $Cr_2AlC$ coatings during application.

**B. Other research topics in collaboration with the MPIE:**

**B1. Quantum mechanically guided design of ultra strong and damage tolerant glasses (In collaboration with G. Dehm & D. Raabe & B. Gault)**

The enhancement of fracture toughness, see Fig. 3, and strength of a cobalt tantalum-based metallic glass thin film with increasing boron content was recently reported [2].

The improvement of the mechanical performance is attributed to the formation of a compositionally lamel-

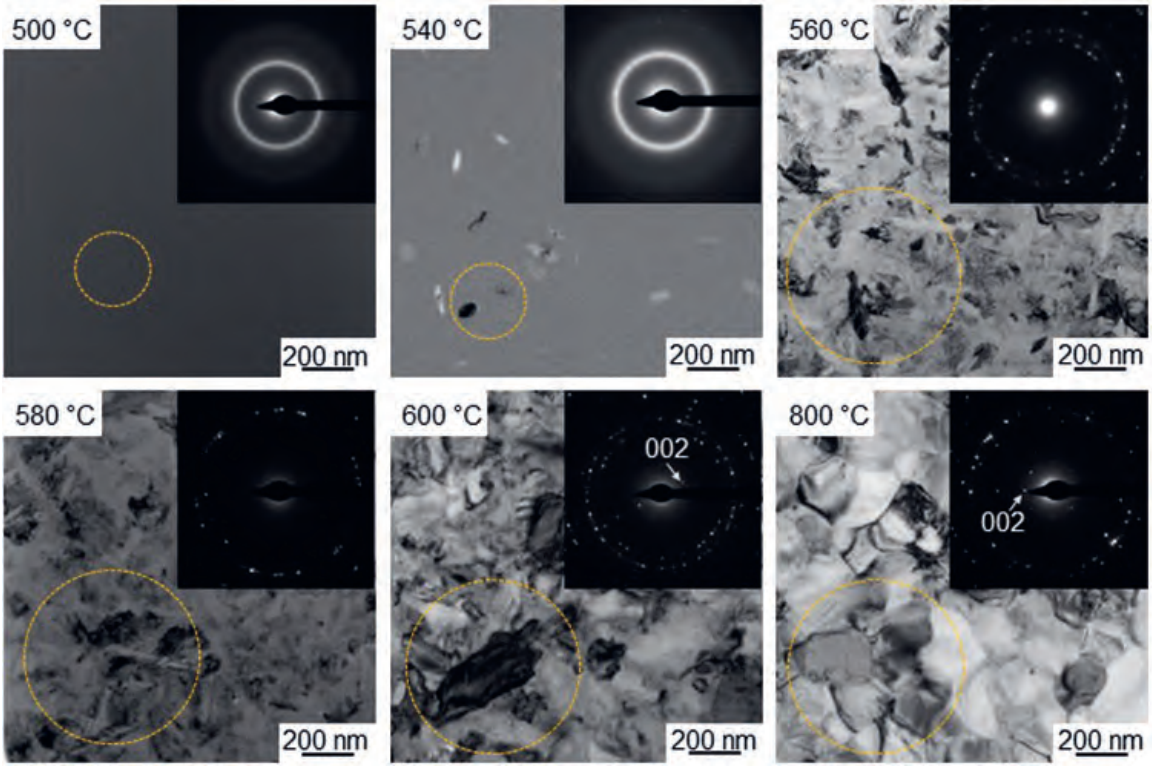


**Fig. 2:** *Bright field images and SAED patterns of FIB lamellas extracted from $Cr_2AlC$ coatings after annealing at 500, 540, 560, 580, 600, and 800 °C in vacuum [unpublished].*

lar compared to uniform glass microstructure, which becomes thinner with increasing boron content as revealed by transmission electron microscopy, see Fig. 4. Compositional variations across the lamellar structure are revealed by atom probe tomography (APT), see Fig. 4.

These findings provide a new design route for cobalt tantalum-based metallic glass thin films with enhanced mechanical performance as a function of boron content. A compositional lamellar structure revealed by TEM shows that the lamella thickness decreases as boron content increases. A substantial compositional difference was observed within the lamellar structure, where boron- and cobalt-rich structures were revealed by APT. As the thickness of the lamellar structure decreases, fracture toughness

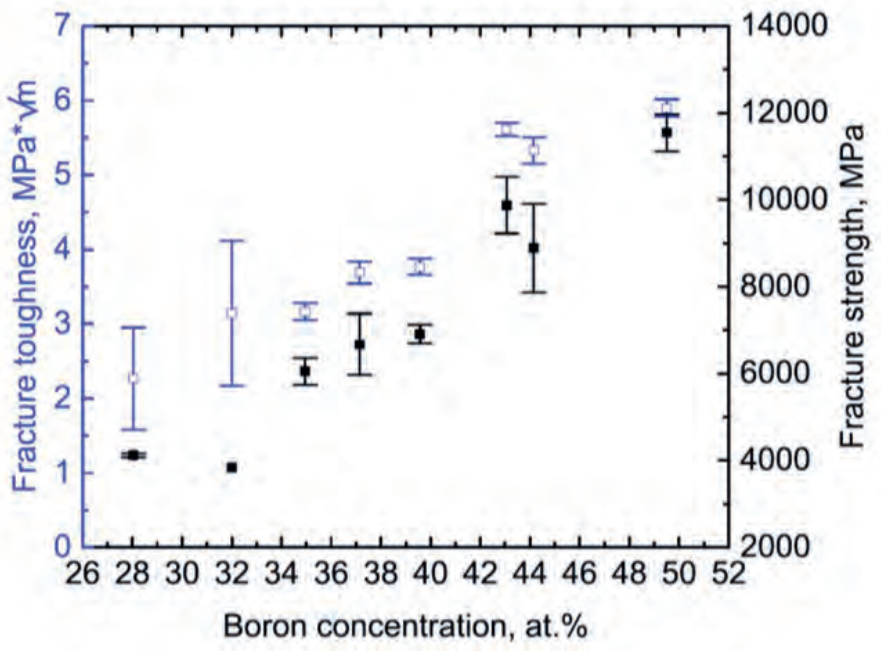


**Fig. 3:** *Micro-mechanical testing of the combinatorial CoTaB metallic glass thin film. Fracture toughness and fracture strength graphs as a function of boron content as revealed by microcantilever bending tests [2].*

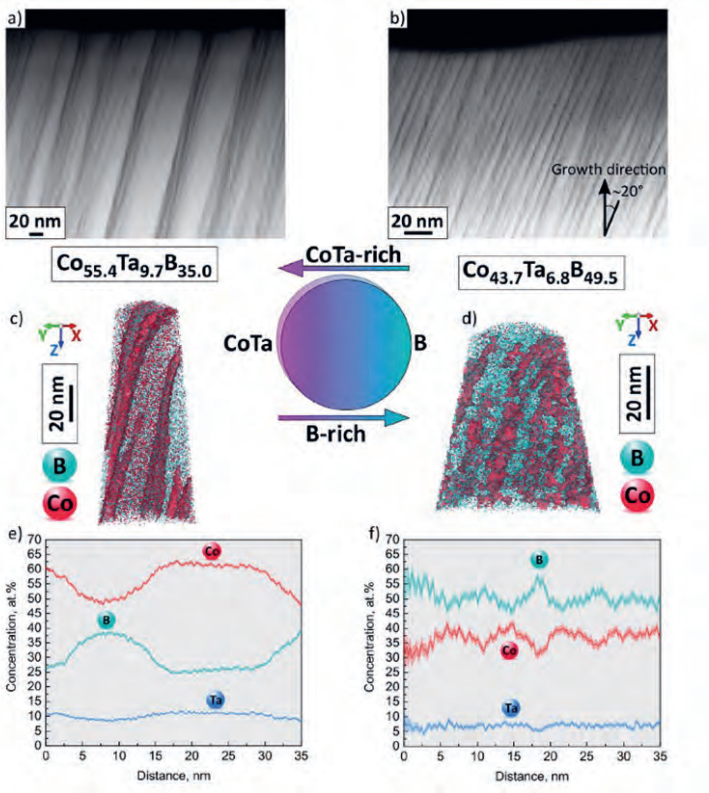


**Fig. 4:** *a, b) HAADF-STEM micrographs revealing the lamellar structure for $Co_{55.4}Ta_{9.7}B_{35.0}$ and $Co_{43.7}Ta_{6.8}B_{49.5}$. c, d) Corresponding APT reconstructions from $Co_{55.4}Ta_{9.7}B_{35.0}$ and $Co_{43.7}Ta_{6.8}B_{49.5}$ compositions. e, f) Compositional profiles perpendicular to lamellar structures revealing the boron and cobalt variations [2].*

and fracture strength are enhanced, suggesting the origin of the enhanced mechanical properties in the nanolaminated structure. The origin of the lamella formation is subject of ongoing research.

### B2. Can high strength and moderate ductility be combined in wear resistant coatings?

A fundamental plasticity study of $X_2BC$ nanolaminates (X=Hf, Mo) in collaboration with C. Scheu & G. Dehm [3-6].

These activities are described on p. 183.

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# Max Planck Research Group on High Temperature Materials

*G. Eggeler [1], A. Kostka [2], X. Wu [3,4,5], L. Cao [1,6]*

[1] Chair of Material Science and Engineering, Ruhr-Universität Bochum
[2] now at: Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-Universität Bochum
[3] Department of Microstructure Physics and Alloy Design (MA)

Since May 2015, Gunther Eggeler, professor for materials science at the Ruhr-Universität Bochum (RUB), leads a new Max Planck Research Group on High Temperature Materials (HTM), which emanated from the Max Planck Fellow Group, which existed from May 2010 until May 2015. The new HTM group seamlessly continues the research activities in the area of high temperature materials. Aleksander Kostka, a scientific member of the previous Max Planck Fellow Group, is now a transmission electron microscope (TEM) scientist at the Ruhr-Universität Bochum. This position allows him to also keep an involvement in the new HTM group. The expertise of the group lies in the field of exploring and explaining microstructural evolution during processing and service of engineering materials. Research of the group in the reporting period has shifted from tempered martensite ferritic steels (last reporting period) to single crystal Ni-base superalloys. Gunther Eggeler is the speaker of the collaborative research center SFB/TR 103 (From Atoms to Turbine Blades – A Scientific Basis for a New Generation of Single Crystal Superalloys), which interacts closely with the TEM and atom probe tomography researchers at the MPIE. Research in the group is focused on elementary processes, which govern microstructural stability and strength of single crystal superalloys. Elementary dislocation processes, which govern low temperature (<800°C) and high stress (>600MPa) creep were studied combining miniature specimen

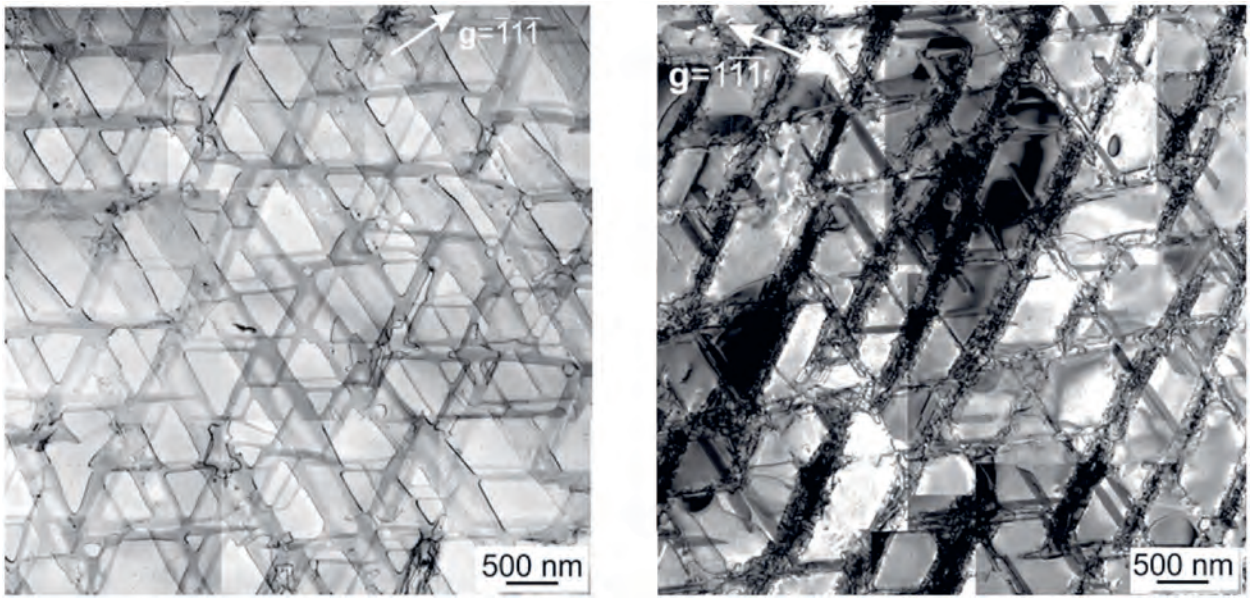


**Fig. 1:** *STEM montages showing dislocation structures after 0.1 (left image) and 0.4% (creep deformation) at 750°C and 800 MPa. TEM foils parallel to a {111} planes. The STEM montages show how dislocations enter the γ-channels. Dislocations must fill the γ-channels before γ'-cutting by planar faults can occur. For details see [1,2]. Single crystal superalloy: ERBO 1 (CMSX4 type).*

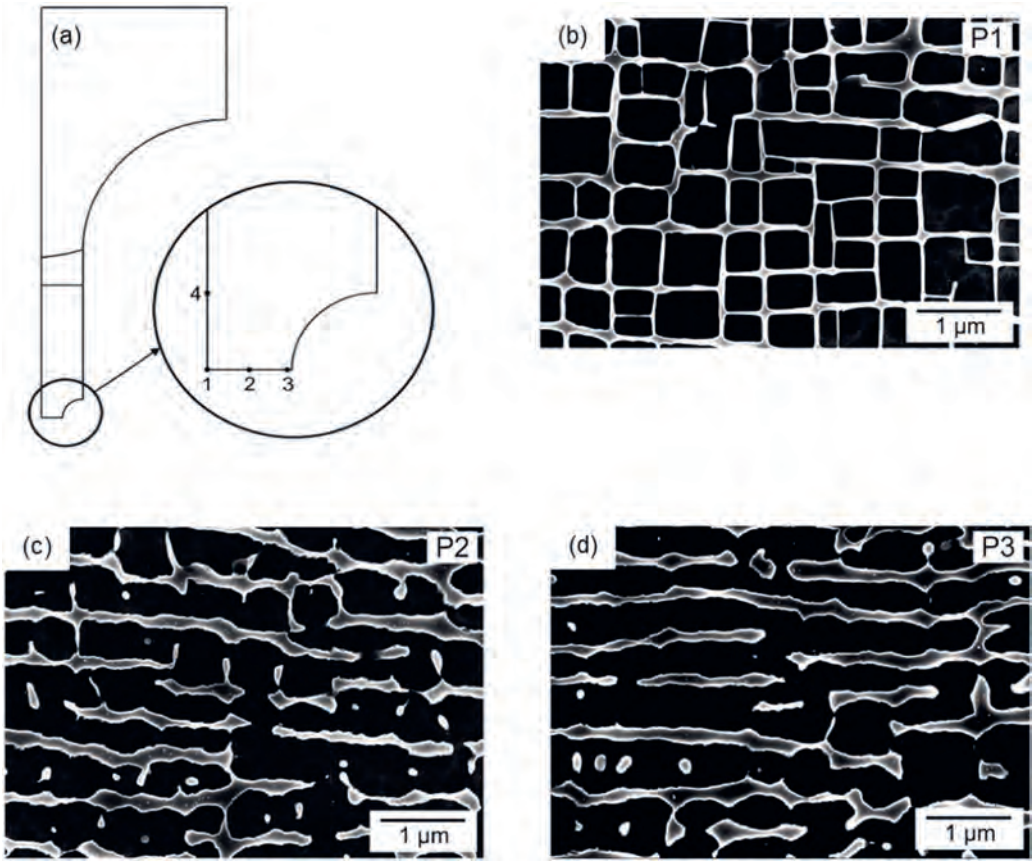


**Fig. 2:** *Heterogeneous microstructure evolution at different radial positions of a circular notched miniature tensile specimen (net section stress: 300 MPa, temperature: 950°C, time of creep exposure: 169 hours). (a) Schematic illustration of specimen (positions P1, P2 and P3 in the notch root cross-section are highlighted). (b), (c) and (d) SEM micrographs showing the γ/γ'-microstructures at positions P1, P2 and P3 as indicated. For details see [4,5]. Single crystal superalloy: ERBO1 (CMSX4 type).*

creep testing with diffraction contrast transmission electron microscopy [1,2]. The effects of defects on local thermodynamic and kinetic equilibria were investigated [3]. Recently the influence of stress state on the directional coarsening of the γ'-phase (rafting), the well known microstructural evolution of the γ/γ'-microstructure under high temperature creep conditions, was studied [4,5].

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# Max Planck Partner Group on Designing Damage Tolerant Functional Oxide Nanostructures

*Group Head: B. N. Jaya*

Indian Institute of Technology Bombay, Powai, India

The group aims at micro-mechanical characterization of functional oxide structures in order to design and develop architectures with increased damage tolerance. In cooperation with N.G. Mathews from the Indian Institute of Technology Bombay and C. Kirchlechner and G. Dehm from the SN department, the damage tolerance of Pb-free Barium Titanate (BTO) is studied at small length scales. BTO is chosen as the model material system for its excellent ferroelectric and piezoelectric properties. The effect of specimen size on yield/failure strength, and slip activity in BTO, impact of domain type, as well as its fracture toughness at small length scales has not been reported so far. The following are preliminary results from experiments on BTO Single Crystal (SX).

The BTO SX micropillar compression studies showed a prominent size effect in yield strength (156% increase) while also displaying duplex slip in samples of 2, 1 and 0.5 µm diameter. Micro-cantilever fracture toughness tests reveal $K_{IC}$ = 1.9 MPam$^{1/2}$, 120% higher than those reported earlier using indentation fracture tests at macro-length scales. On the whole, BTO displays enhanced damage tolerance at small length scales. It was also observed that the interference of the electron beam during *in situ* testing does not have any impact on the load-displacement response of BTO SX. This work will be further extended to polycrystalline BTO thin films and their electro-mechanical response will be used to propose strategies to enhance the damage tolerance of such nanostructures.

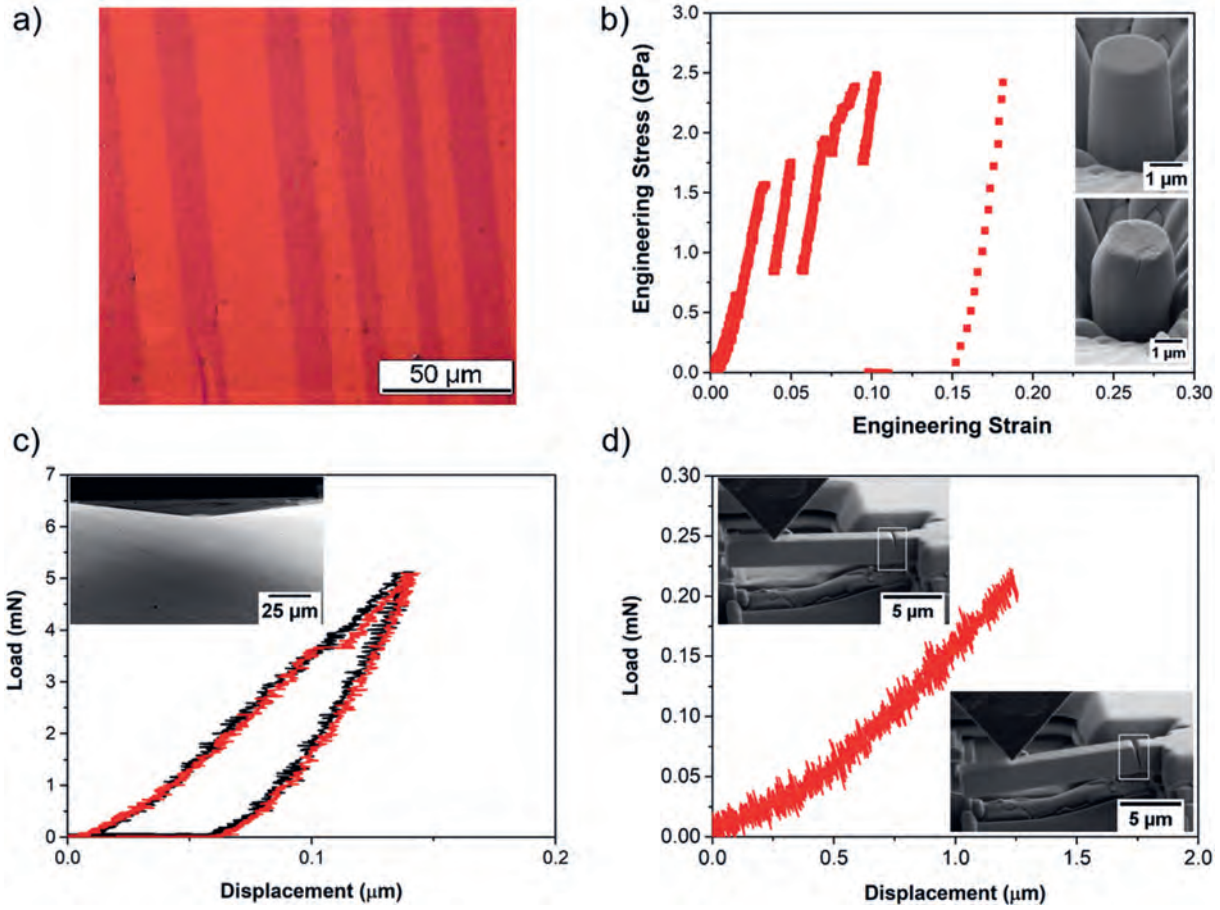


**Fig. 1:** *a) BTO SX under polarized light showing two different ferroelectric domains, b) Micro-pillar compression experiment on BTO SX showing several load drops corresponding to slip activity, c) Nanoindentation tests on a single domain of BTO SX with the electron beam switched on (black curve) and off (red curve) revealing no difference in behaviour, d) Micro-cantilever fracture test showing linear elastic behaviour with catastrophic fracture.*

# Max Planck Partner Group on Combinatorial Design of Novel Rare-Earth Free, High-Entropy Based Permanent Magnets

*Group Head: P. Gokuldoss*

Indian Institute of Technology, Madras, India

Magnetic materials are used to manufacture essential parts of any electrical motor, generator and transformer, finding application in a wide-range from power plants, house hold appliances to automobiles, industrial and commercial sectors. Most of these electrical machines require high performance permanent magnets that can deliver the necessary power. Currently, only rare-earth based permanent magnets are used for such applications, as the rare-earth elements provide the required features for permanent magnetic response, namely, uniaxial magnetic anisotropy. Hence, intense research has been devoted to developing highly-efficient permanent magnets that are either rare-earth free or require only minor additions in order to reduce the cost without compromising energy efficiency.

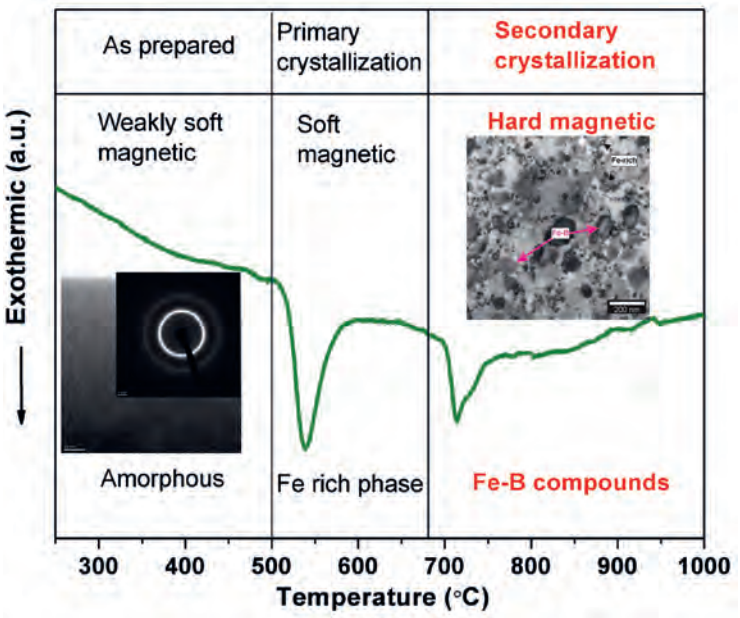


**Fig. 1:** *Phase evolution in rapidly quenched Fe-B based alloys upon heat treatment.*

Development of new rare-earth free permanent magnets has not been so successful till now considering that the phases that can exhibit uniaxial magnetic anisotropy together with high coercivity are difficult to be identified. Most often these phases are located in the compositional centre of phase diagrams within a limited composition range and are stable only in small temperature intervals. Hence, to identify new phases that can suitably be developed into novel high-performance permanent magnets requires a combinatorial approach to alloy design where extensive composition ranges can be screened experimentally within a short time frame and with limited materials expenditure.

This newly launched project thus combinatorially explores multi-component systems based on the concept of high entropy alloys (HEAs). This concept enables experimentally probing compositions that are multi-component in nature and are also located in the middle of phase diagrams. By employing multiple methods of combinatorial screening such as rapid alloy prototyping, combinatorial thin film deposition, reaction sintering, both equilibrium and non-equilibrium phases can be found and identified for their crystal structures and their magnetic properties as a function of composition.

# Max Planck Partner Group on Stress and Defects Driven Phase Transformations

*Group Head: S. Meka*

Indian Institute of Technology, Roorkee, India

This partner group (PG) was awarded at the end of 2016 and has formally started its activities from 1st March 2017. It is carrying out research activities independently as well as in collaboration with the MPIE. The focus of the research group is to investigate phase transformation phenomena that occur as a result of metal-gas reactions, which, in turn, generate stresses and lattice defects in the material. Some examples of the research are given below.

Researchers from the MPIE and IIT Roorkee are working jointly on developing nitride dispersion strengthened steels by combining the gaseous nitriding expertise of researchers at IIT Roorkee and the Additive Manufacturing (AM) expertise at the MPIE. In this project, Fe-2.3 wt.% Al alloy powder was subjected to gaseous nitriding treatment to realize the internal precipitation of AlN in ferrite matrix in addition to the development of iron nitrides. After that, the developed iron nitrides were reduced to iron and $N_2$ gas by hydrogen reduction treatment such that AlN particles remain stable, whereas iron nitrides are unstable. The nitrided-plus-hydrogen-reduced powders were consolidated using spark plasma sintering (SPS). Sintered compacts have indicated a significant increase in hardness as compared to the case of no AlN dispersion was created, i.e., SPSed as received Fe-2.3wt.%Al alloy powder. Detailed characterization revealed a complex microstructure beyond the targeted AlN particles in ferrite matrix: During nitriding, iron-oxides have developed which also got reduced during following hydrogen-reduction treatment. Due to the availability of this oxygen, Al-oxynitrides have developed as layers in powder particles. We will further optimize the process to avoid oxygen contamination in the future. It is also planned to carry out ballmilling of Fe-2.3wt.%Al alloy powder to reduce the particle size and to introduce dislocations which will act as nucleation sites for AlN and thus are expected to refine the particles. The final aim of this project is to use the nitrided and hydrogen-reduced powders in additive manufacturing employing selective laser melting (SLM) to realize AlN dispersion strengthened steel components.

Other research activity which the PG is currently focussing on is to understand gas/solid equilibria, especially to understand the possible establishment of metastable states leading to spinodal decomposition of the system. In this context, iron-based alloys which show the possibility of spinodal decomposition during the process of equilibrating with externally imposed gaseous nitriding and oxidising atmospheres are being explored. Further joint work is underway on the effect of nitride inhibitor particles on secondary recrystallization in electrical steels.

Under this PG activity, researchers from the MPIE had visited IIT Roorkee for scientific discussions on the ongoing collaborative research activities and also to conduct a one day workshop on “microstructural aspects of additive manufacturing” at IIT Roorkee. Additional research stays of members of the PG at the MPIE are planned for 2019.

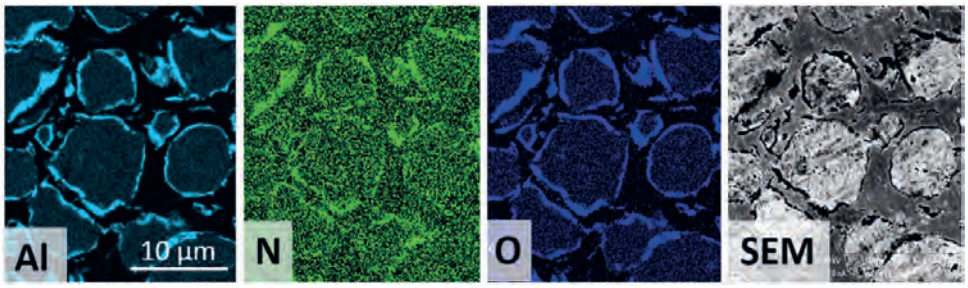


**Fig. 1:** *Microstructure of SPS-sintered Fe-2.3Al powder that had been gas nitrided and hydrogen reduced prior to sintering. A shell of Al-rich oxynitrides around the previous powder particles is visible.*

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# New Research Groups

## Materials Science of Mechanical Contacts

*Group Head: M. Herbig*

Department of Microstructure Physics and Alloy Design (MA)

The non-permanent research group ”Materials Science of Mechanical Contacts” was established in January 2017 with the financial support of the Bundesministerium für Bildung und Forschung (BMBF Junior Research Group on “Material Science for Alternative Energy”). It aims at deepening our understanding of the materials science phenomena associated with intense joint mechanical and environmental contacts. This is key to revealing a broad range of phenomena required for improving crucial engineering components such as bearings, rails, hip implants, extrusion tools, boring heads, cutting inserts or dental fillings.

One main focus of this research group is the study of white-etching-cracks (WECs), which are primarily known to cause failure in bearings and rails, but which are in reality ubiquitous in high carbon steel applications subjected to intense mechanical contacts. This failure mode causes billions of euros costs worldwide each year. The group follows a diversified approach to yield a breakthrough on this long-standing challenge: Specimen failure under controlled laboratory conditions is generated using a customized rolling contact fatigue machine built in-house that simulates test conditions similar to ball bearings but on self-designed alloys. Both, lubrication and loading conditions as well as the electric current flow through the bearing (which is of importance as electric discharge events have been associated with the presence of WECs) can be controlled with this instrument. These specimens are compared to those failed in service using state-of-the-art microscopy. Individual phenomena are investigated separately where possible. Dedicated experiments are conducted to investigate the mechanisms of precipitate decomposition by deformation, heat and electricity. A further project aims at the direct observation of solute hydrogen by atom probe tomography (APT) in deformed pearlite to shed light on the role of hydrogen in the process of cementite decomposition. The fracture toughness of white-etching-layers in rails is determined by cantilever bending tests in the scanning electron microscope.

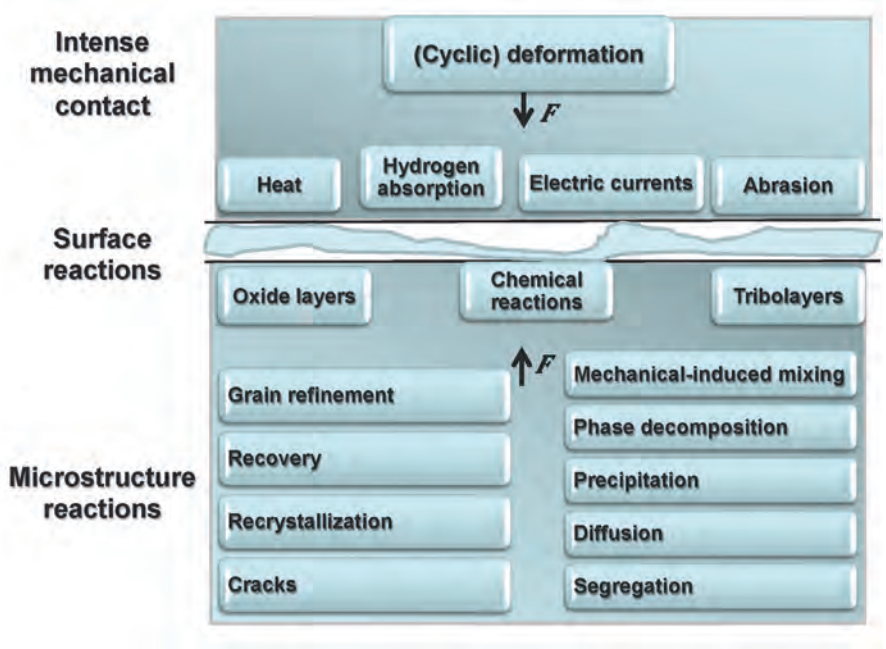


**Fig. 1:** *Microstructure reactions caused by intense mechanical/environmental contacts.*

The contact between two solid bodies subjected to high forces under harsh environmental conditions and large numbers of repetitions involves complex materials science phenomena (Fig. 1): Plastic deformation can lead to fatigue, grain refinement and precipitate decomposition. Frictional heat can cause diffusion, phase transformation, recovery or recrystallization. The presence of air, lubricants or body fluids at the contact point causes oxidation, tribolayers, or even corrosion or hydrogen embrittlement. These processes usually occur simultaneously in service and cannot be tracked *in situ*. The analysis of such phenomena requires combined chemical and structural characterization down to the atomic scale.

The research activities on steels are complemented by research on hip implants where corrosion and wear debris at the contact point between the stem and head leads to adverse tissue reactions, requiring the explantation of 2.5% of all prostheses. Here, correlative transmission electron microscopy and APT give access to the complex body/implant interactions.

# Complex Concentrated Alloys

*Group Head: F. Körmann*

Department of Computational Materials Design (CM)

The Complex Concentrated Alloys (CCA) research group of Fritz Körmann, established in 2018, aims at the computational design and accelerated exploration of multi-component alloys with parameter-free (*ab initio*) computer simulations [1]. A main focus is currently on complex concentrated alloys and related concepts such as multi-principal element alloys and high-entropy alloys. Mechanical [2,3], magnetic [4], thermodynamic [5,6] and other materials properties [7-9] are investigated by means of computer simulations in close collaboration with experimental and theoretical partners at the MPIE and worldwide.

Multicomponent alloys with multiple principal elements including high-entropy alloys and compositionally complex alloys are attracting rapidly growing attention. The endless possibilities to explore new alloys and the hope for better combinations of materials properties have stimulated a remarkable number of research works in the last years. Most of these works have been based on experimental approaches, but *ab initio* calculations have emerged as a powerful approach that complements experiment and serves as a predictive tool for the identification and characterization of promising alloys [1].

The CCA group focuses on the theoretical *ab initio* modelling of phase stabilities and materials properties of multi-principal element alloys by means of density functional theory (DFT) [1]. Concepts and methods are developed to efficiently consider chemical disorder [1-9] and various finite-temperature excitations [3-6,8,9] based on DFT. Different concepts to study crystal and alloy phase stabilities [2,3,5,6], the impact of lattice distortions [7], magnetic transitions [4], and chemical short-range order [6] are objectives of the group. Strategies to study elastic properties, stacking fault energies, and their dependence on, e.g., temperature or alloy composition are evaluated in close collaboration with other departments at the MPIE.

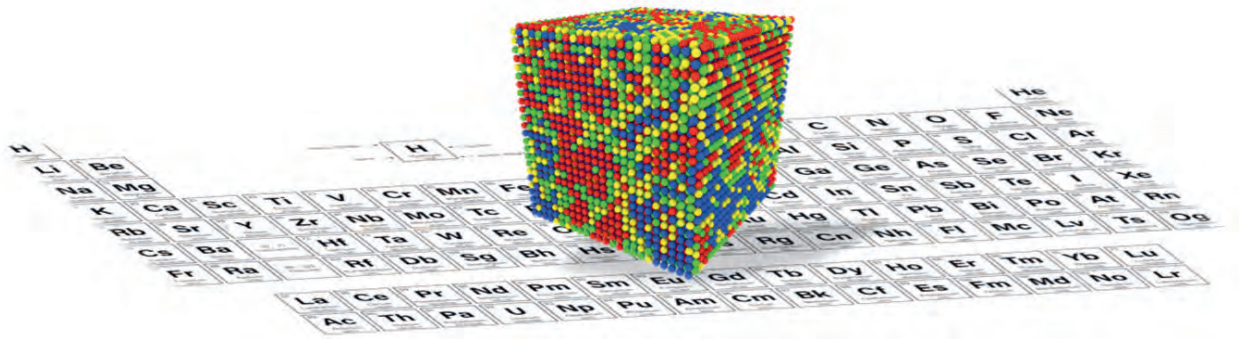

**Fig. 1:** *Sketch of a four-component high entropy alloy. A key aim of the CCA group is to develop the computational methods for screening the large compositional phase space of such multi-component alloys for phase stabilities and outstanding materials property combinations.*

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# High-Entropy Alloys

*Group Head: Z. Li*

Department of Microstructure Physics and Alloy Design (MA)

Funded by the German Research Foundation (DFG), this new group was established in 2017 with the aim to develop novel high-entropy alloys (HEAs) with exceptional mechanical, physical and chemical properties based on the understanding of their structure-properties relations.

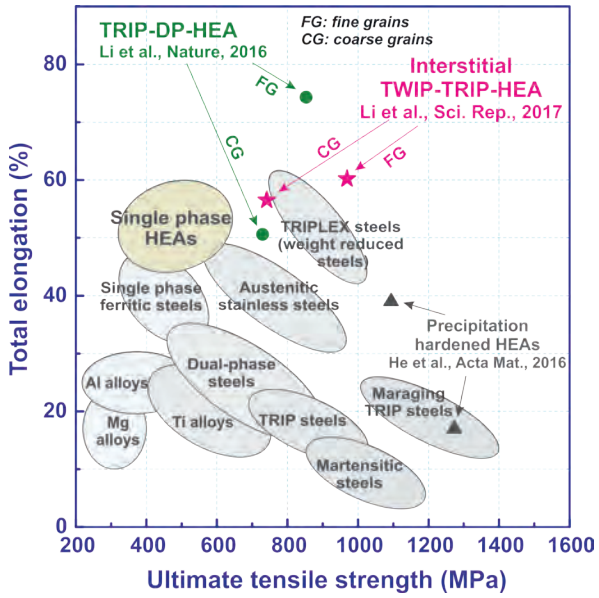


**Fig. 1:** *Strength-ductility profiles of various classes of metallic materials including the new HEAs developed by the group.*

Conventional alloy design over the past centuries has been constrained by the concept of one or two prevalent base elements. As a breakthrough of this restriction, the concept of HEAs opens a new realm of numerous opportunities for investigations in the huge unexplored compositional space of multi-component alloys.

While conventional alloys use strengthening mechanisms such as grain boundaries, dual-phase (DP) structure, dislocation interactions, precipitates and solid solution (e.g. steels, Ti-alloys, Al-alloys), the novel interstitial TWIP-TRIP-HEAs (TWIP: Twinning-induced plasticity; TRIP: Transformation-induced plasticity) concept developed by this new research group combines all available strengthening effects, namely, interstitial and substitutional solid solution, TWIP, TRIP, multiple phases, precipitates, dislocations, stacking faults and grain boundaries. This leads to the exceptional strength-ductility combination of the novel HEAs, exceeding that of most metallic materials.

The research group conducts the state-of-the-art research work employing novel experimental methodologies (Fig. 2), e.g., electron backscatter diffraction (EBSD), electron channeling contrast imaging (ECCI), atom probe tomography (APT) and transmission electron microscopy (TEM), in the following specific aspects:

- Excellent strength-ductility combination of transitional metal HEAs
- Resistances to hydrogen-embrittlement and corrosion of HEAs
- Light-weight high-strength HEAs
- High-temperature refractory high-strength HEAs
- Multifunction of HEAs
- Defects, segregations and thermodynamics in HEAs
- *In situ* observation of deformations in HEAs under electron microscopes

These aspects are strongly interconnected and facilitate an extensive collaboration network with national and international experts.

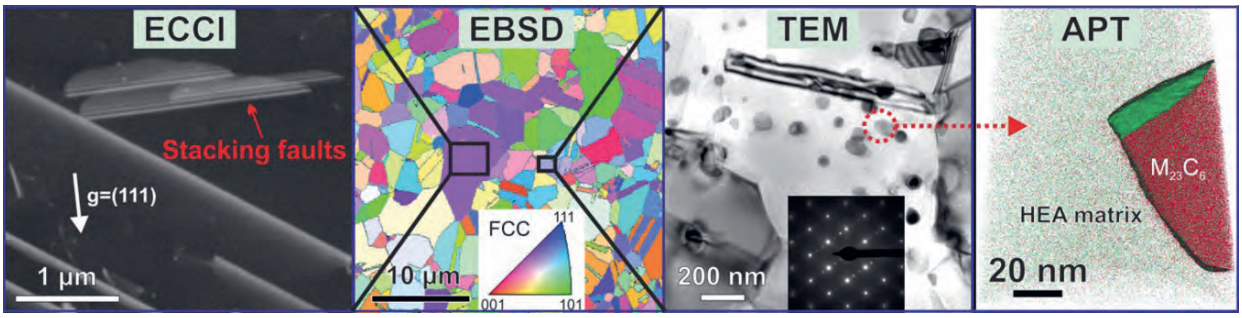


**Fig. 2:** *Representative microstructural information obtained from an interstitial TWIP-TRIP-HEA sample by combining multiple advanced characterization techniques.*

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# New Scientific Laboratories and Facilities

## The LAPLACE Project: Preparation and Transfer of Specimens for Electron Microscopy and Atom Probe Tomography under Ultra-High Vacuum and Cryogenic Conditions

*L.T. Stephenson [1], U. Tezins [1], A. Sturm [1], D. Vogel [2], Y. Chang [1], W. Lu [3], M. Rohwerder [2], D. Raabe [1], B. Gault [1]*

[1] Department of Microstructure Physics and Alloy Design (MA)
[2] Department of Interface Chemistry and Surface Engineering (GO)

The Atom Probe Tomography (APT) group in the MA department is developing integrated protocols for ultra-high vacuum cryogenic specimen transfer between platforms without exposure to atmospheric contamination. This apparatus enables back-and-forth transfers that will allow precise imaging of the specimen at various stages of the analysis. In theory, recording the emitter shape could provide input to improve APT data reconstruction protocols, and a future research direction will be to push for chemical compositional mapping with true atomic resolution. This explains the allusion to the 'Laplace demon', which refers to the statement by Laplace that by knowing the position and nature of all particles in the universe at a given point in time, one could predict the future and know all of the past.

Operating as of May 2018 are four linked platforms; a $N_2$-atmosphere glovebox, two state-of-the-art atom probes, and a scanning electron microscope / Xe-plasma focused ion beam equipped with a cryo-stage (funded by the federal ministry BMBF). It will be complemented with a small reaction chamber to allow for gas charging and surface reactions induced directly on atom probe specimens, which is developed together with the GO department and planned to be installed mid 2019.

Up until now, the outcome of the UHV specimen transfer has allowed the analysis of environmentally-sensitive materials by atom probe tomography, as well as, through cryogenic preservation, specimens that have been specifically modified by chemical reactions at their surface, i.e. deuterium or hydrogen charging. We demonstrated the efficacy of the new protocols by the successful preparation and transfer of delicate samples. First, we prepared a series of specimens from commercially pure Mg and Ti, as well as specimens from a Ti-6Al-2Sn-4Zr-6Mo alloy. Mg is highly sensitive to oxidation and we demonstrated that a thin layer of surface oxide was formed in the high-vacuum chamber of the plasma focussed ion beam instrument [1]. Commercially pure Ti and Ti-alloys are prone to forming hydrides during preparation as shown in Fig. 2. Here, we showed how maintaining the specimen at low temperature during the final stages of sharpening of the needle-shaped specimen could alleviate this issue. The results from APT displayed in Fig. 2 were also confirmed at a larger scale via transmission Kikuchi diffraction and transmission electron microscopy [2]. This result is critical for the success of the ERC-Consolidator project of B. Gault (see p. 70) that aims to precisely measure the H-content in engineering materials to explain their failure in service.

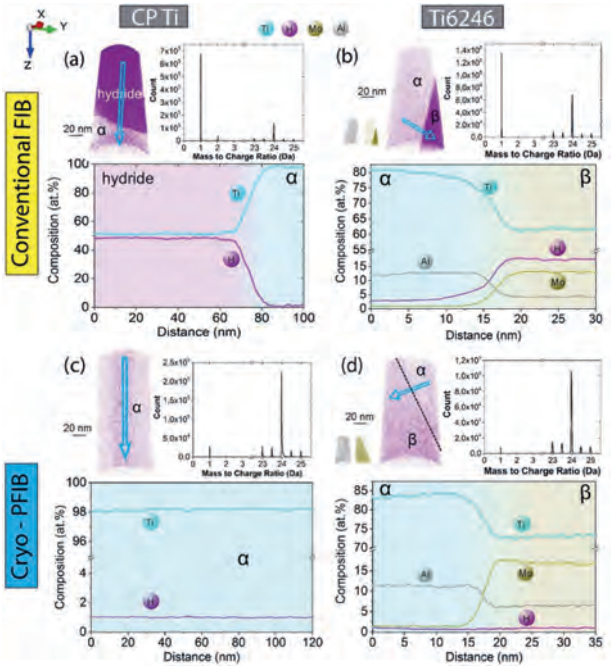


**Fig. 1:** *H distribution map obtained from APT, mass spectrum and composition profile of (a) commercially-pure titanium and (b) a Ti-6Al-2Sn-4Zr-6Mo alloy from specimens prepared by conventional focused ion beam at room temperature; (c)-(d) specimens from similar materials prepared by cryo-plasma focused-ion beam (at approx. -140°C).*

The Laplace project provides unique, state-of-the-art infrastructure for investigations in materials science and also allows for exploring new opportunities. We also demonstrated that the preparation and transfer of ice, which we hope will be an effective carrying medium for analysing suspensions and e.g. nanoparticles, and we recently successfully analysed proteins fibrils [3] involved in Alzheimer disease.

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# Additive Manufacturing and Powder Synthesis Laboratory

*E. A. Jägle*

Department of Microstructure Physics and Alloy Design (MA)

In the group "Alloys for Additive Manufacturing", we perform research to develop alloys that are suitable for use in additive manufacturing (AM). This can mean that they are resistant to typical processing-induced defects such as hot tearing. It can also mean that they exploit particular characteristics of the AM process. The three features of AM that our group focusses on are:

1. the high cooling rates of up to $10^6$ $Ks^{-1}$ after deposition,
2. the powder-technological nature of the process and
3. the possible metal-gas interactions occurring during material build-up.

**Fig. 1:** *Image of the SLM process during operation (left). The "sparks" captured are the typical ejected powder particles that are carried away from the melt pool by the inert gas cross jet. On the right hand side, the gas atomization process is shown (initial experiments).*

To investigate the impact of these features and to be able to develop new alloys, we aim to cover the entire process chain of additive manufacturing in-house. This starts with the design of alloys using thermodynamic databases, in particular using the software Thermocalc. Next, the alloys of interest are cast in rod shape by the metallurgy group. We have designed and built a laboratory-scale gas atomizer that enables us to produce small batches of powder from the cast rods. The powder is then used in our Aconity 3D "Mini" Selective Laser Melting (SLM) research machine to produce specimens which are analysed with the Institute's extensive testing and characterization facilities. We also pursue two other alloy development routes. In the first screening stage, small coupons are produced by arc melting and re-melted in the SLM machine. In the second, the alloy is generated during the process by melting a mixture of powders.

The devices available in the laboratory are designed or selected, to optimally support the research group's mission: To efficiently design and produce new alloys specifically for AM. There are very few atomizers available worldwide in research institutes that are capable to produce small powder batches of just a few hundred grams in the required size range. The atomizer is of the EIGA-type (Electrode Induction Melting Gas Atomization), which enables us to process reactive and refractory metals. Additionally, it is built in a modular fashion, allowing for easy cleaning between experiments and future modifications.

Among the available AM processes, we focus our work on the SLM process because it involves the smallest melt pools and hence the highest cooling rates. Our SLM machine is equipped with a small build platform and therefore requires only little powder. Its build platform heating system allows processing materials up to 800°C, which gives a high degree of freedom to avoid defects and to perform *in situ* heat treatments. In the beam path of the laser, there are two high-speed spot pyrometers for process monitoring. Finally, also this machine is designed for simple powder exchange and minimum cross-contamination.

In addition to the larger machines, the laboratory includes some powder handling equipment such as a sieving station, a powder drying oven, high-energy ball mills as well as a microbalance with a density measurement kit.

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# 3D-Orientation Microscopy by Automated Mechanical Polishing Combined with EBSD and ECCI

*S. Zaefferer [1], P. Konijnenberg [1,2], S.-P. Tsai [1], I. Gonzalez [3], S. Hartke[1]*

[1] Department of Microstructure Physics and Alloy Design (MA)
[2] Bruker Nano
[3] Electronics Group

3D orientation microscopy (3D-ORM) based on electron backscatter diffraction (EBSD)-mapping and serial sectioning is a powerful and versatile tool to obtain insights into the 3-dimensional nature of microstructures. 3D-ORM offers basic morphological data on microstructures, like the 3-dimensional shape and size of crystals, the arrangement of crystals and phases (e.g. neighbourhood or interconnectivity of structures), the 3-dimensional distribution of precipitations, dislocations and the extension and magnitude of elastic and plastic strain fields. The technique should be employed in cases where microstructures cannot be inferred through stereological approaches from sample sections. A particular information, which, in most cases, cannot be inferred in this way is the crystallographic and morphological character of grain and phase boundaries, which, however, determines the physical and chemical properties of these highly important lattice defects. The crystallographic character is described by 5 parameters, namely the misorientation across the boundary (3 parameters) and the boundary plane normal vector (2 parameters). The morphology may be described, for example, by local curvature or faceting of the interface.

Both, the morphological and the crystallographic character, may vary strongly even along one single grain or phase boundary, which means that they need to be determined locally if properties like mobility, corrosion or light emission (in the case of semiconducting materials) are to be explained. So far, 3D-ORM based on serial sectioning by focused ion beam milling (FIB) has been developed at the MPIE and other places worldwide. This technique has the advantage of being easily automatable and delivering precisely spaced sections. Its disadvantages, however, are the severely limited volume that can be investigated with the technique (usually about 20 x 20 x 20 µm³), the inconvenient geometry of the investigated volume, and the often significant beam damage caused by the high-energy ion beam milling. As a consequence we have looked into other techniques of serial sectioning which may be broad ion beam milling, laser ablation and mechanical-chemical surface polishing. For a number of reasons we decided to invest into the mechanical-chemical polishing approach which offers very large volumes to be investigated (in the order of 1000 x 1000 x 100 µm³ or even larger), in principle leads to ideal surface quality with a minimum of damage, and results in ideally flat surfaces which are very well suited for further measurements of, e.g., corrosion or optoelectronic properties. The challenge with this approach is, however, the difficulty of automation and the exact measurement and control of section thicknesses. To overcome these problems we have bought a polishing robot (Saphir XChange, Fa. ATM) and a “Cobot” (i.e. a collaborative robot) (UR5, Universal Robots). Both instruments are connected to a Zeiss Merlin scanning electron microscope with an EBSD and energy dispersive x-ray spectroscopy (EDX) system. The Saphir XChange polishes a sample in a perfectly controlled manner, the UR5 transports the sample to and from the microscope and the microscope performs EBSD and electron channelling contrast imaging (ECCI) measurements on the polished sample surface. To integrate these instruments into one 3D-ORM system we have put together a team of 5 people with different backgrounds, including material science, mechanical engineering, electronics and software design. The system is expected to make first complete runs in early 2019.


**Fig. 1:** *Combination of the Saphir X-Change polishing automata (the main gray box), the UR5 cobot (in the front) and the Zeiss Merlin SEM (behind both in the background). The cobot is currently picking up a sample which has been placed on an exchange table by the polishing automata. It will subsequently open the microscope door, place the sample in the microscope and close the door again.*

# Aberration Corrected Transmission Electron Microscopy Facility

*C. Liebscher [1], V. Kree [1], J. Thomas [1], G. Dehm [1], C. Scheu [2]*

[1] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[2] Max Planck Research Group on Nanoanalytics and Interfaces (NG)

The aberration corrected transmission electron microscopy (TEM) facility was completed with the installation of the image corrected FEI Titan Themis 80-300 (Thermo Fisher Scientific) mid of 2017 illustrated in Fig. 1. Since its commissioning in October 2017, the microscope is available for $C_s$-corrected TEM imaging with a point resolution of down to 80 pm, enabled by a CEOS GmbH aberration corrector. The microscope can be operated at 80, 200 and 300 kV acceleration voltage. Conventional high-resolution imaging can be coupled with through focal series acquisition for exit wave reconstruction. Low dose conditions can flexibly be adjusted to study beam-sensitive materials and to reduce beam-induced artifacts. The microscope is also equipped with a Lorentz lens for imaging magnetic domain walls in materials. It is also possible to operate the microscope in basic scanning TEM (STEM) mode, which can be coupled with energy dispersive X-ray spectroscopy (EDS) through four synchronized EDS detectors (ChemiSTEM).

Currently, the microscope is upgraded with a high speed CMOS (Complementary Metal Oxide Semiconductor) based camera to enable image acquisition with up to 300 frames per second (fps). This is needed to study dynamic events in materials under *in situ* conditions. Since the beginning of 2017, a Gatan model 654 straining holder is available for the FEI microscopes, which allows to strain micron-sized sample *in situ* in the TEM to observe their deformation behaviour. An image of the holder tip, the copper support and the location of a focus ion beam (FIB) prepared sample are shown in Fig. 1.

In May 2018, a DENSsolutions Lightning heating and biasing holder was implemented that allows to heat micron-sized samples up to temperatures of 1300 ºC, and in addition it is possible to apply high electric fields of up to 100 kV/cm at temperatures up to 800 ºC. The tip of the sample holder with electrical contacts and the MEMS (Micro-Electro-Mechanical System) based chip are illustrated in Fig. 1. The novel MEMS based heating/biasing chip design enables unprecedented sample stability with a drift rate of <0.3 nm/min and strongly reduced bulging of the $Si_3N_4$ membrane of <500 nm up to 500ºC.

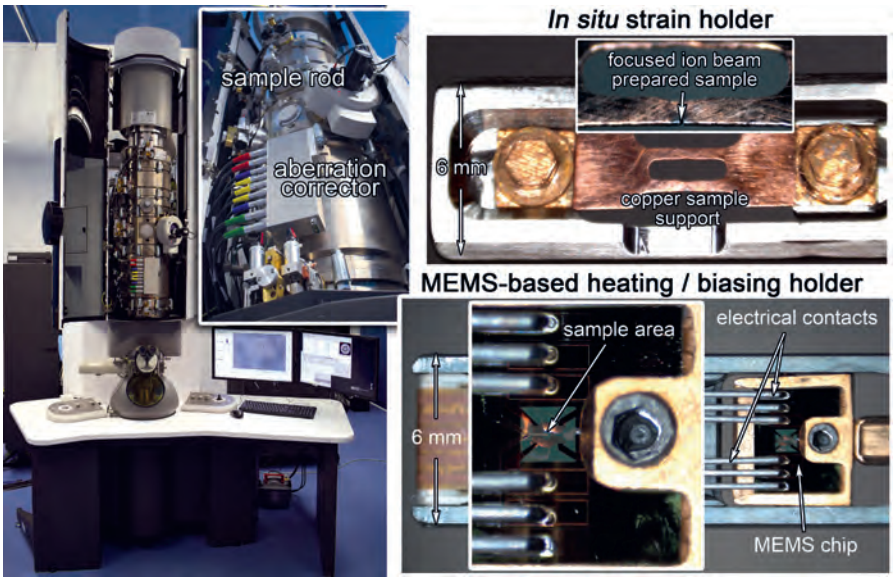


**Fig. 1:** *Image corrected FEI Titan Themis 80-300 (Thermo Fisher Scientific). The insets highlight the aberration corrector and the sample rod. Close up images of the tips of a Gatan model 654 in situ straining holder and a MEMS based DENSsolutions Lightning heating/biasing holder.*

Hence, the aberration corrected transmission electron microscopy facility enables to investigate the sample behaviour *in situ* under an applied strain, temperature or bias and the dynamic evolution of the micro- and nanostructure can be captured with high-speed electron detectors.

# Thermal Analysis Laboratory

*F. Stein, L. Christiansen, A. Bobrowski*

Department of Structure and Nano-/ Micromechanics of Materials (SN)

Thermal analysis serves to study physical properties of materials as a function of temperature. The most versatile methods for this purpose are differential thermal analysis (DTA) and differential scanning calorimetry (DSC). In general, DTA/DSC allows the detection of any type of thermal effect in a material occurring during heating or cooling with a constant rate or when holding at constant temperature.

DTA/DSC is applied at the MPIE in all sorts of projects for various types of materials most of metallic but also of ceramic or even biological nature. The available facilities cover a wide range of temperatures from -196 °C (liquid nitrogen) to 2000 °C. Examples for investigated effects comprise melting behaviour, invariant reactions, order-disorder transitions, magnetic transformations, and martensitic transformations in, e.g., steels, but also in shape memory alloys. Moreover, crystallization/recrystallization, relaxation or decomposition processes and glass transitions in amorphous materials can be studied, metastable states can be identified, and precipitation processes can be detected. In addition, the kinetics of effects as for example slow solid-solid transformations or precipitation reactions can be analysed.

Another important aspect of the DSC method is its capability to generate calorimetric data. By exploiting the heat flow signals, heat capacity can be determined between room temperature and about 1200 °C. Finally, the DTA/DSC instruments can also be perfectly well applied for precisely controlled heat treatments to attain special microstructural states while simultaneously recording the heat flow signal.

The DTA/DSC facilities available in our thermal analysis laboratory comprise a low-temperature device 'DSC1' (Co. Mettler-Toledo) capable of measuring in the range from -196 °C (liquid nitrogen) to 600 °C, and two classical DTA/DSC instruments 'DSC 404 C Pegasus' (Co. Netzsch) and 'Setsys 16/18' (Co. Setaram) working between room temperature and 1650 °C and 1750 °C, respectively. Recently, the thermal analysis laboratory was complemented by an instrument for simultaneous thermal analysis 'STA 449 F3 Jupiter' (Co. Netzsch) combining DTA/DSC with thermogravimetric analysis (TGA). For the development of alloys for applications at very high temperatures, e.g. for the replacement of Ni-based superalloys, there is a need to measure the thermal behaviour up to very high temperatures. The STA instrument possesses a graphite furnace allowing DTA experiments up to 2000 °C. Even though the experiments are performed in a He inert gas atmosphere, metallic materials often show a strong sensitivity for chemical reactions with remaining gaseous impurities and often also with the crucible materials. Therefore, simultaneously to recording the DTA signals, weight changes of the sample are monitored by TGA. The STA instrument is equipped with two furnaces, switching from the graphite furnace to the rhodium furnace allows to apply the STA for heat capacity measurements.

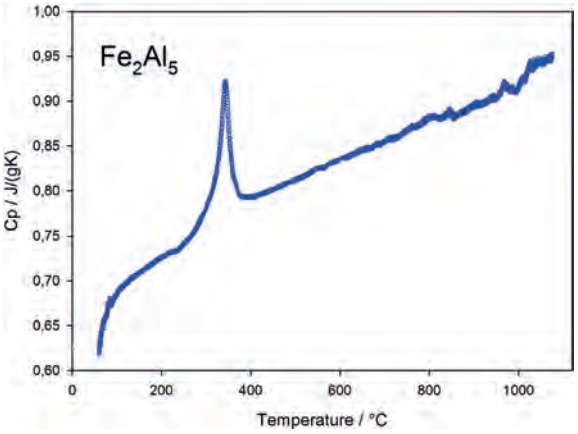


**Fig. 1:** *The picture on the left side shows the opened STA instrument with DSC sample holder and the two furnaces in the position to switch from the 2000 °C graphite furnace (left side) to the rhodium furnace (right side) suited for heat capacity ($C_p$) measurements up to 1200 °C and classical DTA/DSC up to 1650 °C; the diagram shows a $C_p$ measurement of a single-phase $Fe_2Al_5$ intermetallic alloy indicating a structural transformation.*

# Long-term Oriented Method Development

## Understanding the Complexity of Dislocation Structures using 3-Dimensional Electron Channelling Contrast Imaging (3D-ECCI)

*S. Zaefferer [1], P. Konijnenberg [1,2], S.-P. Tsai [1]*

[1] Department of Microstructure Physics and Alloy Design ( MA)
[2] Bruker Nano

The microstructure of a material, i.e. the ensemble of its extended crystal defects (grain and phase boundaries, precipitations, dislocations and stacking faults, elastic and plastic strain fields) , is intrinsically 3-dimensional (3D), even if many techniques for microstructure characterization (light microscopy, transmission electron microscopy (TEM), scanning electron microscopy (SEM) techniques) reveal only 2D sections or shallow 3D projections of it. Nevertheless, the properties of materials and processes of microstructure formation usually depend strongly on the 3D arrangement of defects. This relation is obvious for grain and phase boundaries for which the local crystallographic and morphological character plays an important role for their properties. Moreover, the 3D arrangement is also important for dislocations and their related stress fields. One interesting and fundamental example is the question whether dislocations that are found inside of deformed grains are produced by activation of Frank-Read sources inside of the grain or whether they originate on the grain boundaries. 2D sections of grains almost never explicitly show the location and nature of dislocation sources. Another example is the distribution of dislocations in front of progressing lenticular martensite crystals. In this case dislocations are important for the arrest of the martensite growth due to the loss of lattice coherency. A third example is the distribution of dislocations along triple junctions in deformed grains and the related formation of new crystals during recrystallization.

The observation and quantification of dislocations has long time been a domain of TEM, which, however, requires thin foil samples and therefore, in most cases, impedes a true 3D observation (except for the 100 nm to 200 nm of volume thickness that is observed by the technique). In contrast, the still relatively new electron channelling contrast imaging (ECCI) technique, applied in SEM, allows observation of dislocations and other defects in the first 100 nm thickness below the surface of bulk samples. If this technique is combined with a sufficiently gentle method to remove thin serial sections of a material, it is possible to perform 3D dislocation observation over large volumes and at a large number of locations in a single sample. An appropriate method for serial sectioning is the mechano-chemical polishing with an oxide particle suspension (OPS) of suitable composition. We are currently building up a fully automated system for this approach (see p. 36). We expect that this system will be able to perform sections of minimum thickness of about 50 nm with a surface quality sufficient for ECCI observations which will allow tracing individual dislocations through a large depth of 10 or more sections.

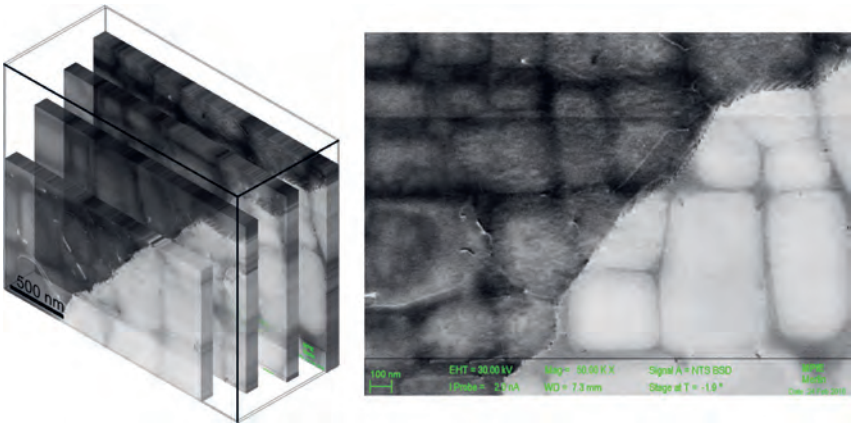


**Fig. 1:** *3D-ECCI on a subgrain boundary in a single crystal superalloy with a γ-γ' microstructure. The left image shows 4 sections with about 150 nm spacing, displayed as semitransparent ECC images. The right side shows the last section. The cuboidal γ' precipitates are clearly visible. The subgrain boundary consists of a network of narrow-spaced dislocations, visible as white lines. The bright and dark sides are due to different channelling conditions on the two sides of the boundary.*

A first test of this method has been pursued by manual polishing of a superalloy with a γ-γ' microstructure. The figure above shows the arrangement of dislocations along a subgrain boundary in this material. The left side displays the 3D arrangement; the right side shows just the last section. Slice thickness is not yet well controlled and the software for imaging the dislocations is not yet well developed. Both will be subject of future developments.

# *In situ* Electron Microscopy Techniques

*C. Liebscher[1], W. Lu[1], S. Lee[1], C. Kirchlechner[1], S. Hieke[2], S. Zhang[2], C. Scheu[2], G. Dehm[1]*

[1] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[2] Independent Max Planck Research Group on Nanoanalytics and Interfaces (NG)

*In situ* electron microscopy offers novel insights into the dynamic evolution of microstructure at elevated temperatures [1-3], high oxygen partial pressures [4], an applied strain [5] or electrical bias at highest possible resolution, even down to the atomic scale. Furthermore, it is possible to probe local chemical and electrochemical reactions of nanomaterials in gaseous and liquid environments [6] by still preserving nanometre resolution. This broad range of *in situ* techniques is currently under development and implementation at the MPIE for both scanning electron (SEM) and transmission electron microscopy (TEM). The aim is to establish methodologies suitable to investigate all levels of microstructural features in advanced material systems.

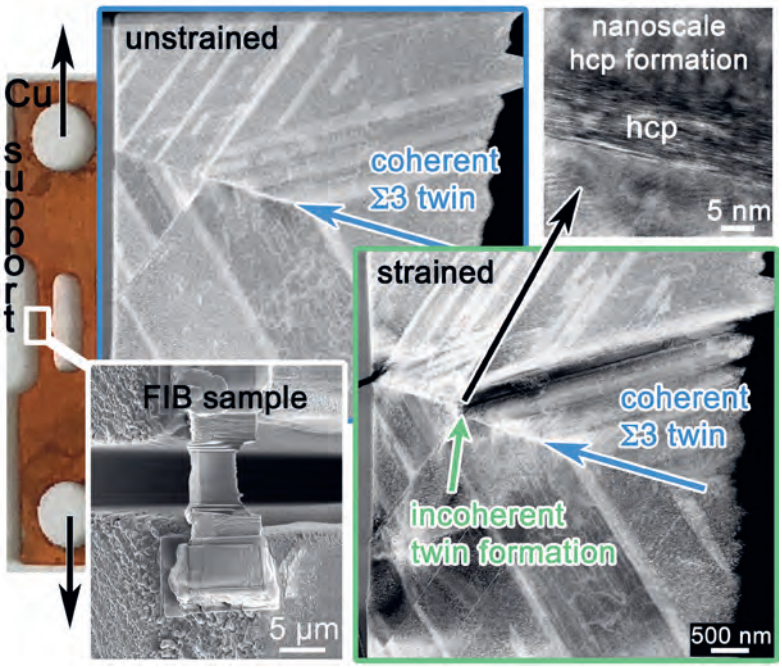


**Fig. 1:** *In situ TEM straining experiment of a dual phase high entropy alloy. The focused ion beam (FIB) prepared sample is welded onto the copper (Cu) support. During straining, an incoherent twin boundary segment is formed by the accumulation of dislocations at the coherent twin. This location serves as the nucleation point for the formation of the hexagonal closed packed (hcp) phase.*

*In situ* straining in the TEM in conjunction with novel imaging techniques provides unprecedented insights into the local deformation mechanisms of complex microstructures. As an example, the deformation induced formation of hexagonal close packed (hcp) phases at a coherent Σ3 twin boundary in the face centred cubic (fcc) grains of a dual phase high entropy alloy (HEA) is illustrated in Fig. 1. These novel alloy systems provide a unique combination of strength and ductility and *in situ* straining experiments are able to unlock the fundamental deformation induced phase transformation mechanisms [5]. *In situ* heating in the TEM [1] enables the determination of phase decomposition pathways and the local diffusion of elements on a nanometre level at temperatures of 1000 °C or more.

As a future perspective, *in situ* heating experiments will be coupled with electrical biasing to determine the effect of electric fields on the phase decomposition of materials and interfaces at atomic resolution. Also, combined *in situ* heating and mechanical loading experiments were developed over the last years and are now ready to investigate fundamental properties (e.g. activation energies for dislocation slip transfer) of plasticity, fracture and fatigue. The ultimate goal of the development of *in situ* electron microscopy techniques is to establish the underlying mechanisms linking microstructure and properties.

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# Submicron 3D Insights into Deforming Microstructures

*C. Kirchlechner [1], J.-B. Molin [1], L. Renversade [1,2], J.-S. Micha [2]*

[1] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[2] CRG-IF BM32 at ESRF, Grenoble, France

Interlinking the mechanical properties of advanced materials to their underlying and evolving defect structure is key to understand and improve their reliability during daily use. For instance, in case of fatigue the properties of interest are the local strain distribution, the density and type of dislocations, crystal orientations and the crystallographic phase. All aforementioned properties are accessible at the sample surface with advanced characterization tools like scanning electron microscopy (SEM) including electron backscatter diffraction (EBSD) and, destructively, by transmission electron microscopy (TEM). But can we measure these properties *in situ*, non-destructively, with submicron precision and in bulk materials?

Within the XMicroFatigue project jointly funded by the German DFG and the French ANR, we are developing a unique tool being able to shed unprecedented light onto buried deforming volumes and interfaces. Together with our French partners from CEA-Grenoble we combined a synchrotron-based Differential Aperture X-ray Microscope (DAXM) [1] with a state-of-the-art micro-deformation rig [2]. The combined apparatus is located at BM32 of the European Synchrotron Radiation Facility (ESRF) and allows for *in situ* Laue microdiffraction experiments as well as a three dimensional reconstruction of the deformed sample volume. A spatial resolution better than 500 nm³ and deviatoric strain sensitivity better than $10^{-4}$ are currently reached.

The first project with this unique tool focusses on the fatigue damage initiation close to grain boundaries in copper. For this purpose micro cantilevers with a diameter of 10 µm are cut by focussed ion beam milling and subsequently cyclically loaded. Laue patterns and the force-displacement response are recorded during loading [3]. In addition, after ¼, ½, ¾ and after a full cycle the three dimensional dislocation structures and strain distributions are mapped with submicron resolution (Fig. 1).

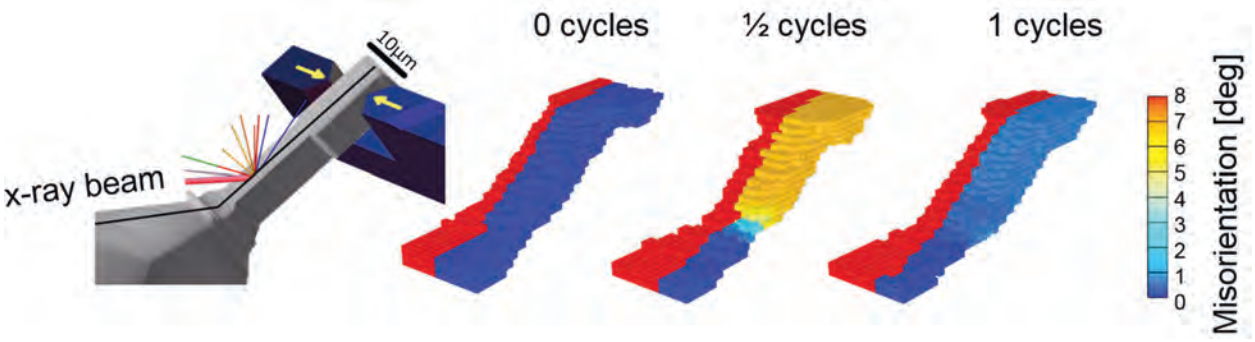


**Fig. 1**: *Bi-crystalline micro fatigue sample. The schematic indicates the location of the grain boundary (solid black line), the loading direction (yellow arrows) and the incoming and diffracted X-ray beams. The 3D point-to base disorientation reconstructions of the initial state, after ½ and a full cycle are plotted.*

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# Environmental Small Scale Mechanics

*S. Brinckmann, J. Duarte, V. G. Arigela, C. Kirchlechner*

Department of Structure and Nano-/ Micromechanics of Materials (SN)

In the past decade, micromechanics have been established to fundamentally understand plasticity and fracture mechanisms and attribute these mechanisms to the microstructural components. At the MPIE, we develop analytical tools to investigate further the influence of environments on the plasticity and fracture mechanisms. High temperature applications in the energy sector require a thorough understanding of failure of microstructural components. Hydrogen is long known as detrimental for steels although the mechanisms at the microstructural length-scale are still not well understood.

Based on a previously build setup [1] for synchrotron experiments, a customized high-temperature microscale loading rig was developed to characterize material systems at their service conditions. This setup (Fig. 1) is being operated in a custom-made steel environmental chamber capable of attaining a vacuum of $10^{-6}$ mbar at temperatures of 600°C. The device also allows testing materials in various gas atmospheres permitting comprehensive understanding of environmental embrittlement phenomena. Moreover, this setup allows microscale mechanical testing using varying test methods (tension, compression, bending and fatigue), geometries, material systems, temperatures and environments.

Nanoindentation is a valuable technique to study hydrogen-microstructure interactions in metallic alloys, due to the small-probed volume and fast sample preparation. *In situ* testing while charging the sample with hydrogen prevents concentration gradients due to hydrogen desorption. Two custom electrochemical cells were built in-house to hydrogen-charge the samples during nanoindentation: "front-side charging" with the sample and the indenter tip immersed in the electrolyte, and "back-side charging" where the analyzed region is outside of the solution (Fig. 2). During front-side charging, surface degradation might occur which possibly reduces the reliability of post deformation analysis. Hence, we tailor the electrolyte and the operating procedures to the material and mechanical loading conditions to minimize the surface alteration and maximize the experimental stability.

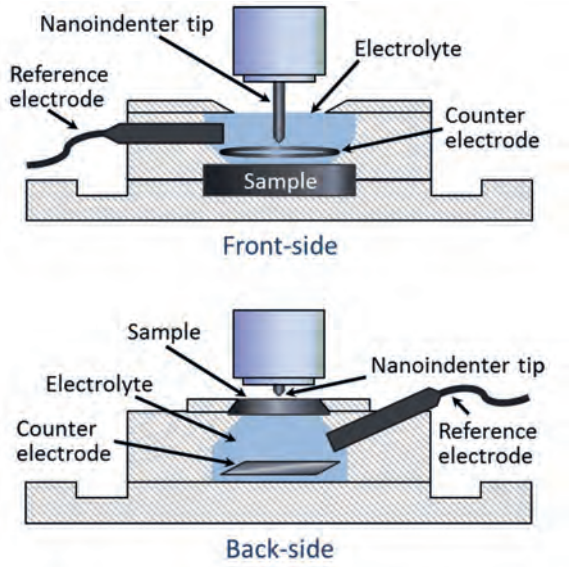


**Fig. 2:** *Schematic of the in-house electrochemical cells to perform in-situ nanoindentation.*

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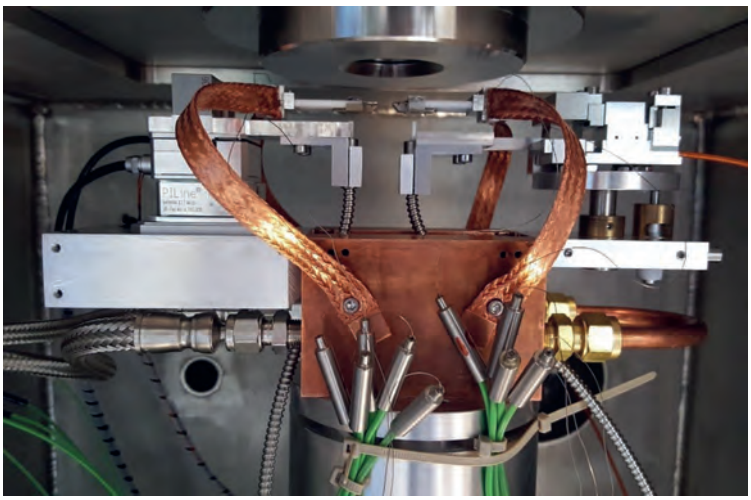

**Fig. 1:** *The high-temperature straining device enclosed in an environmental chamber.*

# Micromechanics along Concentration Profiles in Diffusion Couples

*F. Stein, W. Luo, C. Kirchlechner, S. Brinckmann*

Department of Structure and Nano-/ Micromechanics of Materials (SN)

Mechanical properties of single-phase materials such as solid solutions or intermetallic phases may strongly vary as a function of composition (e.g. solid solution hardening by alloying), but are also well known to be affected by microstructural features such as size and crystallographic orientation of the grains and their morphology. Systematic investigations on the isolated, sole effect of composition often are difficult as for each composition a new alloy has to be prepared having not only a comparable microstructure but also keeping other parameters unchanged such as the level of impurities and the chemical homogeneity. Especially for intermetallic phases, an additional problem is the difficulty to produce flawless macroscopic samples, which are required for classical mechanical compression or bending tests.

To avoid these problems and to circumvent the necessity of preparing large-scaled samples, we follow a completely different approach, in which we use diffusion couples between two single-phase metals or intermetallics. By intimately contacting two pieces of such single-phase materials and holding this arrangement for sufficient times at elevated temperature, extended diffusion zones (in the order of 10 µm to 1 mm) of solid solutions and intermediate phases can develop having concentration gradients that cover the entire homogeneity range of these phases (for an example, see Fig. 1a). Under ideal conditions, large grains with a continuous concentration gradient grow in such diffusion zones.

Position-resolved nanoindentation tests along the concentration gradient (Fig. 1b) then are a simple method to yield information on the composition dependence of hardness and elastic modulus. Furthermore, by FIB (focused ion beam) cutting of small micropillars and microcantilevers at different selected positions in this diffusion zone parallel to the direction of the concentration gradient (Fig. 1c), we can obtain series of single-phase, single crystalline specimens with identical crystallographic orientation but different chemical composition. Then micropillar compression and microcantilever bending tests of these specimens allow a systematic study of composition- and orientation-dependence of strength and fracture toughness, for instance in order to get a better understanding of how the mechanical behaviour is affected by deviations from the ideal, stoichiometric composition of a phase, e.g., by introducing defects such as anti-site atoms in the crystal structure.

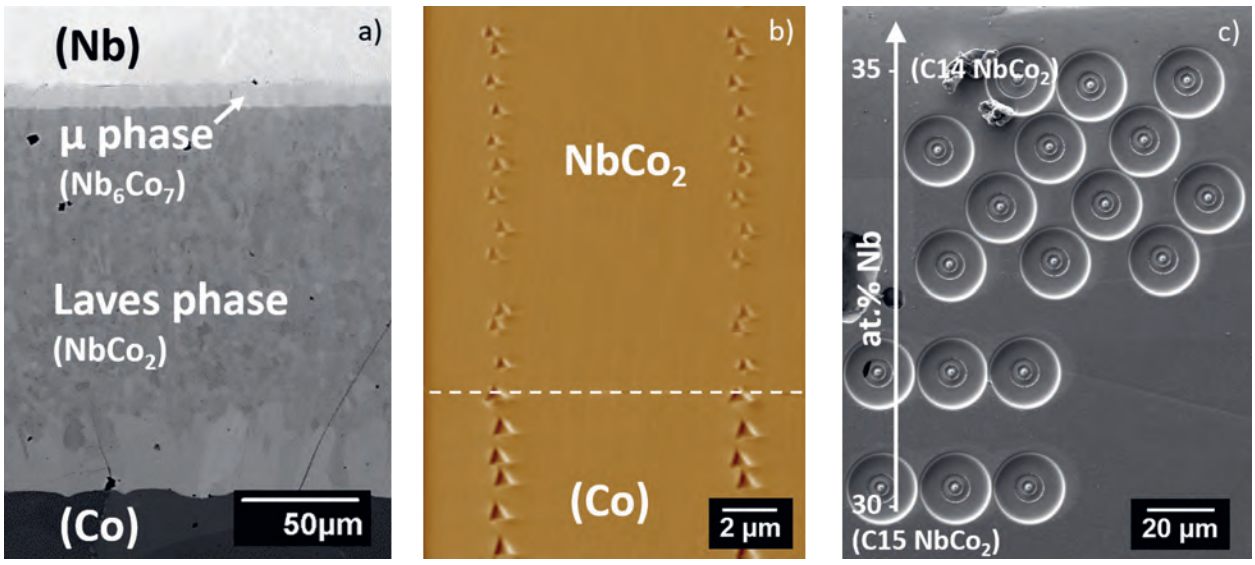


**Fig. 1:** *a) Diffusion couple of pure Co and Nb forming the (Co) and (Nb) solid solutions and two intermetallic phases, which are the Laves phase $NbCo_2$ covering a wide composition range from about 24 to 36 at.% Nb and the µ phase $Nb_6Co_7$ (47 to 55 at.% Nb); b) nanoindents along the concentration gradient near the boundary between (Co) and the Laves phase; and c) series of micropillars cut by FIB along and perpendicular to the concentration gradient in the diffusion zone of the Laves phase (showing the composition range where the structure type of the Laves phase changes from the cubic C15 to the hexagonal C14 variant).*

# Advanced Metallurgical Synthesis and Processing

*H. Springer, E. A. Jägle*

Department of Microstructure Physics and Alloy Design (MA)

The metallurgical synthesis and processing is one of the cornerstones of the Institute, connecting therory and characterisation into the full circle of material development. It represents the basis to investigate micro- and nano-structural phenomena, validate simulations and study complex phase transformations and interfacial reactions. Accordingly a wide range of experiments are performed ranging from single-crystaline model alloys to modified industrial materials. About 500 metallic materials per year are produced for inhouse use across all departments as well as within the scope of external cooperations with scientific and industrial partners. Building on a strong set of basic equipment, the techniques and processes are constantly updated in parallel with the progress in materials development. With ever growing complexity, these innovative alloys are critically dependent on being developed together with their production techniques. At the same time, novel techniques require adapted alloy solutions, as they are opening the path for new concepts and material solutions.

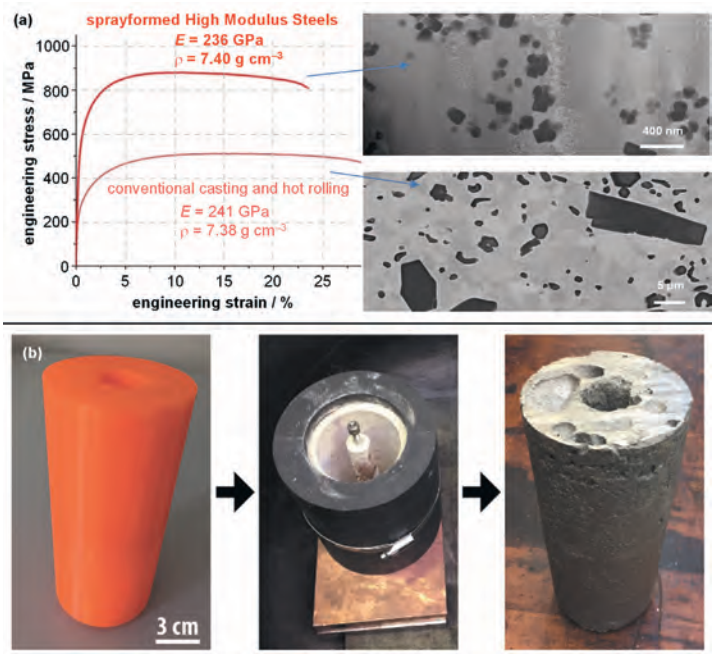


**Fig. 1:** *(a) Nano-structured High Modulus Steels obtained through sprayforming allow for an unprecedented combination of the key material properties for lightweight design. (b) Expendable 3D printed PLA polymer form being used to shape a sand casting mould, together with the final cast near-net shape ingot.*

Additive manufacturing, also referred to as 3D printing, is a prime example where the specific features of a novel technique both represent a challenge for utilising their full potential, as well as offering the possibility to realise materials with property combinations impossible to achieve before. The rapid solidification of the extremely small meltpool – compared to conventional large-scale casting procedures – can be used to achieve supersaturation of alloying elements, which then can be exploited for finely tuned precipitation reactions e.g. in Al-Sc alloys and maraging steels [1,2]. Another interesting pathway lies in utilising the increased solidification kinetics to obtain high modulus steels, which due to the *in situ* formation of nano-scaled $TiB_2$ particles, can overcome the inherent conflicts between density, stiffness, strength and ductility (Fig. 1a), and are therefore prime candidates for future lightweight design solutions [3]. By controlling the interaction between liquid powder particles and gases from the process atmosphere, oxides and nitrides can be synthesised in novel materials for high temperature applications [4]. Furthermore, additive manufacturing techniques can be used complementing the combinatorial high throughput design of structural materials [5], and as a rapid solidification technique which produces bulk samples rather than thin films or foils. 3D printing can also be used to produce expendable polymer shapes for pre-forming casting moulds (Fig. 1b; “lost-PLA casting”).

To fullfill the twin role as both the basis for material development, as well as the driving force for novel material design in highly innovative and competitive fields, new machinery (e.g. a strip casting simulator) are built and new labs are established at the MPIE, in close cooperations between groups inhouse and with external partners.

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# Scanning Kelvin Probe Techniques for Advanced Measurement of Hydrogen and Electrochemical Activity at Buried Interfaces

*M. Rohwerder, C.-H. Wu, W. Krieger*

Department of Interface Chemistry and Surface Engineering (GO)

The utilization of Kelvin Probe (KP) techniques for spatially resolved high sensitivity measurement of hydrogen has been a major break-through for our work on hydrogen in materials [1]. A relatively straight forward approach was hydrogen mapping for supporting research on hydrogen embrittlement that was successfully applied on different materials, see e.g. [2-6].

The key strength of this KP approach for H mapping is that the hydrogen release from the investigated material into an ultra-thin palladium detection layer is directly measured with high local resolution. This release rate is a measure for how fast H can be supplied e.g. to a crack tip. Scanning KP (SKP) is fully quantitative. We are currently working on several concepts for full calibration also for Scanning Kelvin Probe Force Microscopy (for instance by a combination (see [5]).

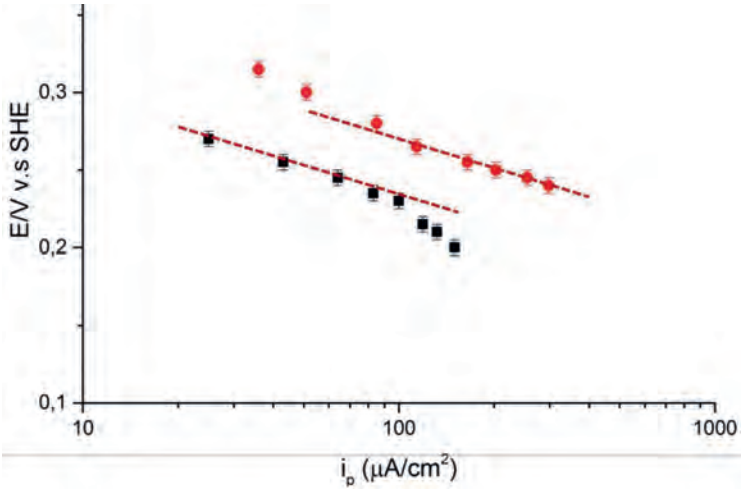


**Fig. 1:** *I(U) relationship between ORR and HOR on two iron(oxide) surfaces, one slightly (black) and one highly defective (red). Atmosphere $O_2$ at about 90% r.h., i.e. the Fe is covered by less than 1 nm of water.*

Another idea is to use the method for detecting corrosion sites through the metal. This is of interest, for instance, for fundamental studies in corrosion science as well as for practical application in the field, e.g. to measure internal corrosion at the outside of a pipeline.

Since often the evaporation of a thin Pd film and providing a dry nitrogen atmosphere is inconvenient or even impossible (such as in the field), alternatives are currently being investigated. Another problem is saturation of the potential change upon reaching certain levels of H activity. This can be circumvented by using another approach where the equilibrium potential between hydrogen oxidation (HOR) and oxygen reduction reactions (ORR) is used for measuring permeation/effusion rates of hydrogen, which was first applied for investigating oxygen reduction at buried interfaces (see [7,8] and p. 66). We found that this can even be applied directly on the iron (oxide) surface (see fig.1).

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# Coupled Electrochemical Scanning Flow Cell-Based Techniques for Electrocatalysis Research

*S. Cherevko [1], O. Kasian [1], S. Geiger [1], M. Ledendecker [1], K.J.J. Mayrhofer [1, 2]*

[1] Department of Interface Chemistry and Surface Engineering (GO)
[2] Helmholtz Institute Erlangen-Nürnberg for Renewable Energy

Electrochemical scanning flow cell (SFC) has been developed in the "Electrocatalysis" group of the GO department to assist in the electrochemical measurements in research areas such as corrosion, fuel cells, water electrolysis, electrosynthesis, etc. Due to its high-throughput nature, this cell transformed typically manual, routine, tedious, and time consuming measurements into fast and automized ones. What made SFC especially powerful, however, is its scaling capability to create new, and unique for electrocatalysis research, coupled techniques such as *in situ* SFC inductively coupled plasma mass spectrometry (*in situ* SFC-ICP-MS), SFC on-line electrochemical mass spectrometry (SFC-OLEMS), and others (see Fig. 1). Recently, employing a set of SFC-based techniques, in this case SFC-ICP-MS and SFC-OLEMS, "Electrocatalysis" group aided in understanding of the water splitting mechanism on iridium,[1-3] a very important and timely topic in the renewable hydrogen production technology.

In the years that past, potential of these techniques has been realized by numerous research groups worldwide, which is supported by a growing number of the high quality scientific works employing *in situ* ICP-MS and similar methods. Both, internal and external developments reveal that, despite the fact that SFC can be considered as a mature technique, the full potential of this technique is still yet to be seen. Development is continuing in the direction of SFC coupling to Raman, infra-red, X-ray based spectroscopies, etc.

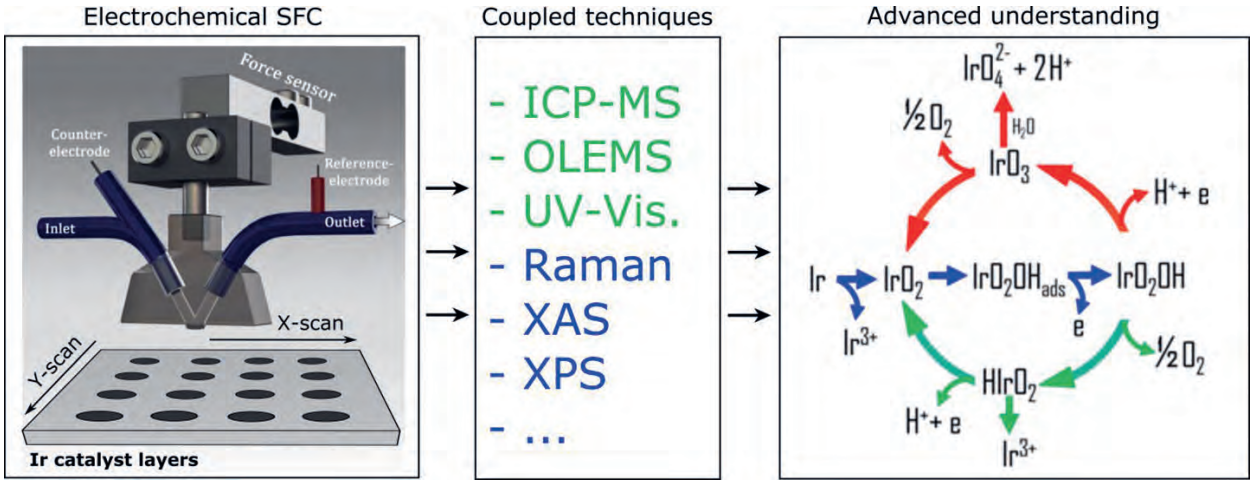


**Fig. 1:** *Concept of the combinatorial reaction analysis by SFC coupled techniques.*

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# *Ab initio* Description of Electrified Interfaces in Electrochemistry and Atom Probe Tomography

*M. Todorova [1], S. Surendralal [1], C. Freysoldt [1], S. Wippermann [2], J. Neugebauer [1]*

[1] Department of Computational Materials Design (CM)
[2] Department of Interface Chemistry and Surface Engineering (GO)

Solid/liquid interfaces are an essential constituent in electrochemistry, electrocatalysis and corrosion. These interfaces are characterized by strong electric fields that originate from finite surface charges and modify adsorption, desorption, interface reconstructions, double layer formation and reactions at the electrode/electrolyte interface. Electric fields (a few $10^{10}$ V/m) are also required for field evaporation, the key mechanism in atom probe tomography (APT). Modelling such electrified interfaces is challenging: while the counter-charges in reality are far away, atomistic simulations must either include artificial ones or introduce special boundary conditions, which may cause additional complications. In consequence, no standard approach is yet available. The groups of C. Freysoldt, M. Todorova and S. Wippermann develop and employ various methods to treat finite electric fields in density-functional theory (DFT).

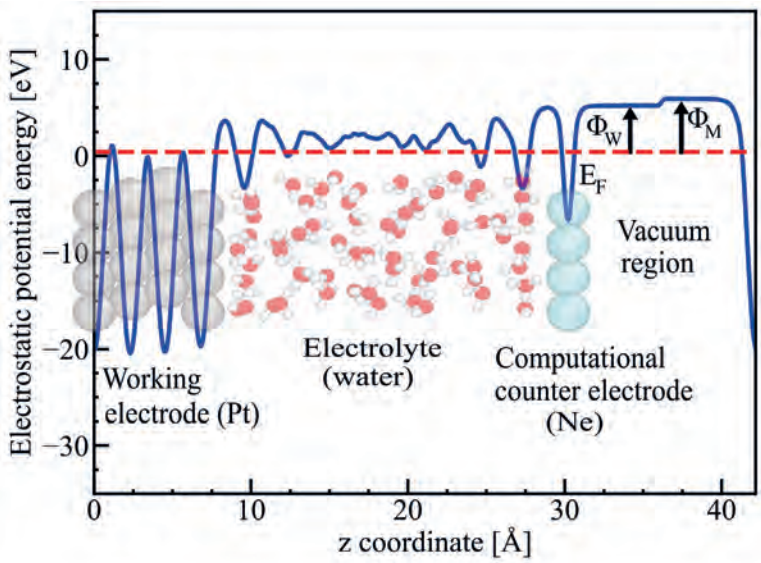


**Fig. 1:** *Supercell-setup of the computational counter electrode. Atoms are shown as spheres (grey: Pt, red: O, white: H, light blue: Ne). The blue line shows the electrostatic potential distribution within the supercell. The Fermi energy of Pt is shown as a red dashed line. The dipole correction, via which the potential of the interface is determined is visible as a jump in the electrostatic potential in the vacuum region, i.e. difference between the work function of the metal ($\Phi_M$) and the work function of the counter electrode ($\Phi_W$).*

Combining concepts from electrochemistry and semiconductor physics, we were able to design a novel approach that allows to study chemical reactions at the electrochemical interface using standard DFT codes [1]. The schematic setup of the approach is shown in Fig. 1 and described in detail on p. 193. An alternative approach is the modern theory of polarization, which introduces an electric field term directly into the DFT Hamiltonian. This allows us to simulate the full electrochemical cell without a vacuum region.

Studying elementary processes at APT tip surfaces by DFT, requires, in contrast, a voltage drop of a few 10 V across the simulation cell. This is much larger than the typical energy scale of valence electrons, precluding any attempts to generate the fields by charged ions. In this case, we model the electrified surface by a charged slab in a periodic cell. In all existing DFT codes the counter charge is smeared out, which produces an uncontrollable distribution of the electric fields. We therefore developed a new approach that places a counter electrode in the centre of the vacuum region together with a discontinuity in the electrostatic potential, a technique known as the “dipole correction” for asymmetric slabs [2]. This combination realizes a single “generalized dipole correction”, which enables, together with further improvements ensuring a proper initialization and suppression of charge fluctuations, surface calculations for fields even beyond the evaporation threshold.

Our development activities aim at solving outstanding questions related to electrified surfaces, and profit from mutual insights generated in the different areas of application. To foster exchange also at an international scale, in March 2017 we conducted a three-day workshop at Ringberg castle on “High Electric Fields in Electrochemistry and Atom Probe Tomography”, to bring together leading scientists from the areas of APT, field-ion microscopy and electrochemistry.

Time scales of electrochemical processes are far beyond the realm of DFT. Future work will in addition explore how to combine the electric field approaches with accelerated sampling techniques or implicit solvent approaches.

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# *Ab initio* Thermodynamics and Long-Term Archiving with the in-house Developed *pyiron* Platform

*J. Janssen, B. Grabowski, T. Hickel, J. Neugebauer*

Department of Computational Materials Design (CM)

A long-term project in the CM department is the development of a Python based platform, called pyiron [1], to handle complex simulation protocols together with the huge amount of generated ab initio and atomistic data. In the following, we discuss two major applications.

*Ab initio thermodynamics:* The CM department is systematically developing and exploring *ab initio* based approaches to describe materials properties over the entire temperature range up to and even beyond melting. This requires novel strategies to compute all relevant entropic contributions, as well as their non-adiabatic coupling phenomena. The systematic achievement of highest precision and efficiency requires combining first principles calculations performed with different codes with advanced statistical sampling methods. One of the strategies – the local anharmonicity (LA) approach – explores, for example, the leading terms of fully anharmonic lattice vibrations. Another strategy (TU-TILD) uses on-the-fly optimized potentials to sample the configuration space. A third one accurately describes paramagnetic disorder using spin-space averaging (SSA).

Therefore, complex simulation protocols that combine distinctly different computer codes and that handle hundreds or thousands of separate calculations have to run on heterogeneous computer architectures. To enable the development and dissemination of these complex simulation protocols, the CM department has developed *pyiron* [1]. Like an integrated development environment (IDE) for programming languages, *pyiron* allows one to interactively implement and test simulation protocols and to upscale them for high-throughput simulations on large computer clusters. The key idea behind this new framework is to provide a single tool with a unified interface for all routines developed and established in the department or externally. This enables the user to focus fully on science rather than having to deal with technicalities and specific input/output formats of the various codes and tools.

While the development of a Python based workbench started back in 2011, the recent developments towards abstraction of the underlying concepts resulted in the release under an open source license in 2018 (www.pyiron.org). This allows the CM department to make newly developed approaches and computational tools accessible to a broad community. Successful examples for the application of *pyiron* include the simulation of the solid-liquid transitions with the two-optimized references thermodynamic integration (TOR-TILD) [2], paramagnetic defect calculations with spin-constraints, *ab initio* calculations under controlled potentiostat conditions for electrochemical systems [3], as well as machine-learning techniques for the calculation of interstitial solution enthalpies. With this versatility, the *pyiron* framework has become more and more established in the CM department. It has further been used in several collaborating institutes, e.g., for a high-throughput framework to validate empirical potentials developed at the Interdisciplinary Centre for Advanced Materials Simulation, ICAMS.


**Fig. 1:** *By using the integrated development environment pyiron, the modelling strategies become easily readable in interactive notebooks (middle). They provide a direct link to the physical concepts and raw data (left) as well as to the final results appearing in publication (right).*

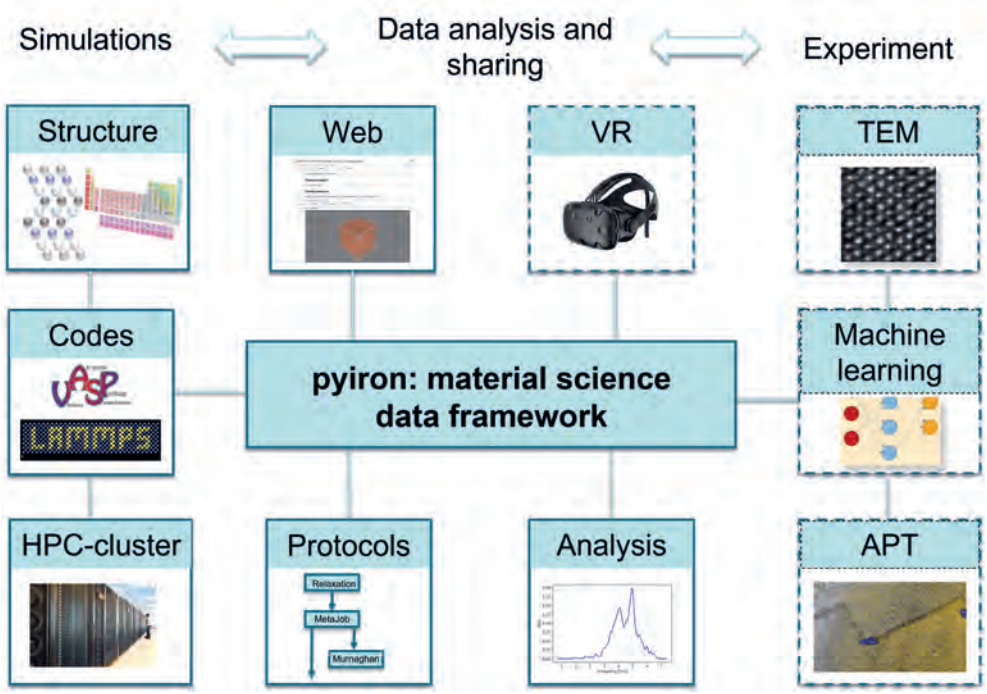


**Fig. 2:** *Overview of the pyiron framework covering all aspects of data generation, collection, storage, sharing, and analysis. While originally developed to support the simulation activities of the CM department it evolved into a versatile tool that can also handle experimental data. The dashed lines mark topics and software modules under development. (VR: Virtual Reality; HPC: High-Performance Computing; APT: Atom Probe Tomography)*

*Long-term archiving:* The last two years showed that the algorithmic concepts and solutions to realize *pyiron* allow applications that are much broader than the original goal of developing and working with complex simulation protocols (see Fig. 2). For example, the fundamental concept of *pyiron* objects allowed to link a computationally highly efficient but complex storage solution combining SQL with the HDF5 file format and a conventional file system with an easy to learn and unified user interface. The experience with such a new hierarchical storage solution based on Python, which reflects the needs of high-throughput simulations with various computer codes, turns out to be easily adaptable to store and process not only the huge datasets generated by the advanced in-house experimental tools but also the complex experimental workflows together with their respective metadata (as explored in BigMax, p.53). Examples are high-resolution TEM (transmission electron microscopy) pictures or atom-probe tomography micrographs.

A major advantage of having a unified platform is that it not only enables an easy transfer of data from simulation to experiment but allows vice versa an easy transfer of knowledge and software tools between the experimental and theoretical activities. Machine learning tools enabled converting a few thousand pictures measured by field ion microscopy (FIM) into a 3D atomistic model [4]. This model was then fed into an atomistic MD (molecular dynamic) simulation to obtain a fully relaxed structure that removes experimental noise and systematic imaging errors. The ensuing high quality data allow one to detect even fine details such as point defects (vacancies) in the sample. Linking data and tools, and providing all details in interactive and ready to use jupyter notebooks, makes *pyiron* a highly productive tool: It allows researchers to handle all the data-related requirements encountered in advanced correlative materials science research projects that require the use of a multitude of experimental and theoretical concepts and tools.

An additional benefit of *pyiron* is its ability to log all the steps of the user in constructing the protocols and achieving the results. Thus, *pyiron* not only stores all the input and output data but automatically also all the metadata related to scientific setup and workflow, such as, e.g., the program and code versions that have been used, the previous calculations/ measurements that have been employed as input or the type of analysis or data conversion that has been implemented. With the ongoing developments, we expect pyiron to become the major tool at the MPIE for an active management of big data in modelling and experiment.

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# The Düsseldorf Advanced Material Simulation Kit: DAMASK

*F. Roters [1], P. Shanthraj [1,2], M. Diehl [1], P. Eisenlohr [1,3], D. Raabe [1]*

[1] Department of Microstructure Physics and Alloy Design (MA)
[2] now at: School of Materials, University of Manchester, UK
[3] now at: Chemical Engineering & Materials Science, Michigan State University, USA

Crystal plasticity modelling has gained considerable momentum in the past 20 years [1]. Developing this field from its original mean-field homogenization approach in conjunction with viscoplastic constitutive hardening rules into an advanced multi-physics continuum field solution strategy requires a long term initiative. Roter's "Theory and Simulation" group is working in this field since 2000. Starting originally from Kalidindi's numerical crystal plasticity integration scheme [2] user subroutines for the commercial FEM packages Abaqus and MSC.Marc were developed.

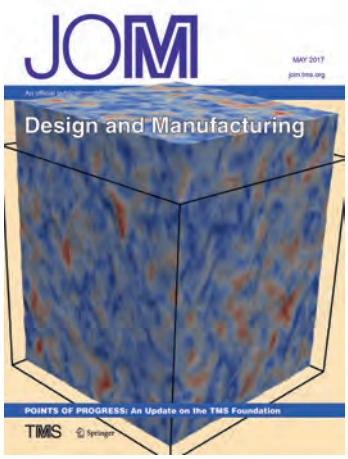


**Fig. 1:** *Cover of May 2017 JOM issue featuring DAMASK RVE.*

The scientific focus of the group is, however, the development of advanced constitutive models based on dislocation densities as internal state variables, which are capable of providing microstructure based predictions [3]. As simulations of different material classes and on different length scales necessitate the use of constitutive descriptions of varying degree of sophistication, it soon turned out that the numerical implementation was not flexible enough to incorporate different constitutive models. Therefore, within the project "Computational Modelling of Polycrystals" (CMC$^n$, the first joined project between the Max Planck and the Fraunhofer Society ever, established in 2006) the development of a flexible framework, for crystal plasticity simulations on all scales from the single crystal up to the engineering component, was initiated. The new code is strictly modularized to allow easy incorporation of additional models on all length scales. In 2010, in collaboration with Prof. R. Lebensohn (LANL, Humboldt awardee at the MPIE at that time), a spectral method based boundary value problem solver, especially suited for RVE simulations (Fig. 1), was added to complement the commercial FEM solvers. In September 2011, a website (https://damask.mpie.de) was launched to release the code to the public domain as free software according to GPL 3. The idea of a flexible open source CP implementation was very well received by the scientific community. Presently, more than 50 groups across the world use DAMASK [4], including universities such as University of California Los Angeles (UCLA), research facilities such as LANL, and multinational companies such as Tata Steel. These groups contribute to the further code development as well, e.g. by adding features such as new or modified constitutive models [5]. In 2015, multi-physics extensions were incorporated into DAMASK to consistently treat coupled problems, such as thermo-mechanics, chemo-mechanics [6], and damage-mechanics [7]. Since early 2016, the code is hosted in a public repository using GitLab (https://magit1.mpie.de) to enable and assist collaborative development among the growing user community.

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# Large-scale and Networking Projects

## The International Max Planck Research School SurMat – Interface Controlled Materials for Energy Conversion (IMPRS-SurMat)

*E. Gattermann [1], S. Wippermann [2]*

[1] Research Coordination Office
[2] Department of Interface Chemistry and Surface Engineering (GO)

The IMPRS-SurMat is an established and highly visible doctoral programme in the field of materials science in North Rhine-Westphalia, existing for 15 years and attracting highly qualified students from all over the world. It plays an essential role in gaining and promoting young scientists for all partner institutes of the school.

As a structured, three-year doctoral programme, the IMPRS-SurMat is coordinated at the Max-Planck-Institut für Eisenforschung (MPIE). Currently, it is in the middle of the third funding period from January 2016 until December 2021. Each running period lasts 6 years. The SurMat was successfully evaluated twice, in 2009 and 2014. The school is open for students with a Master's degree in Materials Science, Physics, Chemistry, or related subjects and offers funding for 3 years.

In 2004, the SurMat was founded by the MPIE, the Max-Planck-Institut für Kohlenforschung in Mülheim and the Ruhr-Universität Bochum. Two new partner institutes joined the SurMat in 2015: the Max-Planck-Institut for Chemical Energy Conversion and the University Duisburg-Essen. Therefore, today the main players of the Rhine-Ruhr region in the fields of materials science and interfaces are interlinked within the IMPRS-SurMat.

The scientific subject "Interface Controlled Materials for Energy Conversion" combines the individual strengths of these partners and focuses on five connected topics:

- Microstructure and physics of defects
- Hydrogen uptake in materials
- Oxygen reduction and evolution reactions
- Materials for future energy systems
- Degradation mechanisms and life extension of materials

The various PhD projects are interdisciplinary with at least two advisors from different academic departments. In addition, the close link between experimental and computational science leads many projects to outstanding results.

Besides the regular funding of the Max Planck Society and the involved partner institutes the SurMat gained additional funding for the third running period from the state North Rhine-Westphalia and from Tata Steel,

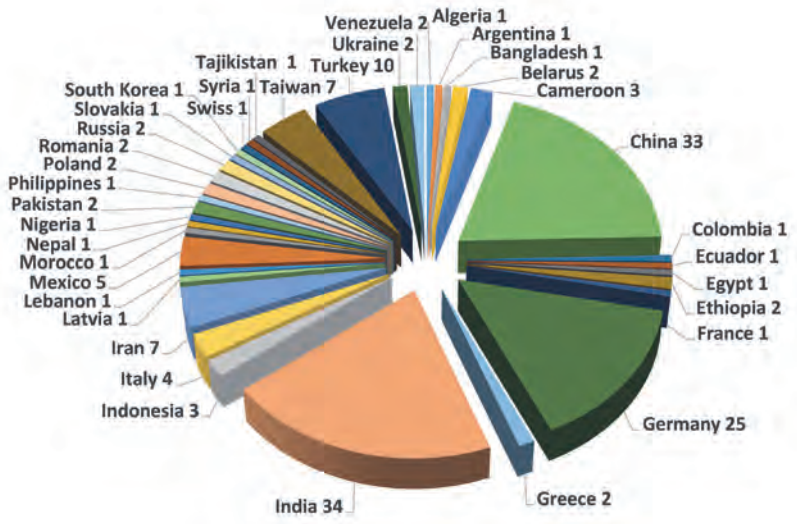


**Fig. 1:** *Origin of IMPRS-SurMat students by countries.*

**Fig. 2:** *IMPRS-SurMat community at the annual retreat in 2018.*

The Netherlands, that supports two projects of SurMat students.

During the first half of the current running period, the new partner institutes integrated very well in the school. Scientists of the University Duisburg-Essen as well as of the MPI for Chemical Energy Conversion started to contribute to SurMat lectures and several talented students started very promising research projects at both institutes. Research at the University Duisburg-Essen focuses amongst others on nanoparticles. The MPI for Chemical Energy Conversion concentrates on Carbon-based materials, e.g. designed for electrochemical applications.

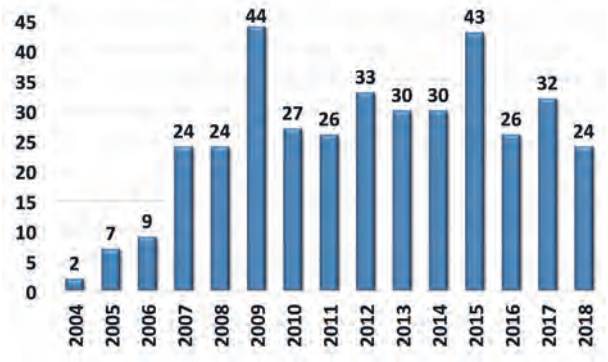


**Fig. 3:** *Number of publications by IMPRS-SurMat students in peer reviewed journals.*

The SurMat hosted already two workshops in the third running period: in fall 2016 the "Materials Day" showcased recent research highlights from the Materials Research Department of the Ruhr-Universität Bochum and the IMPRS-SurMat. The first topical joint Workshop of the IMPRS-SurMat and the IMPRS-RECHARGE "Towards an Atomistic Understanding of Reactions at Surfaces and Interfaces" was conducted at the MPIE in fall 2018. The IMPRS-RECHARGE (International Max Planck Research School on Reactive Structure Analysis for Chemical Reactions) started in 2015 at the MPI for Chemical Energy Conversion. The purpose of this joint workshop was to discuss recent developments, methods and tools to reveal reaction mechanisms and elemental steps at the atomistic scale in catalysis, electrochemistry and corrosion and to identify possible common activities.

In addition, these workshops provided an excellent opportunity for an active exchange of research results and ideas between doctoral students and advisors. Thus, they also enhance the cooperation between the SurMat partner institutes.

For the doctoral students, the school offers a well-balanced curriculum and ensures the best available supervision. The programme is conducted entirely in English and the doctoral degree (Dr. rer. nat. or Dr. Ing.) is conferred by one of the partner universities.

The core curriculum remains to be delivered over years one and two. Until 2018, there was a series of four two-week classes in each term (winter/summer). The SurMat board decided to restructure these classes into five two-day lectures starting from 2019 to focus strongly on the main topics in modern materials and interface science. Furthermore, welcome days for new SurMat students shall be established in 2019. SurMat offers soft skills trainings such as presentation skills, scientific writing and project management, as well as German language courses and career development.

Once per year, the doctoral students send a short report about the progress of their work to the programme coordinator. Subsequently, Thesis Advisory Committee (TAC) meetings take place to discuss the results and plan the next working steps.

Since 2004, 167 students from 37 different countries joined the IMPRS-SurMat. While the majority came from Asia (China, India, Iran), several students originated from Europe, Africa, Middle and South America. For admission, the students have to apply online. Either one or two application rounds are conducted per year. The application process has continuously evolved into an efficient selection procedure. All shortlisted applicants are invited for personal interviews. For the third running period already 61 new students could be won (2015-2018), which means a significant growth of the SurMat community.

Also since 2004, 89 students have successfully finished their doctorate within the IMPRS-SurMat, 19 of them with distinction. The doctoral work requires on average between 3 and 4 years with a genuinely high scientific output. 381 journal articles were published, as well as more than 260 poster and 270 oral presentations on conferences.

# BigMax: Max Planck Research Network on Big-Data-Driven Materials Science

*Z. Peng [1], M. Ashton [2], D. Raabe [1], B. Gault [1], J. Neugebauer [2], C. Freysoldt [2]*

[1] Department of Microstructure Physics and Alloy Design (MA)
[2] Department of Computational Materials Design (CM)

Materials science is data-intensive, with nowadays huge data acquisition rates in a wide array of experimental and computational techniques. Dealing with vast amounts of data is not just a technical challenge, it is an opportunity for new discoveries. A large-scale collaborative MaxNet on Big-Data-Driven Materials Science, i.e. BigMax, blending materials scientists and data scientists was hence recently established. Information extraction from atom probe tomography (APT) is a new playground for machine-learning.

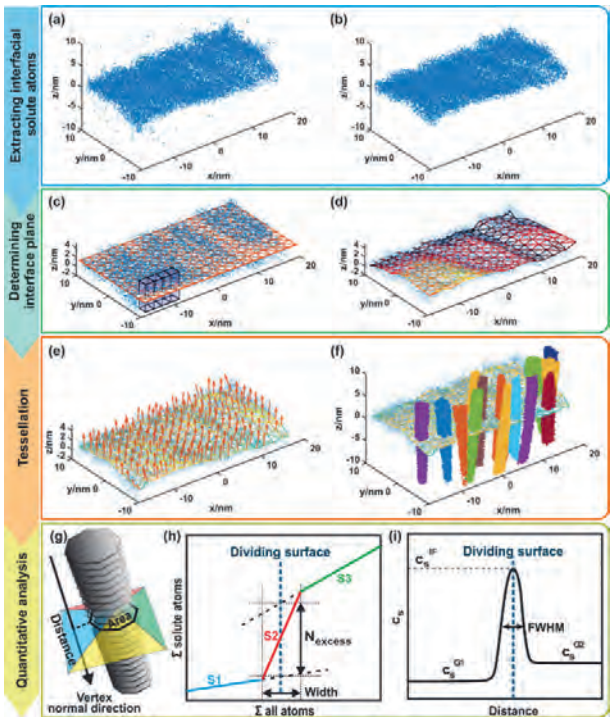


**Fig. 1:** *Interfacial solutes (a) are extracted through DBSCAN (b), PCA is applied to set up the initial interface plane, (c), based on which, the final interface is determined (d). In the third step, the normal direction of each vertex is calculated (e), and the dataset is split in sub-volumes (f) from which profiles are extracted and processed [1].*

Upon processing and reconstruction, APT data is a three-dimensional point cloud from which precise compositional information needs to be extracted. Interphase interfaces and grain boundaries are crucial microstructural features, which generally adopt complex three-dimensional shapes. Therefore obtaining a complete view of the distribution of atomic species near interfaces can be extremely challenging. Two typical machine-learning techniques, a method for finding clusters in point clouds, i.e. DBSCAN, as well as principal component analysis (PCA) were used to find the position of an interface and derive its local orientation. After PCA and DBSCAN, profiles are calculated along the local normal to the surface from which the composition, interfacial width and Gibbsian interfacial excess can be derived and plotted in the form of a two-dimensional map, as shown in Fig. 1.

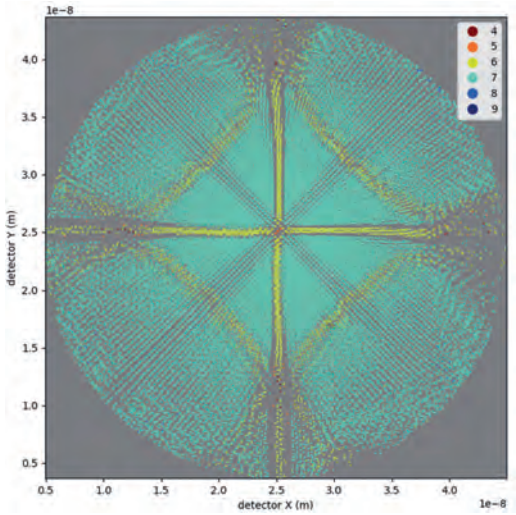


**Fig. 2:** *Detected positions of approximately 50,000 evaporation events for a [110]-oriented tungsten needle simulated in TAPSim. Each detected event is coloured according to the atom's coordination number immediately prior to its evaporation.*

On the other hand, the positions of hundreds of millions of atoms may contain hidden patterns and features relating to material properties. Within the BigMax network, we therefore collaborate with the Fritz-Haber-Institute on establishing structure-property relationships from APT data. In parallel, we pursue novel ideas for improving the reconstruction of the 3D atomic positions from the APT raw data. New algorithms are being developed and trained with APT forward simulations. For instance, Fig. 2 shows a simulated detector hit map, revealing a clear correlation between focussing effects in the pole structure and coordination within the surface. The simulations are augmented by systematic theoretical investigations of the field-evaporation mechanism at the atomic scale.

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# Networking within MAXNET Energy Consortium

*O. Kasian [1], S. Cherevko [1], E. Pizzutilo [1], A. Sarfraz [1], A. Erbe [1,2], K.J.J. Mayrhofer [1,3]*

[1] Department of Interface Chemistry and Surface Engineering (GO)
[2] Norwegian University of Science and Technology
[3] Helmholtz Institute Erlangen-Nürnberg for Renewable Energy

The intermittent nature of renewable energy from wind and solar requires the development of efficient solutions for conversion and storage on the TWh scale. The focus of the MAXNET Energy research cooperation are key reactions for the synthesis of storage molecules and added-value chemicals utilizing renewable energy. The span of the overall projects of the partners thereby ranges from atomistic insights of catalytic reactions to fundamentals of engineering solutions for technical systems [1].

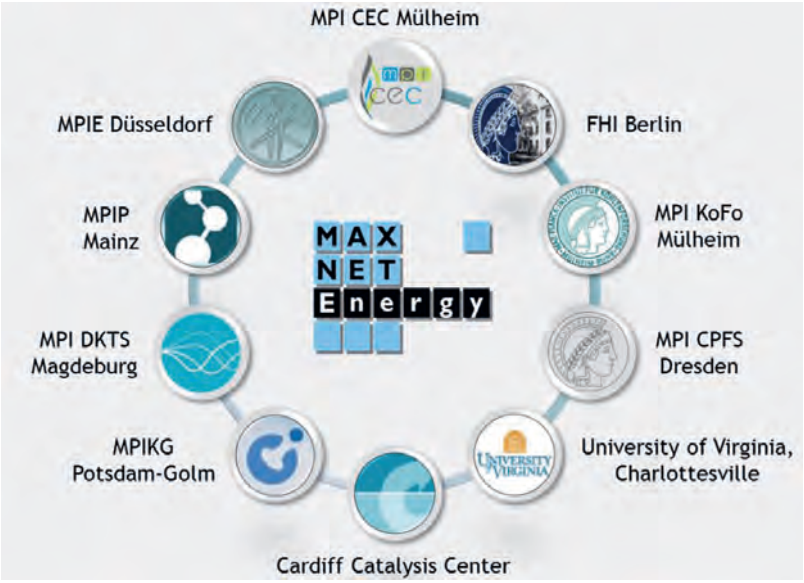


**Fig. 1:** *Partner institutes within the MAXNET Energy network.*

The activities of the GO department within the MAXNET Energy consortium are mainly related to fundamental studies of electrochemical reactions, the catalyst interface and its changes due to different operation conditions . The electrocatalysis group was additionally active in two particular projects in collaboration with the associated Cardiff Catalysis Institute (CCI) on the on-Site production of hydrogen peroxide with Au-Pd catalysts in electrocatalysis and heterogeneous catalysis and on the oxygen evolution reaction (OER) on Ir-Ru mixed oxide nanoparticles, as well as on Ir-modified $TiO_2$ nanotubes in collaboration with the associated University of Virgina. The CCI synthesized well-defined Au-Pd and Ir-Ru-based nanoparticles with different compositions, sizes and supports. The University of Virginia additionally prepared various $TiO_2$-nanotubes as model support materials, which were successfully modified with Ir using physical vapour deposition. Those catalysts were then transferred to the MPIE for their electrochemical and structural characterization. The electrocatalytic performance was fundamentally investigated using the rotating ring disc electrode (RRDE). The microstructural and compositional changes were instead characterized at different stages of the accelerated degradation protocols (SFC-ICP-MS) with identical location TEM (IL-TEM). The strong combination in synthesis of the particular interesting material classes by the partners within MAXNET Energy and the unique characterization techniques at the MPIE led to a comprehensive understanding of the relationship between the structure and activity/stability for the catalysts [2,3,4].

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# Fraunhofer – Max-Planck – Cooperation: Advanced Process and Alloy Design for Laser Additive Manufacturing of Metals (AProLAM)

*E. A. Jägle [1], A. Weisheit [2]*

[1] Department of Microstructure Physics and Alloy Design (MA)
[2] Fraunhofer Institute for Laser Technology ILT, Aachen, Germany

This collaborative research project was active from summer 2015 until the end of 2018. It aimed to combine the expertise of the two participating institutes in Additive Manufacturing (AM) process development and alloy design, respectively. The work focused on two research hypotheses:

(i) Due to the cyclic re-heating of material deposited track-by-track and layer-by-layer in AM, the so-called intrinsic heat treatment, it should be possible to design and fabricate a material that gets precipitation strengthened during the AM process.

(ii) Due to the strong melt pool convection (Marangoni effect) and high cooling and solidification rates during AM, the production of Oxide Dispersion Strengthened (ODS) steels without laborious and costly mechanical alloying and powder compaction should be possible.

precipitation, but also preceding quenching below the martensite start temperature. This allowed us to tailor the process parameters to either avoid or provoke in situ precipitation, illustrating how AM processes can be used to digitally control the material microstructure and hence the properties.

To produce ODS steels via AM, our second hypothesis, we blended micron-sized ferritic steel powders with nano-sized yttria powders. Despite process optimisation, production by LMD did not yield the desired results, with all oxides being lost in slag formation. However, after changing our focus to the Selective Laser Melting (SLM) process, which involves solidification rates that are orders of magnitude higher than in LMD, we could retain up to 35% of the introduced yttria, despite some coarsening of oxides. In a separate process route, we introduced the oxide particles

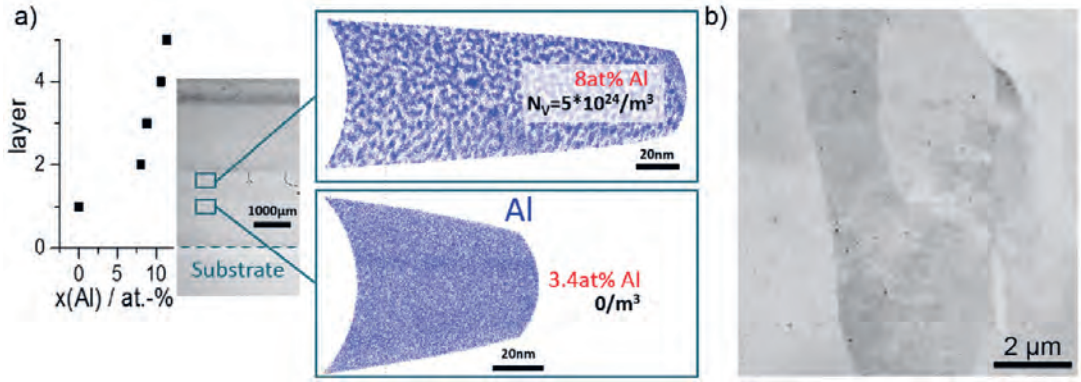


**Fig. 1:** *a) NiAl precipitates in a Fe-19Ni-xAl compositionally graded model maraging steel produced in situ during Laser Metal Deposition. b) Oxide particles in a ferritic stainless steel (Fe-20Cr-5Al-0.5Ti) produced during Selective Laser Melting in a 8% $CO_2$ process atmosphere.*

To test the first hypothesis, we produced samples from highly supersaturated maraging steel model alloys. The AM process in use was Laser Metal Deposition (LMD), in which metal powder is blown by a carrier gas into a melt pool generated by a laser beam. By using two powder feeders simultaneously, we varied the composition of the deposited material, producing compositionally graded Fe-19Ni-xAl specimens. Beyond a certain Al concentration, a very high number density of NiAl precipitates occurred in the material (up to $10^{25}m^{-3}$), as evidenced by Atom Probe Tomography and High Energy X-Ray Diffraction. Crucially, this did not require ageing post-heat treatment, but was a direct result of the intrinsic heat treatment, thus proving our hypothesis. Our model alloys showed promising mechanical properties with tensile strengths up to 1.6 GPa. Extending our research to the Fe-Ni-Ti system, we showed that not only re-heating is required to trigger not by a separate powder, but by an *in situ* reaction of the steel matrix with an oxidising gas atmosphere. We successfully produced ODS steel samples both in LMD with a process atmosphere of Ar+3%$O_2$, as well as in SLM with Ar atmospheres containing from 2% to 100% $CO_2$.

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# Initial Wear: Engineering down to the Atomic Scale

*Z. Peng [1], B. Gault [1], T. Meiners [2], P.-P. Choi [3], C. Liebscher [2], M. Rohwerder [4], D. Raabe [1], M. Friedrichs [5], O. Dambon [5], F. Klocke [5]*

[1] Department of Microstructure Physics and Alloy Design (MA)
[2] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[3] now at: Department of Materials Science & Engineering, Korean Advanced Institute of Science and Technology
[4] Department of Interface Chemistry and Surface Engineering (GO)
[5] Fraunhofer Institute for Production Technology, IPT

Driven by the wide range of applications in laser technology, biomedicine and consumer electronics, etc., the demand for high-quality lenses with complex geometries and small dimensions is rapidly growing. Since direct grinding and polishing of such lenses is not economically competitive, precision glass moulding (PGM) has become a popular manufacturing route. PGM is a replicative technology for efficiently producing high-precision optical lenses in medium or high volumes. PGM is carried out at temperatures ranging from 350 to 800 °C and at a high press force (2–20 kN). The degradation of the moulds is very fast. Production costs are directly related to the moulds' lifetime.

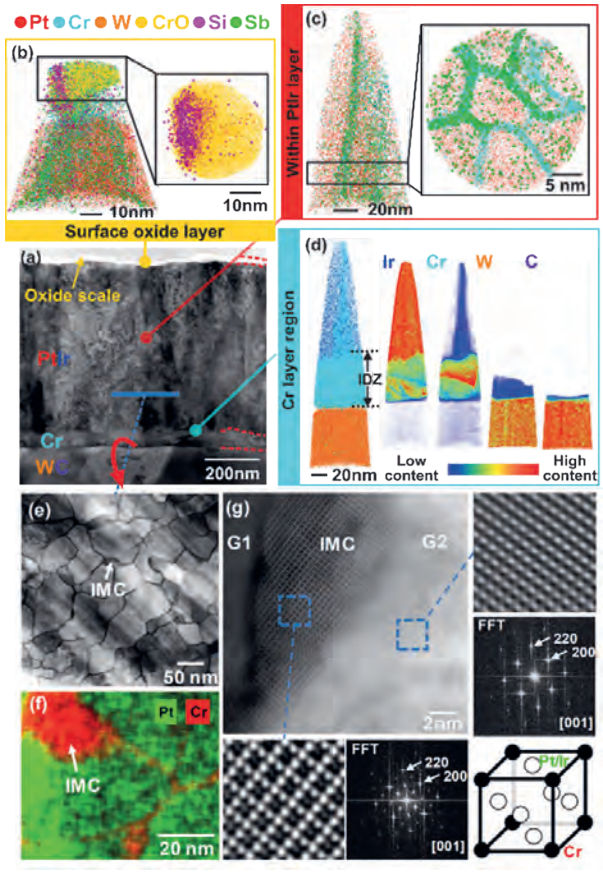


**Fig. 1**: *Representative characterization results of a mould sample after 120 PGM production cycles: (a) cross-sectional STEM image, (b-d) APT results from different regions of the sample, (e) plane view STEM image of the PtIr layer, (f) STEM-EDX map, (g) HR-STEM image resolving the atomic structure of the intermetallic phase (IMC) and a PtIr grain. As the detailed STEM analysis reveals (e-g)), the diffusion and segregation of Cr along the PtIr grain boundaries also lead to heterogeneous precipitation of the $(PtIr)_3Cr$ intermetallic phase.*

Initial Wear's aim was to gain a fundamental understanding of the degradation mechanisms of the mould materials, so as to inform new design strategies for high-performance and high-durability moulds, which is crucial to the PGM industry. To gain insights into the degradation mechanisms, we applied atom probe tomography (APT) and scanning transmission electron microscopy (STEM). APT has the capability to reveal three-dimensional (3D) chemical information with sub-nanometre precision and a sensitivity in the range of tens of part-per-million. STEM allows for precise structural characterisation.

The samples are made of cemented tungsten carbide covered by 20-nm-thick Cr interlayer to enhance adhesion of the main protective coating made of a 600-nm-thick PtIr layer. In controlled laboratory experiments, we found that the degradation is initiated by Cr segregation at the grain boundaries (GBs) in the PtIr and subsequent diffusion to the surface and formation of an oxide layer [1]. Similar degradation processes were also observed in the technical simulation (see fig.1). We found this can be prevented by decreasing the oxygen partial pressure in the environment. Research is ongoing to investigate the underpinnings of these new observations.

In summary, the key steps of the degradation mechanisms are:

1. outward diffusion of Cr atoms along the grain boundaries of the PtIr layer;
2. oxidation of Cr on the surface;
3. bulk interdiffusion between PtIr, Cr, and the WC substrate;
4. penetration of glass fragments into the mould.

To impede the degradation process, we have also tested Ni as an interlayer material, but it behaved even worse. (see [1] for more details). So decreasing the oxygen partial pressure of the processing chamber should be achieved.

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# CarMON - Carbon Metal Oxide Nanohybrids: A Leibniz – Max-Planck Cooperation

*S. Hieke [1], A. Frank [1], V. Presser [2], S. Fleischmann [2], A. Kruth [3], M. Dias [3], S. Peglow [3], C. Scheu [1]*

[1] Independent Max Planck Research Group on Nanoanalytics and Interfaces (NG)
[2] INM – Leibniz Institute for New Materials, Saarbrücken, and Department of Materials Science, Saarland University
[3] INP – Leibniz Institute for Plasma Science and Technology, Greifswald

The CarMON project – short for Carbon-metal oxide nanohybrids – is a collaborative project funded by the Leibniz Association. The project aims to synthesize novel materials and material combinations on the nanoscale for electrochemical applications. CarMON is connecting the Leibniz Institute for Plasma Science and Technology (INP) in Greifswald, the INM - Leibniz Institute for New Materials in Saarbrücken and the independent Max Planck research group on Nanoanalytics and Interfaces (NG) at the MPIE in Düsseldorf. This way, the expertise of the INP regarding plasma-related synthesis and analysis, the competence of the INM in developing new nanomaterials and the abilities at the MPIE concerning advanced (scanning) transmission electron microscopic ((S)TEM) analysis are linked closely, thus enabling new synthesis concepts for novel nanomaterials.

As humanity is facing global warming and fossil fuels are getting scarce, the need for alternative energy concepts – generation and storage – is ever-present. The collaborators aim to hybridize carbonaceous materials and metal oxides, as a synergistic combination of these materials on the nanoscale leads to enhanced properties for various electrochemical applications. In the current project, the search for nanohybrids for electrode appliance in Li-ion batteries and for desalination of water is in the foreground. However, for blending these materials, traditional chemical methods reach their limits regarding defects and imperfections in the crystals which can decrease their performance. Therefore, new synthesis routes are needed and can be found among plasma-assisted processes offering scalable processes at relatively low temperatures and minimal waste.

It is important to control the synthesis and closely link the procedure to properties and crystallinity of the material. Systematic studies varying the deposition parameters for vanadium oxides on silicon have been performed at the INP. The resulting films have been characterized at the MPIE to achieve a deep understanding of the growth behaviour. High-resolution TEM measurements on a $C_s$ image-corrected Titan Themis allow to judge the crystallinity of the as-prepared films. These findings can be complemented by (nanobeam) electron diffraction studies.

Furthermore, electron energy loss spectroscopy investigations performed in scanning TEM enable the allocation of light elements for $MoO_x/MoS_2$ core-shell particles on carbon nanotubes prepared at the INM (Fig. 1). The use of the $C_s$ probe-corrected Titan Themis at the MPIE provides site-specific analytics on the nanoscale, proving the core-shell nature of the samples, as electron energy loss spectroscopy allows to also distinguish light elements like oxygen and sulfur.

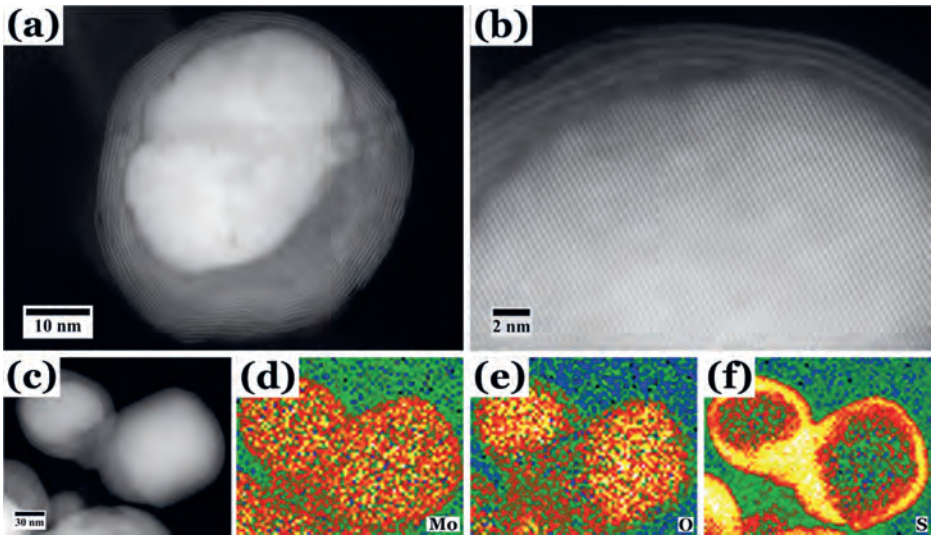


**Fig. 1:** *(a) HAADF STEM image of one $MoO_x$ / $MoS_2$ core-shell particle and (b) detail revealing the shell structure, (c) HAADF STEM image of $MoO_x$ / $MoS_2$ core-shell particles, and (d), (e), (f) corresponding electron energy loss elemental maps of molybdenum, oxygen, and sulfur, respectively.*

# International Scientific Coordination Network Mechanics of Nano-Objects - GDRi MECANO

*G. Dehm [1], D. Raabe [2], C. Kirchlechner [1]*

[1] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[2] Department of Microstructure Physics and Alloy Design (MA)

The International Scientific Coordination Network (GDRi) Mechanics of Nano-Objects (MECANO) is a multinational network initiated by Centre National de la Recherche Scientifique (CNRS) in France. This essentially European network includes 31 French partners (including 4 industrial ones) and 11 laboratories from Germany, Austria, Italy, Switzerland, UK and Ireland. The common ground on which all the partners are working on are condensed matter objects that possess at least one internal or external dimension smaller than a micron. Size effects can appear on various properties due to this structural confinement. However, mechanical size effects are at the core of the MECANO network. GDRi MECANO, which was established in 2012 by Prof. Olivier Thomas (U Marseilles) and is now in its second phase (2016-2019) led by Dr. Marc Legros (CNRS-CEMES Toulouse) brings together physicist, chemists, materials scientists and mechanical engineers. G. Dehm is a member of the Scientific Committee, which meets annually to decide on topics of forthcoming activities. The formation of early career scientists is certainly one of the most important goals that this network aims at.

The scientific questions addressed within MECANO stretch from the synthesis of nanomaterials, manipulation of their properties, to advanced experimental testing and characterization methods for quantitative determination of stress & strain, and defects down to the atomic level, questioning – as always in nanoscience – how well current theories used at the macro- and mesoscale (continuums mechanics, plasticity, elasticity theory, …) can be applied to smaller and smaller length scales.

The GDRi MECANO network promotes scientific discussions and fosters collaborations by organizing (i) general meetings open to all topics, (ii) dedicated workshops on specific topics, and (iii) schools for graduate students to review basics and put recent research developments into perspectives. C. Kirchlechner from the MPIE organized a summer school on “Experimental Nano- and Micromechanics” in 2017 with B. Merle (U Erlangen). The school included hands-on exercises in the laboratories at the MPIE comprising nanoindentation, electron backscatter diffraction, electron channelling contrast imaging, microfracture mechanics, and thin film mechanics. A general GDRi MECANO school was held at 28 Oct. - 2. Nov. 2018 in France with G. Dehm teaching a course on stresses and plasticity in thin films. The GDRi MECANO network is very fruitful in fostering collaborations and exchanges between its partners and the young researchers.

**Fig. 1:** *Participants of the summer school “Experimental Nano- and Micromechanics” held at the MPIE in Düsseldorf from 11-15 September 2017.*

# Development of Cost-Efficient, High-Performance Gas Diffusion Electrodes for Polymer Electrolyte Membrane Fuel Cells with Low Platinum Loading and Newly Developed Hollow Graphitic Spheres as Support Material

*M. Ledendecker [1], D. Göhl [1], K.J.J. Mayrhofer [1,2,3]*

[1] Department of Interface Chemistry and Surface Engineering (GO)
[2] Helmholtz Institute Erlangen-Nürnberg for Renewable Energy
[3] Friedrich-Alexander-Universität Erlangen-Nürnberg

The main goal in catalysis is the development of active, stable and selective catalysts while keeping the material and production costs low. In recent years, the understanding of fundamental catalytic processes has led to considerable improvement in catalyst design with more active and stable catalysts and supports. The joint project comprises different partners in order to develop catalyst/support design strategies from a fundamental, experimental and application point of view and is aimed to establish active and most importantly highly stable fuel cell catalysts and electrodes. The catalyst synthesis and optimization is performed in close collaboration with Prof. Ferdi Schüth at the Max-Planck-Institut für Kohlenforschung (MPI-KOFO). Through the concept of pore-confinement, more stable catalysts towards the oxygen reduction reaction are developed. Together with the Max-Planck-Institut für Chemische Energiekonversion (MPI-CEC) and Ernst Ruska-Centre (ERC)-Jülich, the MPIE as the project leader focuses on mechanistic studies for dissolution and structural degradation of supported nanoparticles. We establish potential boundary conditions for the desired application, point out degradation pathways and develop strategies to overcome stability challenges [1-4]. Fully automated rotating disk electrode (RDE) measurements and the scanning flow cell (SFC) coupled to an inductivly coupled plasma - mass spectrometer (ICP-MS) are the working horses for the in depth characterization (Fig. 1), which are further complemented by HR-STEM, XRD, XPS and atomistic modelling. Promising catalysts are investigated further at the Zentrum für BrennstoffzellenTechnik GmbH in Duisburg and with material technology partners from industry. Moreover, scale-up strategies for synthesis are developed for high performance catalysts in order to pave the path for large-scale applications.

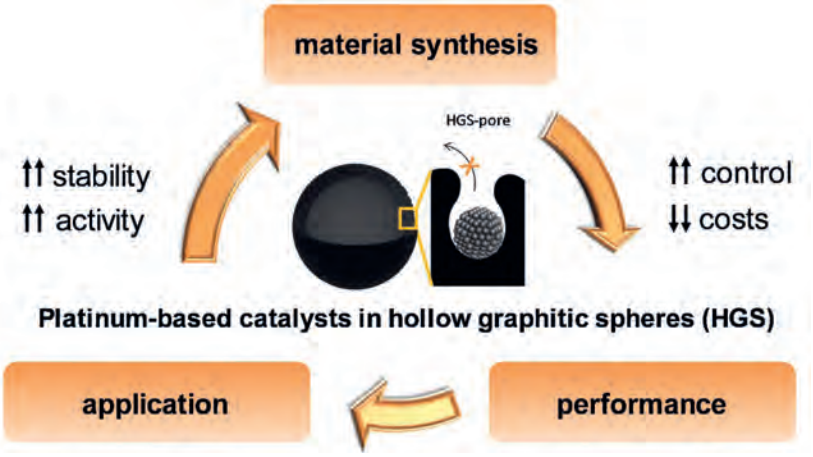


**Fig. 1:** *Overview of the "PtTM@HGS" project. The focus at the MPIE lies in benchmarking catalysts regarding activity, stability and on the elaboration of fundamental processes taking place during catalysis.*

The research project is funded by the Federal Ministry for Economic Affairs and Energy (BMWi) of Germany in the framework of PtTM@HGS (project number 03ET6080A).

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# Compositionally Complex Alloys – High Entropy Alloys (CCA-HEA)

*F. Körmann [1], Y. Ikeda [1], J. Neugebauer [1], Z. Li [2], D. Raabe [2], E. A. Jägle [2], G. Dehm [3], C. Liebscher [3]*

[1] Department of Computational Materials Design (CM)
[2] Department of Microstructure Physics and Alloy Design (MA)
[3] Department of Structure and Nano-/ Micromechanics of Materials (SN)

The recently introduced novel class of materials, referred to as "high entropy alloys" (HEA) for single phase materials or "compositionally complex alloys" (CCA) in case of 2 or more phases contain multiple principal elements and fundamentally differ from conventional alloys with one or two prevalent base elements. This new CCA-HEA concept has opened up a huge compositional space of multicomponent alloys with significant technological potential but also posing new and exciting scientific challenges. The German Research Foundation (DFG) has established in 2017 the Priority Programme "Compositionally Complex Alloys – High Entropy Alloys" to develop CCAs and HEAs with outstanding mechanical properties or materials behaviour.

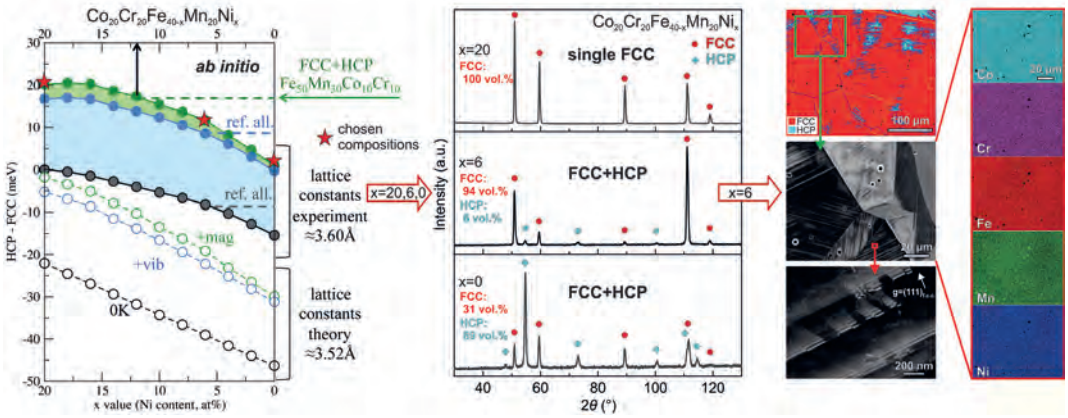


**Fig. 1**: *From left to right: ab initio study of FCC-HCP stability of $Co_{20}Cr_{20}Fe_{40-x}Mn_{20}Ni_x$ alloys, XRD patterns for three HEAs/CCAs with x=20, 6 and 0 at.%, microstructure and elemental distribution of $Co_{20}Cr_{20}Fe_{34}Mn_{20}Ni_6$ [1].*

body-centred cubic CCAs with tailored precipitates based on B2- and/or $L2_1$-phases. In a first step, the phase formation in the rather unexplored composition space of FeAlCr (Mn, Co, Ni, Ti) is explored by high throughput screening and characterization based on thin film deposition techniques. Promising alloy candidates are identified fulfilling the conditions to have a BCC crystal structure and showing either B2, $L2_1$ or both types of precipitate phases followed by a microstructural optimization in terms of precipitate morphology, coherency with the supersaturated BCC matrix and their volume fraction.

(3) "Particle-strengthened Compositionally Complex Alloys - interlinking powder synthesis, additive manufacturing, microstructure evolution and deformation mechanisms" (E. Jägle, G. Dehm, V. Uhlenwinkel/Bremen). Even though it is known that many CCAs contain nano-scaled particles, it is not yet understood if their interaction with gliding dislocations gives rise to strengthening effects following the same laws as for conventional alloys. In this project, the material synthesis follows a powder metallurgical route via gas atomization and additive manufacturing of specimens, allowing rapid compositional screening and minimum inhomogeneity. The research questions will be tackled by investigating nitride and B2-strenghtened FeNiCoCr(Al,Mn)-alloys by a combination of high-resolution analysis employing transmission electron microscopy and atom probe microscopy, mechanical testing and quantitative *in situ* micro-mechanical experiments.

The MPIE is strongly represented in this SPP with three granted projects:

(1) "Interstitial transformation-induced plasticity-assisted quinary compositionally complex alloys: Design, structure and mechanical behaviour (TRIP-iCCAs)" (F. Körmann, Z. Li, D. Raabe). This project proposes a new class of CCAs, namely, interstitially alloyed TRIP-assisted quinary CCAs. Due to the TRIP effect the alloys will have dual-phase structure [1] after strain loading. Interstitial-free quinary CCAs with TRIP effect [2] will first be developed followed by alloying with carbon and nitrogen. This enables the further tuning of the alloy's strain-hardening ability and the introduction of interstitial solid solution strengthening effect. The project employs state-of-the-art theoretical *ab initio* simulation and experimental techniques.

(2) "Tailored precipitation strengthened, compositionally complex FeAlCr (Mn, Co, Ni, Ti) alloys for high temperature applications" (C. Liebscher, K. Pradeep / IIT Madras). This project aims to develop

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# Advanced Combinatorial Alloy Design: High Throughput for Evolutionary Structural Materials

*H. Springer, D. Raabe*

Department of Microstructure Physics and Alloy Design (MA)

The collaborative research centre (SFB) 1232 “Farbige Zustände (coloured states)” targets the establishment of a high-throughput methodology for the accelerated development of innovative structural materials with novel property profiles, as well as their prediction using a heuristic model (Fig. 1). This knowledge based design is relying on systematic investigations neccessary to describe the underlying relationships in the form of so called descriptors. For that purpose, small, fast and effective methods for synthesis and thermo-mechanical processing are being developed and deployed. Based on simplified tests of the mechanical and chemical behaviour, evolution-based search methods are utilised to derive so called predictor functions to forecast the more complex material properties relevant for engineering, such as the stress/strain behaviour during tensile testing.

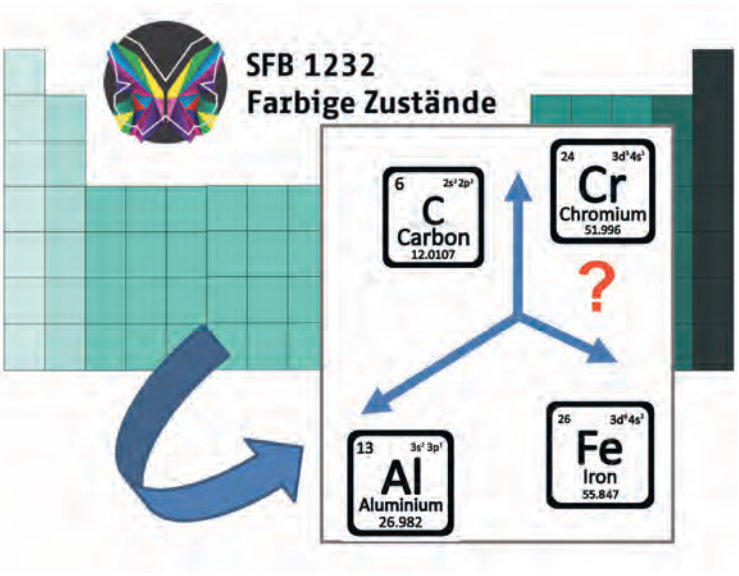


**Fig. 1:** *CRC1232: Identifying and developing innovative structural materials by exploring new ranges of chemical compostions and thermo-mechanical processing parameters.*

A critical point in this high throughput methodology based on small material volumes lies in the necessary transferability of the derived results to industrial volumes of production. This is the one of two objectives for the sub-project “Validation” from the MPIE within the framework of the CRC. The influence of rapid solidification – which the small material volumes in the order of milligrams are subjected to – on microstructures and mechanical properties is investigated with sprayforming techniques, together with partners at the Leibniz-Institut für Werkstofftechnik in Bremen. Furthermore, bulk high throughput methods developed and established at the MPIE, termed rapid alloy prototyping (RAP), are utilised [1]. The highly parallised and standardised sequence of RAP regarding synthesis, processing and characterisation is used to systematically screen the wide range of materials states achievable through chemical and thermo-mechanical variations. Together with literature data, these investigations provide a solid basis for the methodology development. The chosen alloy system Fe–xC–yCr (x = 0 – 1, y = 0 – 20) is especially suited for this purpose due to the numerous complex microstructural phenomena taking place on various scales: Depending on the respective thermo-mechanical variation, mechanisms such as martensitic transformation, austenite reversion, carbon partitioning or carbide precipitiation to name but a few, can be exploited for a vast range of mechanical and chemical properties [2,3]. Additionally to valididating the high throughput methodology, the vast range of investigated materials also offers the unique opportunity to identify yet unknown property combinations. Elucidating their microstructural origins with high resolution characterisation techniques represents the second objective of our sub-project. The MPIE is further involved in the CRC by heading the work group “Suchraumdefinition”, which is concerned with providing metallurgical knowledge to projects more concerned with process engineering, and helps defining the strategic direction in which the material development is headed.

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# Collaborative Research Centre TRR 188: Damage is not Failure

*C. Tian [1], L. Christiansen [1], D. Ponge [2], C. Kirchlechner [1]*

[1] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[2] Department of Microstructure Physics and Alloy Design (MA)

The formation of voids and micro-cracks during plastic deformation of ductile materials occurs not only during service, but also already during the manufacture of engineering components. Typically, the damage imposed during manufacture is quantitatively unknown, which results in uncertainties in prediction of lifetime and defining safety factors. Thus, within the Collaborative Research Centre TRR 188 we want to understand, predict and control the damage evolution during forming of engineering components. The ultimate goal of the research centre is to cut the costs during development of forming parts, to increase the safety and reliability and, concomitantly, reduce the weight of components significantly. The interdisciplinary research strategy comprises mechanical engineers, experts in forming technology, in solid state mechanics and in microstructural physics located at the RWTH Aachen University, at the TU Dortmund and the MPIE. The approach bridges from the micrometre regime (microstructural length scale) up to metres (sample length scale).

At the MPIE we are measuring the local mechanical properties of a dual phase steel (DP800). Besides the size dependent single-phase properties of ferrite, martensite and non-metallic inclusions, we are also developing mechanism-based material laws for interface fracture of the ferrite-martensite interface. The first surprising result shows that the critical resolved shear stress (CRSS) of ferrite is similar for slip on the (110), (112) and (123) slip plane (Fig. 1). These results will be implemented in the crystal plasticity finite element simulations of the cooperating research groups within the TRR188.

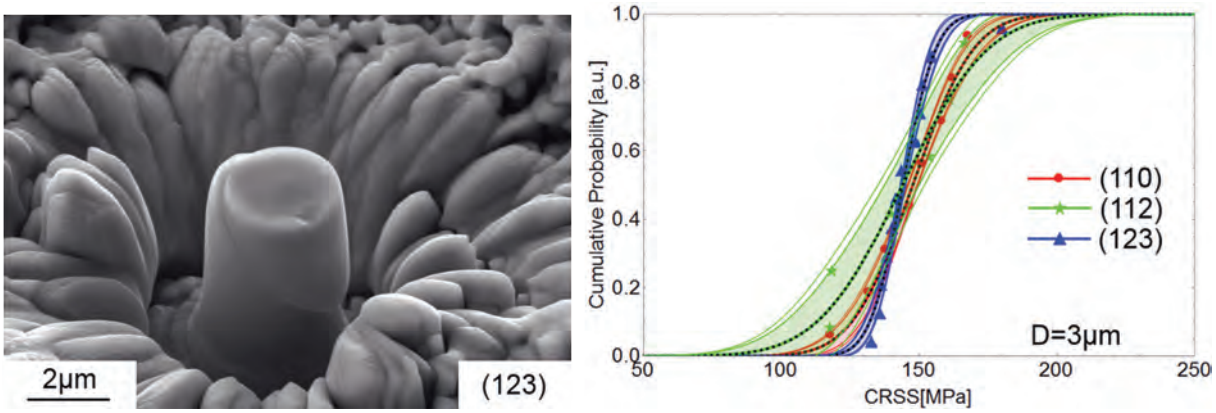


**Fig. 1:** *Ferrite micropillar exhibiting slip on the (123) slip plane. The cumulative probability of the critical resolved shear stress (CRSS) is shown for all three families of slip plane.*

# Gas Turbines of Tomorrow: From Atom to Turbine Blade

*S.K. Makineni [1], J. He [1], P. Kontis [1], X. Wu [2, 3], M. Lenz [4], E. Spiecker [4], S. Neumeier [4], G. Dehm [5], D. Raabe [1], R. Reed [6, 7], J. Cormier [8], G. Eggeler [2, 3], B. Gault [1]*

[1] Department of Microstructure Physics and Alloy Design (MA)
[2] Material Science and Engineering, Ruhr-Universität Bochum
[3] Max Planck Group on High Temperature Materials
[4] Institute of General Materials Properties, Friedrich-Alexander Universität Erlangen-Nürnberg
[5] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[6] Depts. of Engineering Science and Materials, University of Oxford
[7] Alexander von Humboldt Awardee at the MPIE
[8] Institut PPRIMME, CNRS, ENSMA & Université de Poitiers, France

The atom probe tomography (APT) group in the MA department is very active in high-temperature materials, with a strong emphasis on Ni- and Co-based superalloys. Within the second phase of the DFG-funded SFB/TR 103 "From atoms to turbine blades – a scientific basis for a new generation of single crystal superalloys" joint research centre with Ruhr-Universität Bochum and Friedrich-Alexander-Universität Erlangen-Nürnberg, we established a method to facilitate correlative electron microscopy and atom probe tomography [1]. Here, specimen preparation is guided by controlled-electron channelling contrast imaging [2], as seen in Fig. 1. Deployed to investigate the mechanisms of creep deformation in new CoNi-based superalloys, this approach provided insights into the diffusional processes that limit the rate of deformation [3,4]. In Ni-based alloy ERBO-1, we demonstrated that Re was carried by moving dislocations during creep and loses its strengthening effect, thereby likely providing answers to a long-standing debate regarding the role of Re in enhancing the alloy's creep performance.

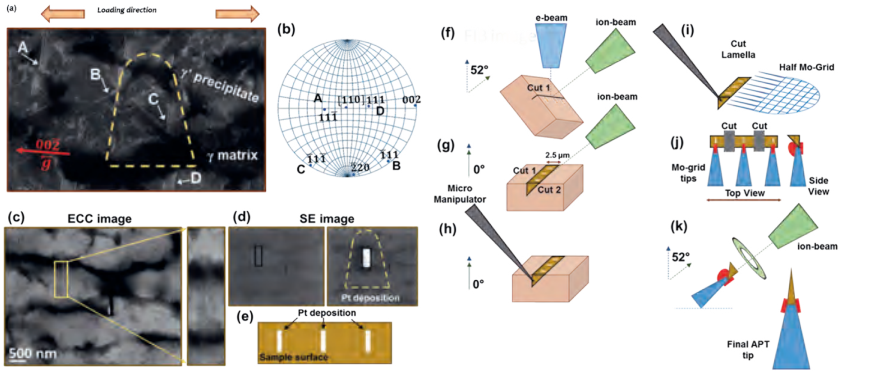


**Fig. 1:** *Complete methodology for targeted specimen preparation from specific crystalline defects using controlled-electron-channelling contrast imaging, transmission electron microscopy and atom probe tomography.*

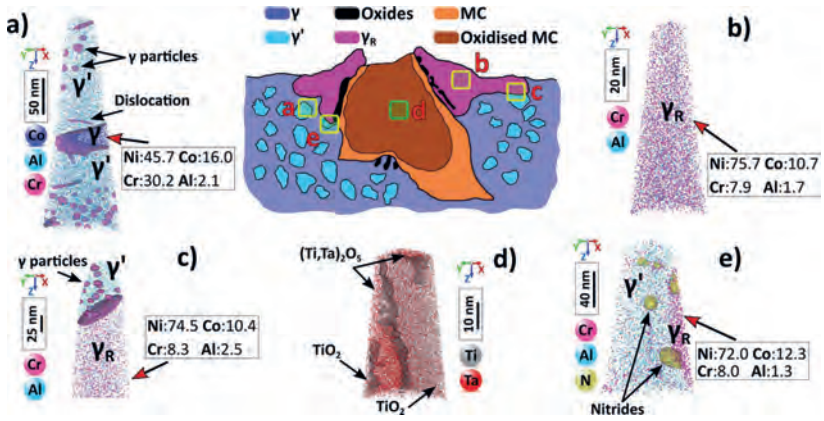


**Fig. 2:** *Summary of APT microstructural characterisation from the surroundings of an oxidised carbide in a multicrystalline Ni-based superalloy [6].*

In parallel, we established new international collaborations with the University of Oxford (UK) [5,6] and the Institut P' a CNRS-laboratory in Poitiers [5] on commercial single crystal and multi-crystalline Ni-based superalloys. We provided evidence of mass transport of specific solutes by or through defects generated during creep or because of the oxidation of intergranular carbides [7]. The possibility that mechanisms such as pipe diffusion could affect high temperature mechanical deformation had been proposed over a decade ago, but we provided the first experimental proof that this was the case, and provided an explanation for how this could affect the local equilibrium and hence the strengthening of the alloy.

Overall, our investigations have thrown light onto the interplay between structural defects and local composition, and hence stability of the alloys in service. Understanding these fundamental aspects is critical to explore new possible alloy design routes to enhance the lifetime of parts, increase operating temperatures and so as to reduce fuel consumption, with clear environmental gains.

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# Metallic Nanowires on the Atomic Scale: Electronic and Vibrational Coupling in Real World Systems

*S. Wippermann*

Department of Interface Chemistry and Surface Engineering (GO)

In 2015, S. Wippermann, head of the Atomistic Modeling Group, joined the FOR 1700 research unit funded by the German Research Foundation (DFG) [1] as a principal investigator. Ideal one-dimensional (1D) electronic systems show fascinating physical properties, such as quantization of conductance, charge density waves (CDW), non-Fermi liquid behaviour and often a variety of instabilities with associated phase transitions. The central topic of the FOR 1700 research group is the exploration and identification of physical systems with 1D electronic properties under explicit consideration of 2D and 3D coupling, their control and manipulation.

These findings are of particular interest because the (8x2) CDW state features associated non-trivial topological electronic properties. The topological properties of this system give rise to fundamental excitations of the CDW, which take the form of topological solitons. Three different types of solitons are observed, carrying a charge of exactly either +1, 0 or -1 electrons, respectively. Soliton-soliton interactions were shown to be topologically protected and to obey an Abelian group. In principle, these fundamental excitations of the CDW can be used as information carriers in new types of information processing. Exactly those electronic states whose excitation

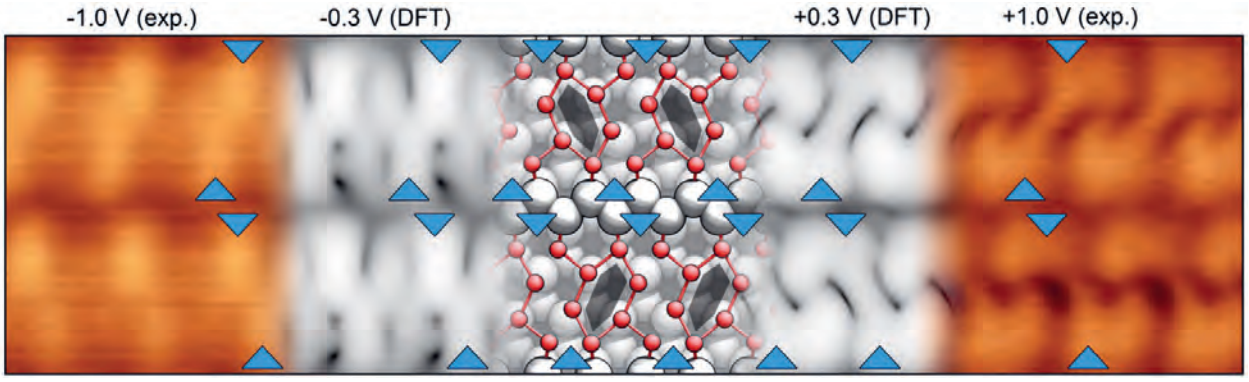


**Fig. 1:** *Structural model of the (8x2) CDW ground state, overlayed with scanning tunnelling microscopy (STM) measurements and density functional theory (DFT) simulations (STM measurements: T. H. Kim, H. W. Yeom, Pohang University of Science and Technology). Red balls and grey spheres represent indium and silicon atoms, respectively.*

The ordered array of indium atomic wires formed at the Si(111)-(4x1)In surface is a particularly interesting model system of this kind. It features a reversible temperature-induced metal-insulator transition at $T < T_C = 120$ K into a CDW ground state with (8x2) translational symmetry. Due to strongly coupled electronic and lattice degrees of freedom, femtosecond laser excitation can induce a non-thermal transition from the semiconducting (8x2) CDW ground state into a metallic supercooled (4x1) state. This transition is completed within 350 fs. We demonstrated that carefully tuned electronic excitations can create non-equilibrium potential energy surfaces that drive structural dynamics at the quantum limit, that is, in a regime where the nuclear motion is directed and deterministic [2].

can drive the transition from the (8x2) into the (4x1) state [2] also couple strongly and selectively to the topological solitons. Currently, we are exploring in detail electron-phonon, electron-soliton and soliton-soliton interactions.

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# Steel-*ab initio* - Quantum Mechanics Guided Design of New Fe-based Materials: A Joint Initiative between the MPIE and RWTH Aachen University

*T. Hickel [1], D. Ponge [2], M. Herbig [2], B. Gault [2], S. Zaefferer [2], F. Roters [2], C. Scheu [3], J. Neugebauer [1], D. Raabe [2]*

[1] Department of Computational Materials Design (CM)
[2] Department of Microstructure Physics and Alloy Design (MA)
[3] Independent Max Planck Research Group on Nanoanalytics and Interfaces (NG)

In 2007 the Max Planck Institute (MPIE) and RWTH Aachen University jointly initiated a collaborative research centre (Sonderforschungsbereich, SFB 761) on quantum-mechanics guided design of new Fe-based materials. The initiative is funded by the German Research Foundation (DFG). Speaker and chairman of the project is Prof. Wolfgang Bleck (Institute of Ferrous Metallurgy, RWTH) and vice-chairman is Prof. Dierk Raabe (MPIE). Due to several successful evaluations, the project is now running in the third four-year funding period, which started in July 2015. In this period, the MPIE is heading seven partial projects, involving scientists from three departments.

The key idea of the SFB 761 is to develop a new set of methods for materials and process design based on *ab initio* calculations in conjunction with advanced characterization and metallurgical alloy development tools. The first phase of the project focussed on the ternary Fe-Mn-C system, forming the basis of high manganese steels. During the second phase the alloying spectrum was extended to Fe-Mn-Al-C. A key quantity in the investigations was the stacking fault energy, which serves as a central link between atomic structure simulations and engineering applications. Now, in the third phase, the material spectrum is again extended towards steels with either medium Mn or higher Al content. This opens another spectrum of physical questions, where in particular phase boundaries (α/γ and γ/κ) become important. Other focus topics of the third period are strain hardening engineering and hydrogen management in these steels.

The MPIE contributes with theory and experiments to the success of this project. *Ab initio* methods are not only used for the prediction of key thermodynamic parameters, but turned out to become increasingly important for understanding the different strengthening mechanisms (TWIP, TRIP, shear band formation). In combination with constitutive models, the extraordinary deformation behaviour with high strain hardening values can even be quantitatively predicted. On the experimental side, in particular correlative studies that combine high-resolution electron microscopy and atom probe tomography provided a combined knowledge of the local structure and chemistry on the atomic scale. This technique was, for example used, to resolve the formation of kappa-carbides, since their superstructure arrangement yields an additional strengthening mechanism in these materials.

The new methods and insights developed within the SFB 761 have an impact beyond the project consortium. A couple of transfer projects are established to allow industrial partners to benefit from these results. One of them, which is run by the MPIE, evaluates the sensitivity of high-Mn steels that contain Cr carbides to hydrogen embrittlement. Additionally, the SFB 761 has initiated a series of international conferences on medium- and high-Mn steels. The 4th edition of this conference will take place in April 2019 in Aachen and is co-organized by the MPIE.

More details on SFB761 are available on http://www.stahl-abinitio.de.

**Fig. 1:** *The SFB 761 team during a meeting in June 2018.*

# Activities within the Cluster of Excellence "Ruhr Explores Solvation" (RESOLV)

*M. Todorova [1], M. Rohwerder [2], A. Erbe [2], J. Neugebauer [1]*

[1] Department of Computational Materials Design (CM)
[2] Department of Interface Chemistry and Surface Engineering (GO)

The Cluster of Excellence RESOLV (Ruhr Explores Solvation Science) was established in November 2012 at the Ruhr-Universität Bochum (RUB). Prof. Dr. Martina Havenith-Newen (Physical Chemistry 2, RUB) is speaker of the cluster in which several departments from RUB, groups from TU Dortmund, University Duisburg-Essen, Fraunhofer UMSICHT Oberhausen, Max-Planck-Institut für Kohlenforschung (Mülheim a. d. Ruhr), Max-Planck-Institute for Chemical Energy Conversion (Mülheim a. d. Ruhr) and the MPIE participate.

With their expertise in interface science, two departments of the MPIE, "Interface Chemistry and Surface Engineering" (GO) and "Computational Materials Design" (CM), are strongly involved in research area C of RESOLV "Ion Solvation and Charge Transfer at Interfaces". Most projects with MPIE involvement call for a strong collaboration between experimentalists and theorists. Two RESOLV-doctoral students, whose main working focus was at the GO department, graduated during the reporting period. One of them worked on a project, which helped to understand the effect of the electric double layer structure on tribology phenomena by force measurements. The second one used interface vibrational spectroscopy to investigate the electrode potential triggered de-solvation of a germanium electrode during a surface transformation. An almost completed third project focuses on the defect evolution in zinc oxide growing on zinc, and the defect formation on ZnO single crystals. Fundamental work in progress investigates the interfacial structure and energy level alignment at immersed electrodes. (see p. 107). The project based in the CM department focuses on the impact of the solvent on the surface structure. Using *ab initio* techniques it could show that solvents have little impact on metallic surfaces but hugely impact semiconducting and insulating surfaces (see p. 89). Ongoing work is addressing questions related to nano-catalysts in wet environments, internal polarisation effects and surface reactivity.

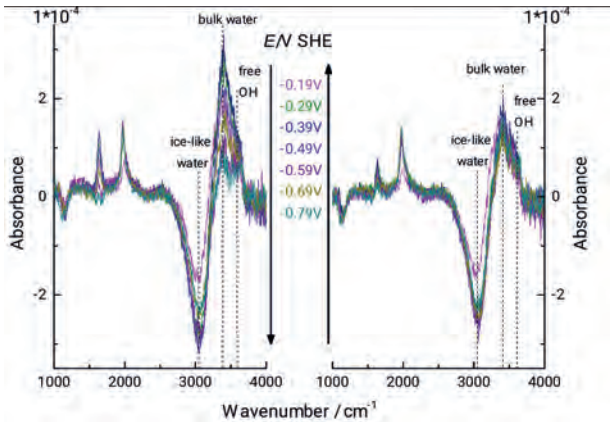


**Fig. 1:** *Infrared difference absorbance spectra of interfacial water at Ge(100) in contact with 0.1 M $HClO_4$ at different potentials. At the lowest electrode potentials, the surface is H-terminated, which interrupts the hydrogen-bond network to the interface. As a result, the vibrational mode of non-hydrogen bound OH is observed at ~3750 $cm^{-1}$ [1].*

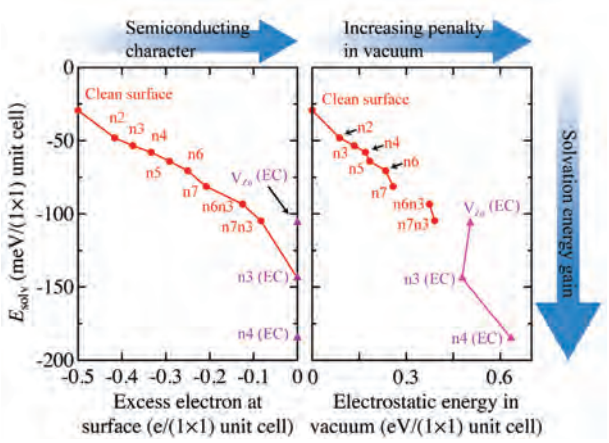


**Fig. 2:** *Solvation energies of ZnO(0001)-Zn surface structures plotted as a function of (left) the excess electrons at the surface and (right) the electrostatic energy of surface phases referenced to that of the clean surface. In contrast to structures with metallic character, structures with semiconducting character, in particular those with a high electrostatic penalty in vacuum, experience a strong energy gain due to solvation [2].*

In 2017, the Cluster of Excellence RESOLV applied for an extension for a second funding period. The submitted proposal outline was one of the 88 proposals (out of 195 submitted) which were successful. The presentation and defence of the subsequently submitted full proposal took place in Berlin in June 2018, with Prof. Neugebauer (CM) being one of the 15 RESOLV PIs participating in the event. The decision that RESOLV is one of 57 Clusters of Excellence to receive funding for the next 7 years was announced in September 2018.

More details about RESOLV are found at https://solvation.de/

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# Interdisciplinary Centre for Advanced Materials Simulation – ICAMS

*J. Neugebauer [1], T. Hickel [1], D. Raabe [2]*

[1] Department of Computational Materials Design (CM)
[2] Department of Microstructure Physics and Alloy Design (MA)

The Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), which has been initiated in 2005 by the MPIE and has been founded in 2008, has become one of the leading institutions for scale bridging materials modelling. It includes the departments for Atomistic Modeling and Simulation (headed by R. Drautz), Scale Bridging Thermodynamic and Kinetic Simulation (I. Steinbach), and Micromechanical and Macroscopic Modeling (A. Hartmaier) (Fig. 1). After the initial startup period of five years with substantial financial support from an industrial consortium, the state of North Rhine-Westphalia and the European Union, the institute has now become a regular unit within the Ruhr University Bochum and beyond. It serves as an integral part of the Material Research Department within the university, but also of the Materials Chain of the University Alliance Ruhr. The latter combines the research activities in the field of materials science and technology at the three Ruhr Area universities Ruhr-Universität Bochum, TU Dortmund University, and the University of Duisburg-Essen.

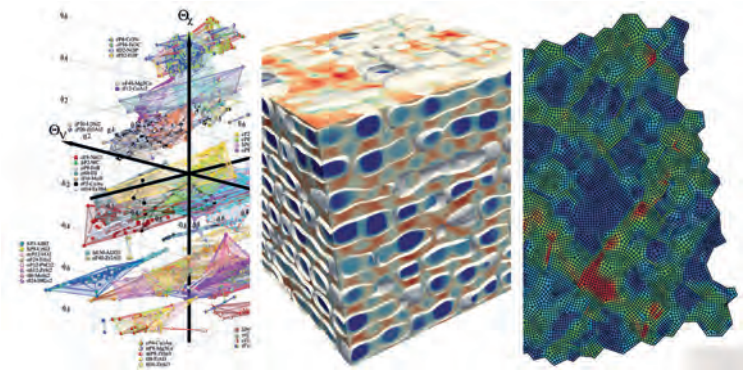

**Fig. 1:** *The three departments of ICAMS combine simulations at different scales, resulting into (from left) atomic structure maps, phase field and finite element simulations as typical images.*

Structurally, the MPIE is embedded into ICAMS via the Advanced Study Group (ASG) “Modeling”, which supports the multiscale concept in particular at the most fundamental scale, which is dominated by electronic interactions and individual atomic processes. The link between ICAMS and the MPIE is further deepened within two large-scale projects supported by the German Research Foundation (DFG) that have been attracted in the past years: Within the Collaborative Research Centre (SFB/Transregio 103) “From Atoms to Turbine” joint research on the characterization of superalloys is performed. The MPIE is further participating in the Priority Program (SPP1713) “Chemomechanics” that is coordinated by I. Steinbach. Its associated projects investigate the interplay of mechanical and chemical forces in metals and polymers. Various other projects, e.g. within the Max Planck Research School SURMAT, have led to an increasing amount of PhD theses that are jointly supervised by members of both institutions. Also, lectures within the ICAMS Master of Science program “Materials Science and Simulation” (MSS) are partially held by members of the MPIE.

**Fig. 2:** *Participants at the 10 Years ICAMS International Symposium, taking place 25-27June 2018 in Bochum. The directors Ralf Drautz, Alexander Hartmaier, and Ingo Steinbach (from left) are standing in the first row.*

The strong collaboration between the MPIE and ICAMS is documented by a large number of publications, a significant amount of attracted third-party funding, but in particular by its scientific outreach. Several workshops (e.g. Ringberg Unary Workshop 2013, ADIS workshops 2014, 2016, 2018) and symposia at international conferences are jointly organized with the MPIE. Regular retreats are performed together with the CM department. The ICAMS Advanced Discussions are meanwhile an established institution. The 10 Years ICAMS International Symposium in June 2018 (Fig. 2), belonging to this series of events, gave a perfect chance to look back at a very successful decade and to look forward to many more years of exciting materials research.

# Knowledge and Technology Platform for Prediction of Durability and Lifetime of Organic Coated Metals under Long-Term Environmental Corrosion

*M. Rohwerder*

Department of Interface Chemistry and Surface Engineering (GO)

This is a joint project with the Free University of Brussels (VUB), within the framework of the Research Foundation - Flanders (FWO), in close contact with about twenty cooperating partners from industry, which started operationally in September 2018 at the MPIE.

The motivation behind this project is that at the current state of the art, lifetime and aging assessment of coated metal are performed by means of experimental testing, combining accelerated testing and field testing.

The limitation of the first is that the conditions of the accelerated testing are not representative for the real environmental conditions and that there is no proven relationship between accelerated laboratory testing and field performance data. The limitation of the second is that it takes several years (5 to 10 years). This seriously impedes organic coating development.

The only way to realize a substantial decrease in the development time of new materials is to introduce modelling in the design cycle. What is needed to realize a breakthrough in this field is a tool that can predict quantitatively and dynamically the corrosion behaviour of organic coated metals.

The scientific motivation for the project is to build a knowledge and technology platform required for achieving such a prediction of durability behaviour and estimation of lifetime of organic coated metals under long-term environmental aging and corrosion conditions. This is a very challenging task, as corrosion of an organic coated metal is the result of an intense interplay between several physical phenomena that need to be understood and modelled. The task of the MPIE will be to identify the underlying processes of the corrosion driven coating delamination and to provide experimental access to key parameters enabling us for its reliable simulation.

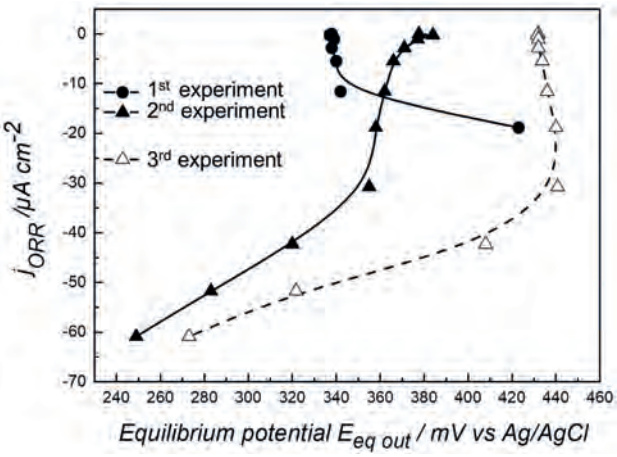


**Fig. 1:** *Example for I(U) curves obtained at a buried interface: three subsequent I(U) curves obtained on PVB/Pd model samples. In the first scan increasing interfacial degradation results in increasing potentials despite increasing cathodic current density. In the subsequent runs further degradation occurs.*

One task will be a standard characterization of delamination behaviour and the migration of cations at the coating/metal interface. Of crucial importance for this will be a recently developed hydrogen permeation based potentiometric method for obtaining full I(U) curves for oxygen reduction at buried interfaces [1,2]. By observing time dependent changes in the kinetics also information about the corresponding interfacial degradation can be assessed (see fig.1).

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# Research Awards

## ERC Advanced Grant: GB-CORRELATE: Correlating the State and Properties of Grain Boundaries

*G. Dehm*

Department of Structure and Nano-/Micromechanics of Materials (SN)

In August 2018 the new ERC Advanced Grant dedicated to Prof. G. Dehm started with the research project GB-CORRELATE. Grain boundaries (GB) are omnipresent defects in structural and most functional materials. While they are known to strongly influence the electrical, magnetic, thermal or mechanical properties of materials, surprisingly little is known on grain boundary phases, their transitions and how they can be applied to advance materials' design. This is in stark contrast to bulk and surface phases and their transitions - i.e. changes in the arrangements of atoms in the volume or at the surface of materials - where thermodynamic and atomistic concepts are well established since a long time. This lack of a complete exploration of grain boundaries is due to their structural and chemical complexity, their internal defects and previously, insufficient characterization techniques. GB-CORRELATE is tackling these challenges by combining correlated atomic resolved microscopy, spectroscopy and tomography with computational approaches. GB-CORRELATE finds perfect scientific conditions at the MPIE due to the strong in-house collaborations between the different departments.

The complexity of grain boundaries with their large number of macroscopic and microscopic degrees of freedom is approached by a hierarchical strategy: dedicated bicrystals in form of bulk materials and thin films are the reference point to identify

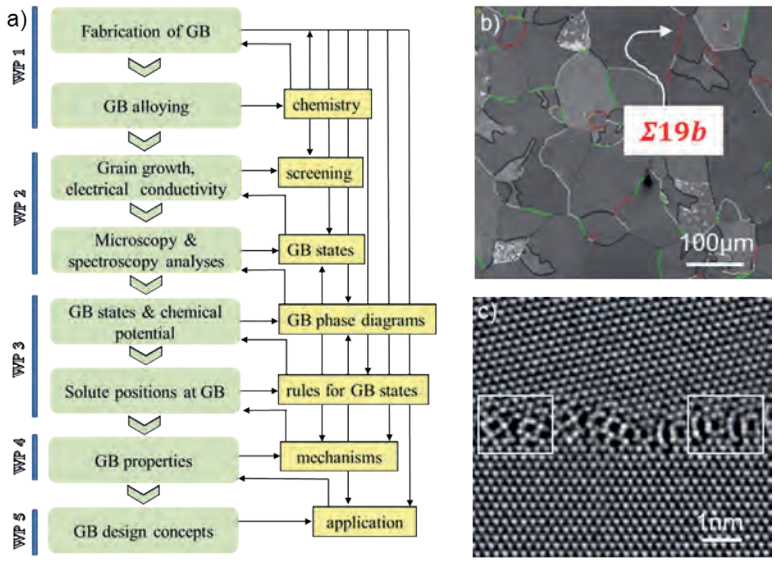


**Fig. 1:** *a) Overview on the work packages (WP) and their tasks within GB-CORRELATE. b) Oligocrystalline Cu film where different grain boundary misorientations are indicated by different colours; red lines mark ∑19b grain boundaries. (c) Atomic resolved scanning transmission electron micrograph of a ∑19b grain boundary with two different structural units (white boxes). Microscopy images are courtesy of T. Meiners.*

In addition to the structural exploration of grain boundaries, *in situ* micromechanical experiments will be performed to interlink grain boundary phases and mechanical properties. Grain growth experiments coupled with microscopy techniques such as electron backscatter diffraction and scanning electron microscopy will allow extracting changes in mobility of individual grain boundaries due to phase transitions in a high throughput approach. The project aims to predict and resolve grain boundary phase transitions, to establish guidelines for them, to correlate them with property changes and finally to provide design criteria for grain boundary engineering.

phase transitions. Cu, Al, and Cu- or Al-based alloys are employed as face-centred-cubic prototype materials with different stacking fault energies and melting temperatures. Growing oligocrystalline and strongly (111) textured polycrystalline thin films introduces further defects like triple lines but still provides access to the atomistic grain boundary structure due to a common zone axis for atomic resolved electron microscopy studies of neighbouring grains. The strategy of GB-CORRELATE is summarized in Fig. 1a, while Fig. 1b provides a first example of grain boundaries in an oligocrystalline Cu film, where two different grain boundary structures within a ∑19b grain boundary are resolved (Fig. 1c).

# ERC Consolidator Grant: SHINE: How to See Hydrogen Atoms in Materials

*B. Gault*

Department of Microstructure Physics and Alloy Design (MA)

Despite being ubiquitous in nature, observing hydrogen (H) in matter is a formidable challenge. Hydrogen is elusive to scientific scrutiny like no other element, because of its low weight and extreme mobility. There is no doubt that H is a prime candidate for enabling future low-carbon emission manufacturing and power supply chains, but, as known for over 120 years, H is also at the origin of a strong and often sudden embrittlement phenomenon which has resulted in many catastrophic failures of engineering alloys and structures. Guided by promising preliminary results obtained on Ti-based alloys, summarised in Fig. 1, I decided to pursue a project targeting quantifying and locating H within materials. These results were the first obtained at the MPIE, where we could demonstrate the capacity of atom probe tomography (APT) to characterise stable hydrides, which are thought to be responsible for brittle fracture of a range of Ti-based alloys [1]. This Consolidator project funded by the European Research Council (ERC) is called SHINE as an abbreviation for 'Seeing Hydrogen IN mEtals'. Here, I ambition to exploit the unique facilities developed in the Atom Probe Tomography group at the MPIE to perform direct imaging and quantification of H atoms in candidate metallic alloys and materials for H-storage. The infrastructure of the Laplace Project allows for the preparation (see p. 34), electrochemical and, soon, gaseous charging of hydrogen or deuterium under highly controlled conditions. Following the transfer of the specimen under ultra-high vacuum and cryogenic conditions [1], these specimens can be investigated. Atom probe tomography will be the principal method of a correlative microscopy and spectroscopy approach to investigate materials where precise knowledge of the distribution of H is crucial. Informed by experimental data, modelling and simulations will provide a mechanistic understanding of the behaviour of H in materials.

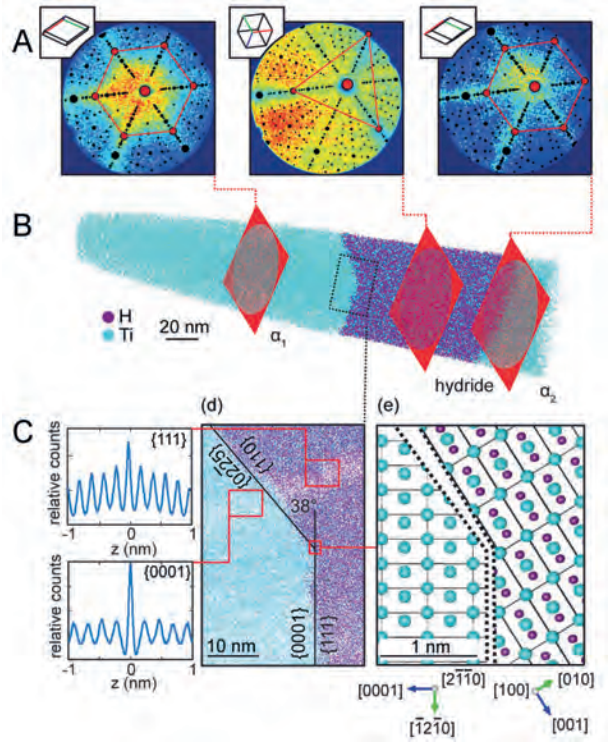


**Fig. 1:** *Atom probe crystallography analysis of a hydride precipitated at an α low-angle grain boundary in Ti-2Fe: (a) patterns formed on the detector during the analysis exhibiting the typical symmetries from the local crystalline phase highlighted by the superimposed stereograms; (b) APT reconstruction and (c) spatial distribution maps revealing the presence of atomic planes in the tomographic reconstruction near the α-Ti/hydride interface shown in (d); (e) model of the faceted α/hydride interface [1].*

Over the five years of the project, which started in February 2018, three PhD students and two post-doctoral scientists will work alongside the PI. This research is pursued in close collaboration with the department of Computational Materials Design, where two of the early-stage researchers are expected to be based. The expertise of the Interface Chemistry and Surface Engineering department will also come to support the development of novel hardware for gas-charging and UHV processing of metallic alloys. New data-processing methods, including possibly exploiting machine-learning approaches, will be established to maximise data quality.

The results from SHINE will be three-dimensional hydrogen mapping at the near-atomic scale that will provide new insights of the behaviour of H in the complex and dynamic microstructures of engineering materials. By relating this fundamental knowledge with observed physical properties, we will enable unprecedented precision in the prediction of material behaviour, and therefore pave the way for new materials design and manufacturing strategies to enhance their performance and durability. All these applications have relevance to a 'low-carbon-emission economy' that humanity must develop in the 21st century.

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# ERC Starting Grant: TIME-BRIDGE: Time-Scale Bridging Potentials for Realistic Molecular Dynamics Simulations

*B. Grabowski*

Department of Computational Materials Design (CM)

The European Research Council (ERC) rewards the most prestigious and competitive scientific funding in Europe. The criterion for selection is scientific excellence. In 2015, Dr. B. Grabowski was awarded an ERC Starting Research Grant for his innovative project proposal: *TIME-BRIDGE: Time-scale bridging potentials for realistic molecular dynamics simulations*.

The main aim of TIME-BRIDGE is to design novel methodologies that enable a more realistic atomistic simulation of materials. The challenge of present-day atomistic simulation techniques is to model 1) long time scales, 2) large system sizes with high accuracy and 3) to connect faithfully to experimental measurements. The general strategy of TIME-BRIDGE is therefore building upon three main pillars that focus on tackling these challenges under a common framework with steady exchange of ideas and expertise. A very good scientific progress was achieved during the first half of the funding period as evidenced by 20 publications in renowened journals and by many (>30) dissemination events on national and international level.

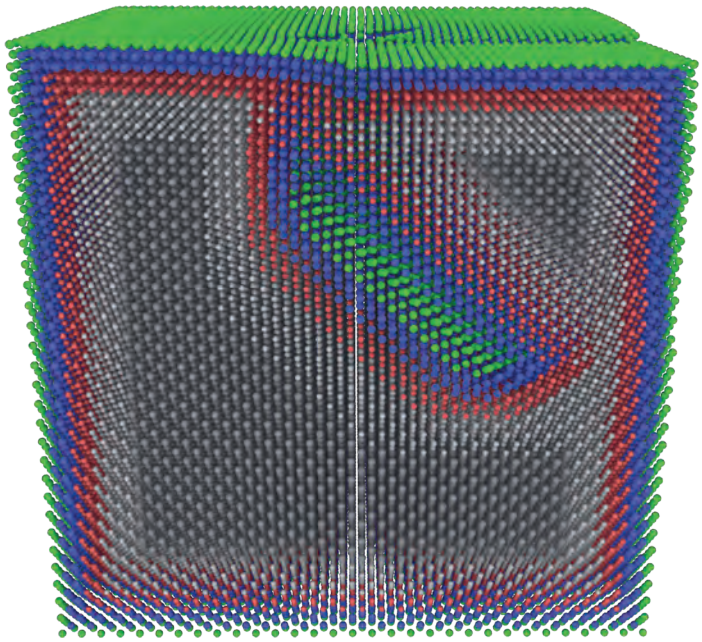

**Fig. 1:** *Partially indented nanopillar with an activated dislocation. The dark gray atoms are described by continuum theory (finite element method), blue and green atoms are treated by molecular dynamics and the other colours indicate buffer atoms.*

For example, we have investigated the possibility to use a new hyperdynamics potential (based on Smooth Overlap of Atomic Positions (SOAP)) for accelerating molecular dynamics simulations (A. Nematollahi). Our results show that this potential is able to differentiate between transition and equilibrium states for various types of simulations. Further, we have developed a new technique that bridges from the nano- to meso-scale by coupling atomistic calculations to continuum models (L. Huber). To achieve this, we use a state-of-the-art force-based coupling method between molecular mechanics (MM) and linear elasticity represented using the finite element method (FEM). We have now extended this technique to be fully adaptive in MM and FEM domains, even at finite temperatures. This adaptivity allows the MM domain to remain small, tracking defects which require atomistic resolution even as they are migrating through the system (see fig. 1). Within TIME-BRIDGE also small scale *in situ* compression experiments on nanopillars are performed to understand the size scaling of rare events such as dislocation motion and interaction with grain boundaries (N. Peter in collaboration with C. Kirchlechner from the SN department).

The TIME-BRIDGE project has a horizon of five years. Over this period, the funding covers three post docs, and a senior scientist.

# ERC Starting Grant: CSI.interface: A Molecular Interface Science Approach: Decoding Single Molecular Reactions and Interactions at Dynamic Solid/Liquid Interfaces

*M. Valtiner*

Now at: Group Applied Interface Physics, Institute of Applied Physics, Vienna University of Technology

In 2016 Dr. M. Valtiner was awarded the prestigious ERC Starting Grant for his project: „CSI.interface - A molecular interface science approach: Decoding single molecular reactions and interactions at dynamic solid/liquid interfaces“.

Generating a detailed molecular understanding of complex, simultaneous interactions at reactive/dynamic solid/fluid interfaces is one of the biggest contemporary scientific challenges across disciplines. Whether it is during corrosive coating degradation, in biological adhesion, or during adaptive interfacial redox-cycle feedback in strongly adhesive seawater organisms: It is a large number of similar or dissimilar molecule/molecule, molecule/surface and competing interactions with ions/water that mediate complex macroscopic properties at crowded solid/liquid interfaces. How do single molecular interactions at dynamic, reactive or steady state interfaces translate into a macroscopically observable outcome? A truly molecular-level understanding of the complex length scale and chemistry dependent nonlinearities at interactive and reactive solid/liquid interfaces in 2D, let alone in 3D is missing.

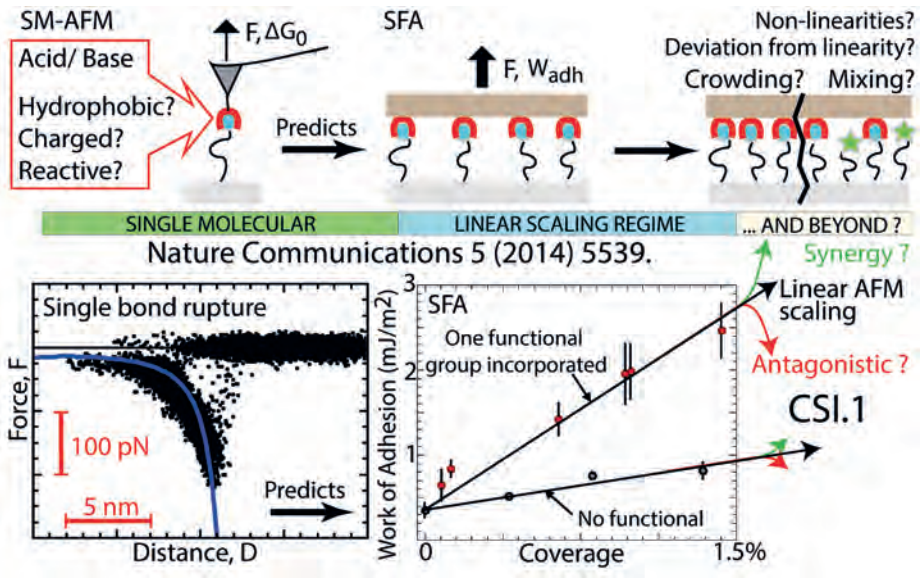


**Fig. 1:** *Bottom: The team of M. Valtiner showed how work of adhesion ($W_{adh}$) can be directly predicted from SM-AFM in a linear scaling regime. Top: In this ERC project this work will extend this to interfacial crowding, molecular mixing including the role of water, ions as well as interfacial reactions at all levels (single to integrating large numbers of interacting molecules).*

With the CSI.interface approach a predictive molecular insight into this complexity will be provided. The group of Dr. Valtiner will develop a comprehensive approach and tools in order to predict macroscopic properties/observables - such as interfacial adhesion or steady-state dynamics of redox cycles - based on single molecule experiments.

Combining Atomic Force Microscopy (AFM) based single molecule force spectroscopy and macroscopic Surface Forces Apparatus (SFA) experiments CSI.interface will (1) derive rules for describing nonlinearities observed in complex, crowded (water and ions) and chemically diverse adhesive solid/liquid interfaces; (2) uniquely characterize all relevant kinetic parameters (interaction free energy and transition states) of electrochemical and adhesive reactions/interactions of single molecules at chemically defined surfaces as well as electrified single crystal surfaces and step edges. Complementary, (3) a novel molecular force apparatus will be built in order to measure single-molecule steady-state dynamics of both redox cycles as well as binding unbinding cycles of specific interactions, and how these react to environmental triggers. CSI.interface goes well beyond present applications of AFM and SFA and has the long-term potential to revolutionize the understanding of interfacial interaction under steady-state, responsive and dynamic conditions. This work will pave the road for knowledge based designing of next-generation technologies in gluing, coating, bio-adhesion, materials design and much beyond.

M. Valtiner was offered a position at Vienna University of Technology and is now full professor, heading the Group “Applied Interface Physics“.

# ERC Co-Investigator Grant: SMARTMET: Utilizing Phase Instability to Design Alloys with Enhanced Mechanical Stability

*C.C. Tasan [1], J. Zhang [1], D. Raabe [1], B. Grabowski [2], L. Huang [2], J. Neugebauer [2]*

[1] Department of Microstructure Physics and Alloy Design (MA)
[2] Department of Computational Materials Design (CM)

Prof. D. Raabe and Prof. J. Neugebauer were awarded an ERC Co-Investigator Grant, the most prestigious and competitive scientific funding in Europe. The project proposal: "SMARTMET: Adaptive nanostructures in next generation metallic materials" was embedded into the Adaptive Structural Materials (ASM) group lead by Dr. C.C. Tasan (experiments) and Dr. B. Grabowski (theory) and worked on during the period 2012 to 2017.

The overarching aim of SMARTMET was the design of advanced metallic alloys with adaptive nanostructures by utilizing mechanically unstable phases. More specifically, the SMARTMET target was to break the well-known inverse strength-ductility challenge, which puts an apparent limit to the mechanical optimization of advanced engineering alloys. The solution approach we have introduced in SMARTMET was to develop new alloy design strategies based on the counter-intuitive approach of utilizing phase instability rather than phase stability. This target was pursued by the joint use of experiments and atomic-scale theoretical tools. The goals of SMARTMET have been reached leading to significant achievements in advanced alloys as evidenced by the more than 50 related publications in high impact journals.

As a representative example Fig. 1 shows the results achieved by bringing the SMARTMET idea into the field of high entropy alloys (HEAs). While over the past decade, these HEAs, also referred to as compositionally complex alloys or multi-principal element alloys, have drawn attention in the context of entropy driven stabilization of a specific phase, we changed this approach and rendered them more instable. Taking such a mechanistic perspective we developed entirely new HEA variants such as TWIP, TRIP, and dual phase HEAs with excellent mechanical properties (Fig. 1).

For this purpose several of the new mechanistically designed HE alloy variants violated some of the original HEA rules, such as using less than 5 alloying elements and the use of minority alloy ingredients below 5 %. Allowing for such compositional deviations from the original HEA rules was justified by three aspects: theory showed that the mixing entropy curves assume a shallow shape so that deviations from equimolar compositions do not alter the entropy configuration substantially. Second, the necessity for compositional tuning of a specific magnitude of the stacking fault energy or similar thermodynamic key quantity is more important than yielding maximum entropy. Third, when striving for excellent mechanical properties, avoiding brittle intermetallic phases is much more important than obeying static alloy design rules.

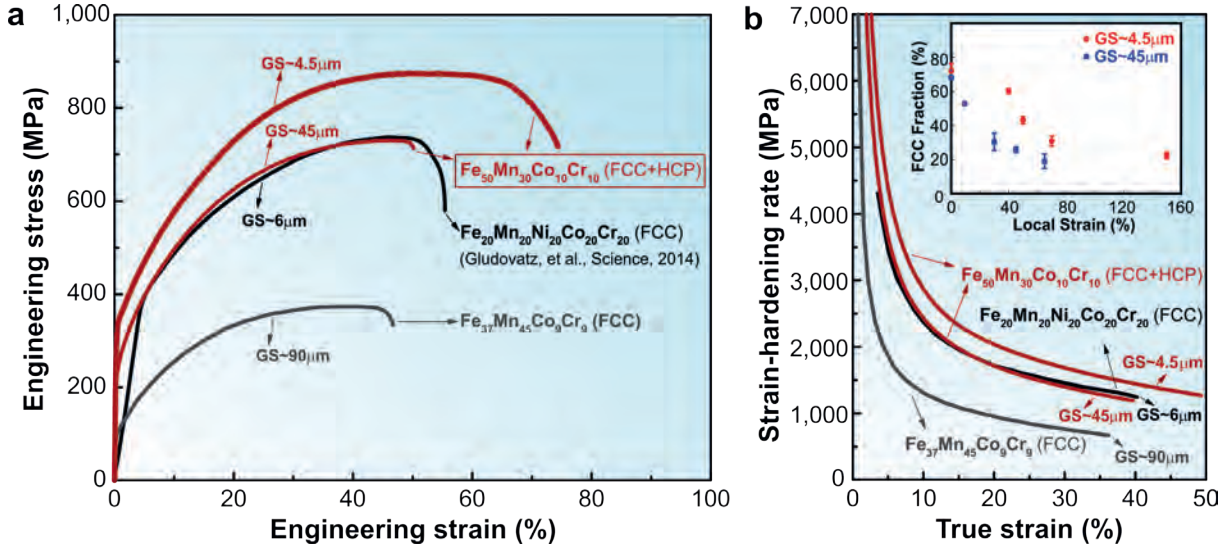


**Fig. 1:** *Mechanical behaviour of the TRIP-DP-HEAs compared to various single-phase HEAs. Ref: Nature 534 (2016) 227.*

# Heinz Maier-Leibnitz Award

*C. Kirchlechner*

Department of Structure and Nano-/Micromechanics of Materials (SN)

Since 1977, the German Research Foundation (DFG) annually awards about 10 early career scientists across various disciplines with the prestigious Heinz Maier-Leibnitz Award. The prize is named after the former president of the DFG and aimed for honoring young researchers and supporting them to pursue their scientific career. In May 2017, Dr. Christoph Kirchlechner, head of the Nano- and Micromechanics group in the SN department of the MPIE was the first time awardee coming from the MPIE in Düsseldorf. The award was presented by the federal minister of education and research, Prof. Johanna Wanka, and the president of the DFG, Prof. Peter Strohschneider in Berlin.

Dr. Christoph Kirchlechner is focusing on the mechanical properties of materials at the micron and submicron scale with special interests on interface fracture and plasticity. His toolbox comprises several electron and X-ray based in situ techniques, such as X-ray Laue microdiffraction (μLaue), which he conducts at the European Synchrotron Radiation Facility (ESRF, Grenoble, France). During the last five years Dr. Kirchlechner has used this technique to shed light on fundamentals of dislocation-grain boundary slip transfer mechanisms, a process of utmost importance for the manufacture and application of all engineering materials. Dr. Kirchlechner and his team could show that – in a certain size regime – the prominent Hall-Petch type hardening is a grain size and – at least at low strains – not a grain boundary effect. Furthermore, they were able to measure the dislocation transmission stress through grain boundaries [1], its strain rate sensitivity [2] and activation volume (submitted to Acta Materialia) for the first time.

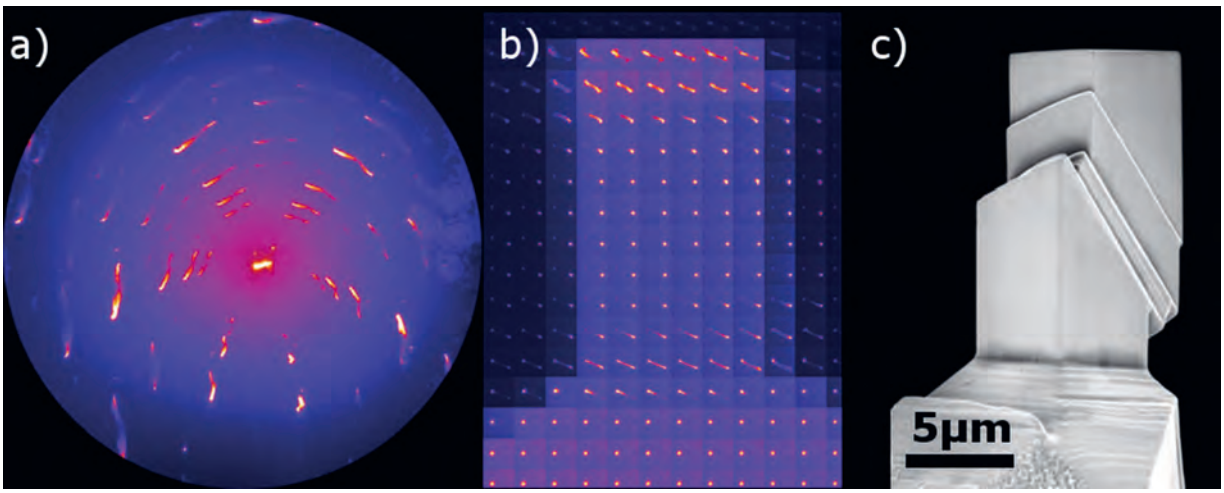


**Fig. 1:** *(a) A full Laue microdiffraction pattern recorded with a 1μm sized synchrotron beam on deformed tungsten. (b) A mosaic composition of Laue patterns recorded across the copper pillar presented in (c).*

## References

1. Malyar, N.V.; Micha, J.S.; Dehm, G.; Kirchlechner, C.: Acta Mater. 129 (2017) 91.
2. Malyar, N.V.; Dehm, G.; Kirchlechner, C.: Scr. Mater. 138 (2017) 88.

# NWO Grant: How to Mix the Perfect High-Entropy Alloy Cocktail

*F. Körmann*

Department of Computational Materials Design (CM)

The Dutch Research Organisation (NWO) supports the research of Dr. Fritz Körmann, project group leader in the CM department and researcher at the Delft University of Technology in the Netherlands with 800.000 euros for five years. The funding enables researchers to establish a research group in the Netherlands and to develop their own line of research. The research topic of Körmann is complex alloys including the new materials class of High-Entropy Alloys (HEAs). Metallic alloys constitute one of the oldest developments of sciences for thousands of years. It is therefore surprising when a new class of metallic alloys is discovered. High Entropy Alloys (HEAs) are such a class and have received great attention recently in terms of the underlying physics responsible for their formation as well as unusual physical and materials properties. HEAs reveal auspicious magnetic and outstanding mechanical properties, making them candidates for next-generation of technological applications. Whereas traditional alloys usually contain 1-2 main components, HEAs are comprised of 4-6 elements in high or even equal concentrations and crystalize into surprisingly simple lattice structures with randomly dispersed atomic species. Prototype examples are CrMnFeCoNi base HEAs. So far more than 30 different elements have been used resulting into more than hundreds of reported HEAs. Still this is only a marginal fraction of the immense number of possible combinations, leaving an overwhelming number of alloys with presumably superior properties unexplored. Further, basic mechanisms such as the relation of strength and chemical complexity are still poorly understood.

In this project we will address these issues by developing a fully parameter-free computational framework to predict materials properties of multi-component alloys. High-throughput first-principles computations will be performed to cope with the large configuration space, focusing in particular on stability and intrinsic materials properties, such as the stacking fault energy and local atomic fluctuations, which can be linked to macroscopic mechanical properties and mechanisms (e.g. twinning induced plasticity). As envisioned by the Materials Genome Initiative, this work represents a computational guide for the discovery and design of materials with specifically desired properties. This will greatly facilitate experimental efforts by narrowing down the large number of possible materials to well-defined promising candidate alloys, and thus greatly accelerate the exploration of hitherto unexplored materials with extreme properties for technological applications.

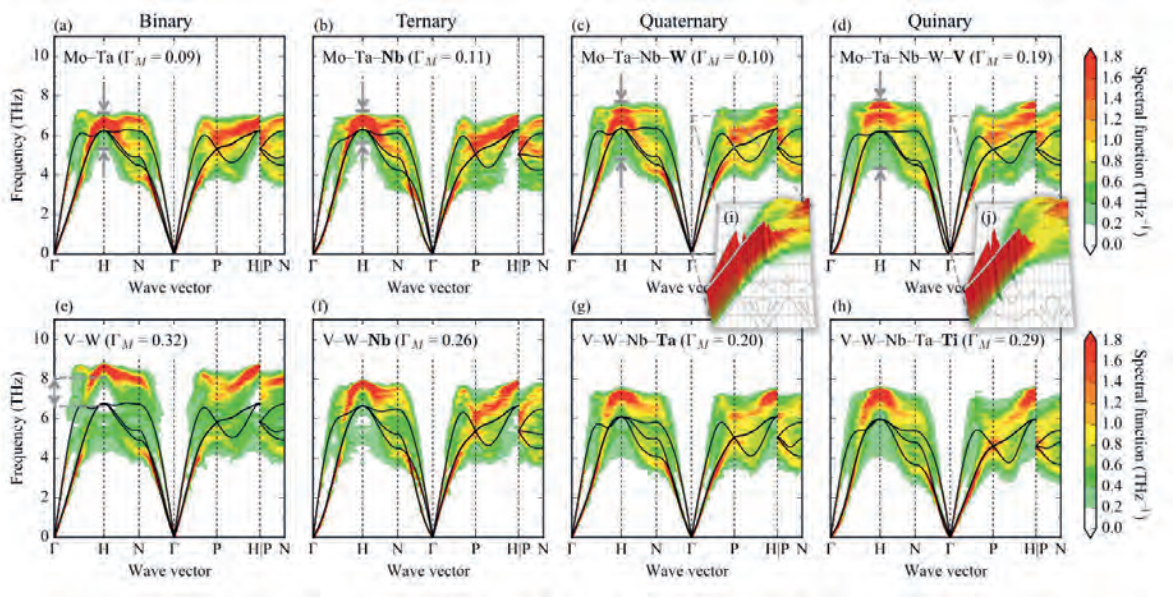


**Fig. 1:** *Broadening of phonon spectra with increasing number of constituent elements: From binaries to 5-component high entropy alloys. The added element for each alloy from left to right is shown in bold. Phonon spectra derived by employing averaged force constants and masses are shown for comparison as black solid lines. Insets (e) and (f) provide 3D representations of the long-wavelength phonon spectra for MoTaNbW and MoTaNbWV. Further details given in [1].*

## References

1. Körmann, F.; Ikeda, Y.; Grabowski, B.; Sluiter, M.H.F.: npj Comput Mater 3 (2017) 36.

# Heisenberg Fellowship

*R. D. Kamachali*

Department of Computational Materials Design (CM)
Department of Microstructure Physics and Alloy Design (MA)

The Heisenberg Programme by the German Research Foundation (DFG) is dedicated to promote young, highly-qualified researchers heading for professorship. It is one of the most renowned funding schemes of the DFG, named after German physicist Werner Heisenberg. The fellowship is supporting the awarded scientist in conducting independent researches for three years and can be extended to another two years. In October 2017, Dr. Reza Darvishi Kamachali was awarded the prestigious Heisenberg Fellowship to pursue his research on "Studying and Design of Chemo-mechanically Heterogeneous Microstructures Using Full-field and Mean-field Modelling".

The current fellowship is hosted by the departments of Computational Materials Design and Microstructure Physics and Alloy Design where scale-bridging studies across atomistic simulations and precise experimentation and characterization is highly developed. By combining mesoscale full-field simulations with mean-field modelling, Dr. Kamachali aims to further bridge the researches at the MPIE on the microstructure level. The strategy of the research is portrayed in the figure above. While mesoscale full-field simulations enable analyzing virtual microstructure evolution in full details, mean-field modelling allows the discovering of applied interrelationships between bulk material properties and the material's microstructure. Complex steels, aluminum alloys and high entropy alloys are potential materials of the research.

Dr. Kamachali is an expert in thermodynamics and kinetics of microstructure evolution. He conducted several researches on grain growth and nano-grain growth, recrystallization and precipitation in aluminum alloys. Dr. Kamachali is a principle investigator in the Priority Programme SPP1713 "Strong coupling of thermo-chemical and thermo-mechanical states in applied materials" where he developed a concept of chemo-mechanical coupling applicable in solid-state microstructure evolution [1,2]. He previously was leading the research group of Solid-solid Interface Kinetics at the Interdisciplinary Centre for Advanced Material Simulation, Ruhr-Universität Bochum.

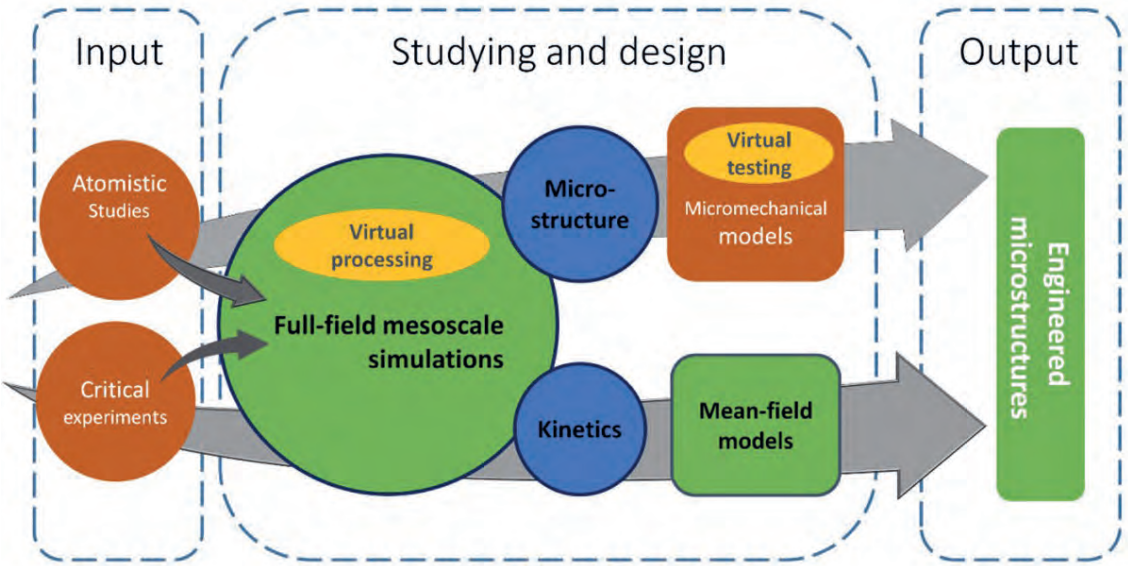


**Fig. 1:** *A strategy of a computationally-guided microstructure design.*

## References

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2. Schwarze, C.; Gupta, A.; Hickel, T.; Kamachali, R.D.: Phys Rev B 95 (2017) 174101.

# Research Funding

*K. Hübel*

Research Coordination Office

### Professional Support in Research Funding

In the past six years Dr. Katja Hübel provided professional support in national, European and international research funding to the scientists of the MPIE with the aim of increasing the career prospectives of our junior scientists. She gave advice on all kinds of funding from individual (e.g. Humboldt Research Fellowship for Postdoctoral Researchers, Marie Skłodowska-Curie Individual Fellowship or ERC Grants) to project funding (e.g. Horizon 2020, German Ministry for Science & Education and German Research Foundation). Furthermore special attention was drawn to prizes and awards (e.g. Leopoldina Preis, Adolf-Martens-Preis and Deutscher Studienpreis).

### Competitive Applications

Professional and administrative assistance was provided for researchers throughout the whole process of application. Support was given in identifying the right funding scheme fitting to the scientific profile or project needs, in proposal writing as well as in budget calculation. For networking projects coordination of the project partners was offered.

Yearly, Katja Hübel is organizing together with Viola Tegethoff from the Max Planck Institute for Radio Astronomy (Bonn) and the National Contact Point ERC a Workshop “Writing competitive ERC Starting and Consolidator Grant proposals“. This workshop is a special offer to junior scientists at Max Planck Institutes in North Rhine-Westphalia.

### Interview Training

Especially applications for group leader funding often include interviews. Those are intensively practiced with participation of the Research Coordinator, the Public Relations Officer (see p. 83) and of course experienced scientific colleagues.

### Project Management

Support in project management was also given. This included assistance in setting scientific project reports as well as in financial reporting. Project reporting was done in close collaboration with the MPIE administration.

### Career Development

A special focus was set on the career development of young scientists. This included not only finding the right funding scheme that fits to their scientific profiles but also strategic advice for their career development. Furthermore Katja Hübel yearly gives a talk “Competitive Proposal Writing“ in order to qualify the researcher for writing high-quality, well-structured proposals.

Support was given to junior scientists working at the MPIE as well as to prospective junior scientists planning to work at the MPIE.

**Fig. 1:** *Dr. Baptiste Gault was awarded with the Consolidator Grant of the European Research Council for his research about hydrogen mapping. Advanced characterization techniques such as atom probe tomography as seen in the photo, will be used.*

### Selected Research Funding (2013 – 2018)

*Prof. Gerhard Dehm* received an ERC Advanced Grant for the project “GB-CORRELATE - Correlating the State and Properties of Grain Boundaries”, Mar 2018.

*Dr. Baptiste Gault* received an ERC Consolidator Grant for the project “SHINE - Seeing Hydrogen in Matter”, Feb 2018.

*Dr. Blazej Grabowski* received an ERC Starting Grant of the European Research Council Jul 2015.

*Dr. Michael Herbig* received 1.468 Mio € funding by the BMBF for his junior research group “Materials Science of Mechanical Contacts”, Sep 2016.

*Dr. Cem Tasan* former leader of the group “Adaptive Structural Materials” (until Dec 2015) won the Freigeist Fellowship of the Volkswagen Foundation, Jun 2015.

*Dr. Markus Valtiner* received an ERC Starting Grant for the project “CSI.interface - A molecular interface science approach: Decoding single molecular reactions and interactions at dynamic solid/liquid interfaces”, Dec 2015.

# Promotion of Young Scientists

*K. Hübel*

We are highly committed to promoting young scientists at all career stages. The success of our intense coaching and training initiative is outlined in the following:

**Scientific Honours and Apprenticeship Awards**

Our excellent junior researchers are rewarded with prestigious scientific honours. In 2017 the MPIE reached the 3rd best position in the Humboldt-Ranking among all non-university research organizations in Germany. In the last six years, our young scientists got a total of 115 prizes, awards and prestigious grants like ERC Starting and Consolidator Grants or a Freigeist Fellowship. The great success of our researchers is also due to the expert support in writing competitive proposals of our Research Coordinator Dr. Katja Hübel (see p. 77). Not only our scientists get honoured, the MPIE is also successfully educating apprentices. From 2013 - 2018 our trainees won 3 times the Apprentice Prize of the IHK (Chamber of Commerce), Düsseldorf and also 3 times the Apprentice Prize of the Max Planck Society.

**Scientific Output**

Our training, coaching and mentoring efforts result in a high scientific output and are also reflected by the career development of our youngsters. In the last six years junior scientists were author on 4 Nature papers, 12 Nature Communications and on 3 Science papers. Our young scientists are encouraged and financially supported to present their research results in international conferences, which is in addition supporting their networking activities and their recognition within the scientific community.

In the past 6 years, more than 10 of our junior scientists secured international professorship appointments at leading research institutes and universities like the Massachusetts Institute of Technology (MIT)/USA or the Imperial College London/UK. We support our senior postdoctoral researchers as well as our group leaders in doing their next career steps. The directors are sharing their expertise on selection committees for becoming university professor by training the interview situation with the respective researcher. Also applicants for the Max Planck Research Groups are prepared for the Selection Symposium. Prof. Christina Scheu is the "MPIE Female Science Career Mentor" supporting female senior postdoctoral researchers as well as young group leaders on their way to become a professor (see p. 81).

**Teaching and Supervision**

Teaching expertise and supervision activities are important prerequisites for an academic career. We encourage our researchers to do both which is facilitated by our connections to the Ruhr-Universität Bochum and the RWTH Aachen University.

**From Researchers for Researchers**

We convey the importance on acting in concert and of efficient interdepartmental research to our junior scientists – a spirit which is fortunately taken over. Our PhD students organize MPIE Lectures, where the group leaders and directors share their knowledge on different experimental and theoretical methods to the audience. Also interdepartmental meetings are organized on a regular basis to further develop our interdepartmental research projects. In addition, the MPIE supports the PhD representatives in organizing Career Talks with speakers from industry as well as diverse Softskill trainings.

**Public Relations**

To attract also the next generation of scientists (pupils and students) the Institute's Public Relations Officer Yasmin Ahmed Salem is organizing a variety of events (see p. 83). The Institute participates in the Researchers' Night in Düsseldorf, we open our laboratories yearly during the Girls' Day, the MPIE is organizing Kids' Labs and we are participating in the Science Days of the Theodor-Fliedner grammar school. Researchers get a PR Coaching if they are invited to give an interview or if a short TV-movie is made to present their research. Also schools are coming to visit our Institute on a regular basis and the departments host pupils for 1-2 weeks of internships. Additionally, summer interns for students are provided by the institute and including a well-established summer internship programme with the students of materials science from the University of Cambridge (UK).

**Applications of Excellent Researchers**

To get excellent junior researchers, the MPIE has a doctoral progamme the „International Max Planck Research School for Interface Controlled Materials for Energy Conversion (IMPRS-SurMat)" (see p. 51). Postdoctoral researchers from abroad can apply for a PostDoc Scholarships (up to 10 years after PhD) or a Research Scholarships (more than 10 years after PhD). In all career stages speculative applications are possible.

# International Office

*S. H. Zwaka*

Research Coordination Office

While the international researchers at the Institute were previously supported to different degrees by their respective departments and groups, in 2018 the board of directors of the MPIE decided to create an International Office at the Institute. By deciding to centralise and structure the support for the Institute's foreign scientists, the directors decided to follow the example of other Max Planck Institutes, research institutes and universities in Germany.

In September 2018, Sophia Helena Zwaka started working at the MPIE to set up an International Office. In order to create a fitting concept for the MPIE, during the first month, she talked to various parties at the Institute including the directors, assistants and secretaries of the directors as well as group leaders, PhD representatives and postdoctoral students.

The International Office aims at assisting the Institute's international scientists during their onboarding process and stay in Germany. This is to be achieved via personal support and the timely provision of relevant information via email, events and the Institute's intranet. Advice and information are offered regarding all aspects of everyday life in Germany including German bureaucracy, housing and family life.

During the first months after the official presentation of the International Office amongst the staff of the MPIE, Sophia Helena Zwaka has provided support in the following aspects: Providing information on visa processes and supporting the scientists in obtaining the adequate residence permit. Finding housing on short notice, which has been facilitated by the decision of the International Office to create a list of landlords who rent out their apartments on a regular basis. Furthermore, information on matters regarding health insurance and the ccupational pension scheme were provided upon request. Zwaka has also supported researchers residing in Germany with their families, by helping with visa and employment matters for spouses, as well as providing information for the application for public child benefit (Kindergeld) and guidance for researchers planning to have a child in Germany.

The majority of researchers who have sought support from the International Office came from the following countries: China, India and Iran.

In order to offer centrally available information, the International Office has created a checklist as an overview on the first steps in Germany. It aims at making relevant information available to every researcher by updating the Institute's intranet and to organise regular events. The organisation of a Welcome Coffee aims at improving interdepartmental communication and at better integrating new international employees by answering any lingering question on administrative processes. A second event aims at explaining the administrative procedures of the Institute to the foreign scientists. To facilitate the comprehension of administrative processes, the International Office works closely together with the HR department. Zwaka aims to facilitate communication between administration and researchers, by explaining the Institute's operating agreements and translating for the administration.

The International Office also plans to coordinate the provision of German classes in 2019, to organise information sessions on topics requested by the scientist and to create a buddy system, were every new foreign employee at the Institute has a buddy - a more experienced employee - in order to offer advice and support in the first weeks at the MPIE.

# PhD Representatives

*V. G. Arigela, J. B. Molin, R. S. Varanasi, A. Hariharan, S. Surendralal, L. Sreekala, P. Beley, M. Pander, J. S. M. Ochoa*

The PhD representatives are the interdepartmental representation of the PhD students at the Max-Planck-Institut für Eisenforschung (MPIE). Annually the MPIE' s PhD students elect one external representative and eight internal representatives (two per department). We are responsible for maintaining and promoting the interdisciplinary cooperation among the PhD students at the MPIE but also in close contact with the other PhD students of the Max Planck Society by engaging within the PhDnet, a platform for exchange among doctoral students of all Max Planck Institutes. Moreover, we provide our fellow colleagues at the MPIE with up-to-date information about stipend and contract possibilities, insurance information and other upcoming and important topics for a better research and living experience. And we exchange important topics with the management of the Institute. We also serve as a bridge to the newly formed $N^2$, a common platform for doctoral students from Max Planck institutes, Leibnitz and the Helmholtz institutes.

**Fig. 1:** *During the visit to Dillinger Hütte, a steel manufacturer in Saarland, Germany. The PhD students are standing next to the longest steel slab ever produced by the company.*

The PhD representatives organize soft skill courses for PhD students biannually covering topics such as scientific writing, presentation, and leadership skills. Additionally, career talks are organized to give PhD students and postdoctoral fellows a platform to network with industry and gain insight into job opportunities from different industrial sectors. During the 2016-18 period, career talks with companies like Tata Steel and Dillinger received much positive feedback. The career talks are followed by visits to the respective manufacturing plants. Moreover, we coordinate with leading international research institutions to organize career events for students who opt to stay in academia. 2018 the National Institute of Materials Science, Japan, visited the MPIE and introduced their center and job opportunities. The MPIE lecture series, which was launched in 2015 to bolster the knowledge transfer in the Institute, flourished well in the past years. The lectures are organized by the PhD representatives, recorded and made available online for the in-house researchers. Exemplary lectures were delivered covering a wide variety of topics such as how to write competitive research proposals or how to use and interpret data from electron backscatter diffraction. The lectures are given by experienced MPIE group leaders. We also coordinate with the doctoral programme of the Institute IMPRS- SurMat to extend the reach to partner institutes and universities. The PhD representatives play an active role in social events of the institute throughout the year, such as the annual Christmas party.

# Equal Opportunities

*S. Degner, C. Scheu*

During the last three years the MPIE has taken several measures to reconcile the demands of family and career.

Firstly, we introduced the family-service of the Max Planck Society to our employees in 2016; the "pme-Familienservice" offers support in childcare, recruitment of daycare-nannies/ daycare-solutions, emergency-nanny in case of child´s sickness, Au-Pairs, private "Kindergarten"/ nursery, programmes during school holidays, backup-service, eldercare, supervision of children and elder persons in general (homecare) and a hotline. The Institute is regulary providing current information on different offers of the "pme-Familienservice" via Intranet as well as via flyers and e-mail.

Secondly, we worked on finding a daycare facility for children (so called KiTa) near the Institute to be able to reserve some places for employees having small children (≤ three years). The reason for that is the lack of KiTa-places in Düsseldorf - especially for the group under three years. Especially our researchers from abroad encounter a lot of problems to get such places for their children. Starting in summer 2017 with two so called "Belegplätze" (places reserved for the MPIE) we increased the number in 2018 to four due to the huge demand.

As some situations in life of our employees may be challenging, the Institute tries to meet the needs of these employees in regard of working time and place.

In spring 2018, Simone Degner was elected as Gender Equality Officer. As one of the first measures she plans a parent-child-room within the next year to improve the flexibility for our staff in difficult childcare-situations.

**Fig. 1:** *Since summer 2017, MPIE employees are able to access places at a private children daycare centre, a so-called KiTa.*

Since October 2018, Prof. Christina Scheu is our "MPIE Female Science Career Mentor". In her function she is supporting female senior postdoctoral researchers as well as young group leaders on their way to become a professor. She has long-standing expertise in coaching as she was already a mentor for female habilitation candidates at the Ludwig-Maximilians-University in Munich. Currently, she has six mentees, from which one got a research grant to establish her own group. Prior to the official start of the mentoring programme, Prof. Scheu was involved in coaching a female scientists who got promoted to a professor position abroad.

The Institute successfully nominated Dr. Olga Kasian for the "Sign Up! Career Building Programme For Excellent Female Post Docs in the Max Planck Society".

# Alumni Networking

*B. Kohlhaas*

The MPIE has a long tradition: in over 100 years, thousands of scientists have done research at our Institute, thus establishing the basis for their careers or using it as a milestone for promising scientific careers both in academic research and in industry.

**Fig. 1:** *The President of the MPG Prof. M. Stratmann, giving a speech at the Milestone Anniversary (Katja Velmans, MPIE GmbH).*

Over the years, a considerable number of employees have worked in various areas and departments and have contributed to the Institute's scientific success. In order to promote a lively exchange among the former Institute members, our Alumni Network was founded in 2003 with currently 1000 members.

The close contact to our alumni as well as to our active employees, is more than just a tradition for us. It is part of our Institute's philosophy and culture: a motor for synergy between research and practice.

**What does "Alumni Network" mean?**

An alumni network is an association of alumni, originally consisting of former university students.

Today, the term commonly refers to people who have spent a certain part of their lives at a company, school or university and have reached the next steps of their own further education. Trainees, students, active and former employees belong to the target group of alumni networks.

**Who are Alumni?**

Anybody who wants to stay in contact, even after his or her time at the Institute, can register as alumni. All former employees of the Institute - whether scientifically active or not - are alumni. This includes visiting scientists who were at least six months at the Institute, trainees, undergraduates, graduate students, fellows and postdocs as well as retired colleagues.

**What are the aims of the Alumni Network?**

The network cultivates contacts and shares experiences. A major intention is to establish a platform for discussions of common interests and problems, and for sharing both professional and personal experiences - across workspaces and generations, across national borders.

**Keep in Touch**

The alumni network helps not only to stay in contact with former colleagues, but also to forge new links with current Institute members, thus supporting an active and beneficial exchange for all.

The members of the alumni network are updated about news, events and actions of the MPIE by e-mail.

Special alumni meetings with scientific lectures and a full social programme allow members to meet colleagues, share experiences and forge ties that may lead to new collaborations.

**Fig. 2:** *Networking at the 100 years anniversary (Katja Velmans, MPIE GmbH).*

In addition, one can inform about Alumni News and easily join the Network online https://alumni.mpie.de.

**Alumni Meeting 2017 at the Milestone Anniversary**

In 2017, we looked back over a history of 100 years of the Max-Planck-Institut für Eisenforschung GmbH. This gave us the opportunity to invite all of MPIE's former colleagues to a festive event. **On 6th of October** we celebrated our **Milestone Anniversary** with an official ceremony followed by a buffet and a party! More than 500 guests attended the successful event, including alumni and current MPIE employees.

# The Institute in Public

*Y. Ahmed Salem*

Research Coordination Office

The MPIE's Public Relations (PR) are based on two main pillars: press relations and events. Some examples of the work between 2016-2018 are highlighted here.

**Press Relations**

The press relations of the MPIE consist of press releases, short news, articles and other printed and online publications, which are written or supervised by the PR Officer.

Throughout the years 2016-2018, the **press releases** issued new research projects with special funding, awards and important scientific publications. This way, our latest findings were illustrated to a broader public, revealing the importance and depth of our research. Press releases are send out to journalists, published on the MPIE website and in the idw, an online service offering latest news to a wider range of interested journalists and people from industry and academia.

Examples of press releases in the reporting time:

11 Oct 2016: Was Windkraftanlagen mit Bahnschienen gemeinsam haben (engl.: What wind turbines and railway tracks have in common) (Funding of the German Ministry for Education and Research to Dr. Michael Herbig)

1 Feb 2017: Gum metals pave the way for new applications (Publication in Nature Communications)

9 April 2018: Oxygen: A blessing and curse for nanostructured alloying (Publication in Nature Communications)

15 Aug 2018: Designing nanocrystals for more efficient optoelectronics (Publication in Nature Nanotechnology)

28 Nov 2018: How oxygen can enhance strength and ductility of high-entropy alloys (Publication in Nature)

**News** are scientific highlights that are presented on the website and are mainly about awards to our scientists or events taking place at or being organized by the MPIE. News appear more often and give an up to date insight on what is happening at the Institute.

Examples of news in the reporting time:

11 April 2016: Martin Friák wins Best Poster Award of the German Physical Society

10 Jul 2017: Enrico Pizzutilo at the 67th Lindau Nobel Laureate Meeting

20 Sep 2018: First Health Day at the Max-Planck-Institut für Eisenforschung

The **MPIE newsletter** appears twice a year. Since 2014, the newsletter focusses on one research topic per edition thus showing the interdepartmental collaboration and different approaches and aspects of one highlight. The topics are either chosen or suggested by the press officer and always contain participation of at least three departments. The newsletter is distributed to industrial partners, journalists and at events in and outside the MPIE. Between 2016 and 2018 the topics were: high entropy alloys, high temperature oxidation, grain boundaries, big data and intermetallics.

Each year all Max Planck Institutes contribute with one or two articles to the **Yearbook of the Max Planck Society**. Since 2017, the Max Planck Society asks the Institutes to hand in articles, which are generally understandable and deal with society's hot topics in order to reach the target group of politicians and decision makers. Thus, the MPIE's PR Officer got in charge of writing the article for the yearbook. The first article was about bone-like steels that prevent materials' fatigue. This article was based on a publication in the prestigeous journal "Science". The vice presidents of the Max Planck Society chose the MPIE's article to be printed in a special book that contains only 15 out of over 80 articles of the yearbook, and which is distributed to politicians showing the relevance of the research in the Max Planck Society.

**Events**

**Promotion of Young Scientists**

To encourage young people to enter research, the PR participates in and organizes various events for children, pupils and students. One example are the **kids' labs**, which started in the jubilee year of the Institute. The PR advertised the event via e-mail, newspaper, posters and on the MPIE's website and was overwhelmed by the positive feedback. In 2017, a kids' lab for five to eight years old children was


**Fig. 1:** *During the Girls' Day 2018 at the MPIE.*

organized giving them the chance to make small experiments on their own. In 2018, another kids' lab was organized during the Max Planck Day (see below). Three **pupils' universities** were organized and held by Dr. Stefan Zaefferer, group leader in the Department of Microstructure Physics and Alloy Design, two of them in 2017 as part of the 100 years jubilee programme and one in 2018 for a class of a primary school in Flingern, a region of Düsseldorf. The Institute also participates at the yearly nationwide **Girls' Days**, where girls have the chance to experience one day as an employee in a field where women are underrepresented. This day is mainly organized by the Research Coordinator (see p.77) and advertised by the PR Officer. Another activity to promote pupils are the **Science Days** of the nearby Theodor Fliedner grammar school. The school organizes yearly an event where companies and research institutes can present their work to the pupils in order to fascinate them for natural sciences. We participate in this programme since its upcoming in 2012 and the PR Officer chooses the doctoral students who present their work and trains them in giving a presentation to pupils. Students who participated in the reporting period were: 2016 - Waldemar Krieger and Julian Rechmann (Department of Interface Chemistry and Surface Engineering); 2017 – Michael Ackers (Department of Microstructure Physics and Alloy Design); 2018 – Caroline Fink (Department of Structure and Nano-Micromechanics of Materials). Groups of **students visit** the MPIE on a regular basis. Hereby the PR Officer organizes a day at the Institute, giving the students a chance to get an insight of the research and possibilities to do a masters or Ph.D. degree. Students and pupils are also welcome to do an **internship** at the MPIE. The internship applications either directly go to the scientists and are handled there, or they reach the Research Coordination Office and are distributed among the departments. Especially the pupils are often supervised by the trainers of the six apprenticeships.

### Events for the Broad Public

**KopfSalat** is an event series taking place twice a year at the MPIE and inviting speakers from all fields of research to give generally understandable talks to a broad public. It is organized by the PR and intends to foster the popularity of the Institute in and around Düsseldorf. Having started in 2014 with around 70 visitors, KopfSalat now has a huge fan community with about 180 visitors per talk. Since 2018 the KopfSalat takes place in the newly build event facilities of hall 9 allowing such a huge audience. The event is announced through the PR mailing list, which in 2018 contained about 300 subscribers, in the local newspaper, different online and social media sites and through post cards that are distributed in the neighbourhood of the Institute, at the Heinrich Heine University Düsseldorf, at the Adult Education Centre Düsseldorf and the town libraries. Besides external speakers, also MPIE scientists gave talks:

**Fig. 2:** *The kids' lab during the Max Planck Day at the MPIE.*

Dr. Christoph Kirchlechner on modern microscopy using synchrotron facilities (2016), Prof. Dierk Raabe on materials research from the very beginnings till now (2017), and Dr. Christoph Freysoldt on big Data and artificial intelligence in materials science (2018).

The **Max Planck Day** took place for the first time on 14 September 2018. The Max Planck Society celebrated Max Planck's 160 years anniversary, his receipt of the Nobel Prize 100 years ago and the Max Planck Society's 70 years jubilee as the successor of the Kaiser Wilhelm Society. The MPIE's PR Officer was part of the organization task force and developed with colleagues from other Max Planck Institutes and the headquarters of the Max Planck Society the concept of this day. It was decided to offer events at

the Max Planck Institutes as well as central events in Munich and Berlin. Two events took place at the MPIE: a kids' lab for children between five and eight years with numerous interactive experiments and a KopfSalat-talk by Dr. Christoph Freysoldt (see above). At the same time a team of MPIE-scientists went to the central event in Munich, a science marketplace, to present their research about additive manufacturing using the exponates created at the Communicate Science Competition for the 100 years celebration (see below), and to take part at a science


**Fig. 3:** *Armin Laschet, Prime Minister of North Rhine-Westphalia, during his speech at the ceremonial act on 6th October 2017. Copyright: Katja Velmans, Max-Planck-Institut für Eisenforschung GmbH*

slam where researchers from different Max Planck Institutes explained their work in brief and entertaining talks. The same science slammer who took part at this science slam, Aniruddha Dutta, doctoral student in the Department of Microstructure Physics and Alloy Design, won in November 2018 the German Science Slam Championship.

**Special Event: 100 Years Ceremony**

In 2017, the Institute celebrated its 100 years anniversary with different events and publications starting from January 2017 and ending with a scientific symposium and a ceremonial act with over 550 guests in October. The preparations started one year before by defining the target groups and how to reach them. The MPIE's first image film, presented during the 100 years ceremony, was produced and is since then available on the website and used at various Institute's presentations. Moreover, an image brochure was created that presents the MPIE's research, its history and overall philosophy. The historic text was researched and written by a special agency, and is now available both on the website and as a flyer, both in German and English. To involve the broad public more into the 100 years celebrations, the PR organized almost monthly events as two pupils' universities, one kids' lab and four KopfSalat talks (see above). A "Communicate Science Competition" amongst the MPIE staff was organized, where scientists and technicians participated to present their research through (interactive) exhibits. These exhibits were presented during the ceremonial act and are now used whenever our research should be explained to a broad public.

**Training and Consultant Service**

The PR Officer is engaged in the training of scientists concerning presentation skills and event organization. Hereby the PR Officer works in close collaboration with the Research Coordinator to train scientists for their interviews that are part of the application procedure to receive research funding. Moreover, the PR Officer attends rehearsals for talks which are supposed to be given to a broad public or to non-researchers. Additionally, help is given in the organization of scientific conferences and events in the Institute, like the TEM-APT opening in November 2018, where the PR Officer was member of the organizing team. This close connection between PR and research gives mutual benefit as the PR Officer gets a closer insight into current research topics and the MPIE scientists get information on how to organize events with up to 200 people and what is needed for advertisement and marketing.

## PART II.

# THE DEPARTMENTS

(in alphabetical order)

# Department of Computational Materials Design

*J. Neugebauer*

## Scientific Objective and Department Structure

The department of Computational Materials Design **develops, implements, and applies *ab initio* guided computational methodologies and toolsets that allow for an accurate prediction of properties of advanced structural and functional materials in realistic environments**. A challenge in overcoming materials limitations and designing such materials is that their technological relevant properties are typically directly related to a high complexity in chemistry, atomic geometry and microstructure. Over the last reporting period, the department has pushed the development of methods both with respect to accuracy and computational efficiency. These developments enabled *ab initio* guided atomistic approaches to handle a completely new level of complexity.

Examples are computational tools that allow us to predict materials properties up to the melting temperature for technologically highly attractive materials such as, e.g., ultra-high strength steels, light-weight alloys, high-entropy alloys, or magnetocaloric materials. This required the development of algorithms that allow us to compute the various entropic contributions - chemical, electronic, vibrational and magnetic. Several breakthroughs, often achieved through a joint effort of the scientific research groups of the department, allow us now to include non-adiabatic coupling contributions such as electron-phonon or magnon-phonon interactions. In contrast to common belief, these mechanisms turned out to be highly relevant and crucial to describe phenomena that were hitherto out of reach for fully parameter-free *ab initio* approaches.

The **group of Tilmann Hickel** used and extended these approaches to address a wide range of technologically relevant materials topics related to high-strength steels, light-weight and Heusler alloys, magnetocaloric materials, super-conductors, as well as to systematically identify processes and failure mechanisms such as hydrogen embrittlement. Based on this broad expertise he very successfully established a large number of joint co-operations and large-scale projects with partners from industry and academia. The **group of Blazej Grabowski** successfully extended the TILD (Thermodynamic Integration using Langevin Dynamics) family of efficient thermodynamic sampling approaches to describe not only solids but also melts. In the last three years, he furthermore developed a variety of coarsegraining techniques that allowed his group to describe systems, such as grain boundaries or

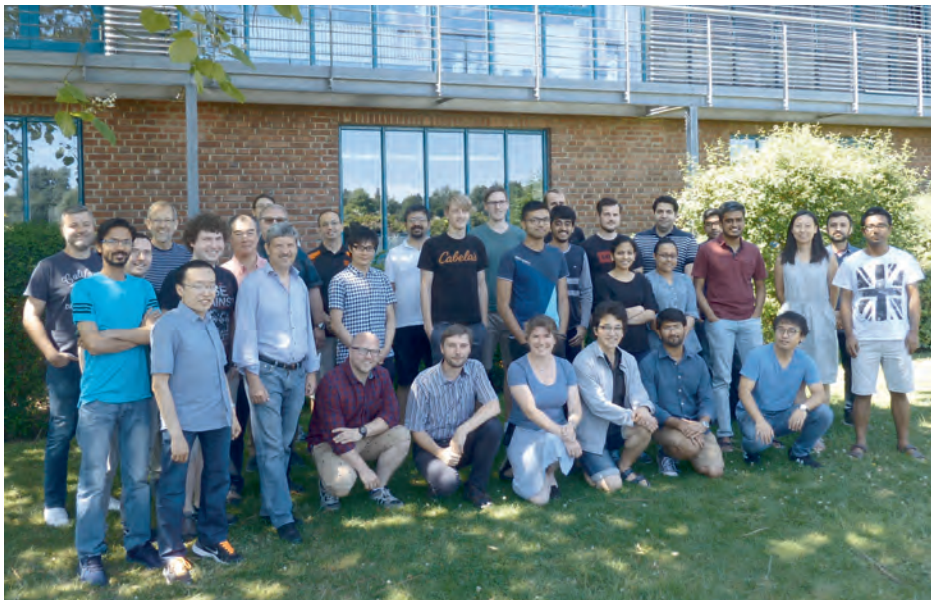

**Fig. 1:** *The CM department (2018).*

nano-composites consisting of millions of atoms, over large time scales. **Fritz Körmann** broadened his expertise in describing magnetic phenomena to the modelling of compositionally complex alloys in his newly (Summer 2017) founded group.

Methodological breakthroughs also opened new research opportunities in other fields: Transferring concepts from semiconductor physics to electrochemistry, the **group headed by Mira Todorova** developed an approach that allows a fully *ab initio* computation of reactions in an electrochemical cell. Using these new developments made it possible to address very fundamental questions, such as the impact of a solvent on the structure of oxide passivation layers or the fundamental mechanisms that control Mg corrosion.

Several methodological breakthroughs were also achieved in the **group of Christoph Freysoldt**. Important examples are new approaches to treat large electric fields and charges in systems with reduced dimensions or a highly efficient approach to perform atomic relaxations. The electrostatic tools provided, for example, new insight into the mechanisms controlling the resolution of atom probe tomography and an additional close link to the activities in the experimental departments. The **group of Liverios Lymperakis** achieved important methodological developments on thermodynamic and kinetic surface phase diagrams.

The **availability of our in-house developed computational methodologies and tools** provided a firm basis for highly successful collaborations with the other departments at the MPIE. These cover materials science topics such as understanding and designing, e.g., ultra-high strength steels or ductilization of Mg alloys, as well as providing new theoretical concepts such as machine learning techniques to enhance resolution and interpretation of experimental techniques (see p.53). These interdepartmental activities resulted in more than 50 joint publications over the last 6 years. They also strengthened existing and opened new collaborations with external partners, resulting in several projects funded, e.g., by the German Research Foundation (DFG), the Ministry for Science and Education (BMBF) or the EU.

This ability to address critical materials science questions by developing new methodological concepts and the respective computational tools enabled the department to publish in high-ranking journals in the Nature family, in Phys. Rev. Lett, etc. Since these highly accurate and computationally efficient approaches require highly complex simulation protocols, it was difficult to disseminate them within the department as well as to external partners. To address this issue the department developed over the last years *pyiron* [1,2] – a platform that provides an integrated development environment to implement and test these methodological tools. Pyiron provides the users with a single standardised interface to run these complex protocols and allows easy upscaling to high throughput studies. As a result, the time needed to become acquainted with the new tools is dramatically reduced, productivity is boosted and the exchange with external partners is simplified. The new pyiron platform also turned out to be instrumental in linking the various method developments by members of the department, opening the large amount of computed data to big data analytics and machine learning.

Pyiron is provided as open source to the scientific community. Other developments are provided as open source as well. Examples are a toolbox for automatically creating arbitrary coincidence site lattice (CSL) grain boundaries [3,4] developed by Sherry Hadian or the tools [5] created by Christoph Freysoldt to compute charged defects in low dimensional systems.

The high international visibility of these developments and studies **opened prestigious job opportunities for several members of the department**. For example, Martin Friák – a former group leader – became head of a joint experimental and theoretical group at the Czech Academy of Sciences in Brno. Robert Spatschek, head of a W2 group, became professor at the RWTH Aachen and head of a section at the Forschungszentrum Jülich. Blazej Grabowski, who is currently a group leader, received an offer for a W3-professorship position at the University of Stuttgart. Former PhD students or PostDocs – Sangheon Lee, Won-Seok Ko, Poulumi Dey and Anoop Kishore Vatti – obtained assistant professor positions in Korea, the Netherlands or India. Chris Race – a former Humboldt fellow – is now a Royal Society University Research Fellow and Senior Research Fellow at the University of Manchester.

To foster collaborations with leading experts worldwide, members of the department actively engaged in initiating and organizing international workshops and symposia. Examples are the workshop on grain boundary migration (S. Hadian), the continuation of the successful biennial workshop series Ab initio Description of Iron and Steel (ADIS; T. Hickel) and the international workshop series on electrochemistry (M. Todorova, C. Freysoldt). Furthermore, several symposia at international conferences such as the DPG (T. Hickel, J. Neugebauer), MRS (J. Neugebauer), TMS (T. Hickel), MMM (J. Neugebauer, T. Hickel) or MSE (S. Hadian) were organised (see p. 232).

The broad expertise in various aspects of materials modelling made the department also very attractive for international guests: During the reporting period the department hosted two Humboldt Fellows (R. Hadian, G. Leyson) and one Humboldt Research Award winner (M. Finnis). M. Ashton just received a Humboldt Fellowship. The high quality and visibility

**Fig. 2:** *The ADIS2018 workshop in Ringberg was one of several workshops organized by the CM department.*

of their research enabled members of the department to **receive highly competitive and prestigious research grants**. Blazej Grabowski received an ERC starting grant. Fritz Körmann successfully applied for a VIDI-Prize of the Dutch Science Foundation.

Due to the expertise of the department in developing tools for big data analytics and advanced data storage with focus on computational materials science, members of the department became highly active in national and international community activities related to digitalization in materials science. Jörg Neugebauer became, e.g., founder and chair of the expert committee "Digital transformation in materials engineering" of the Association of German Engineers (VDI). He was also elected as member of the DFG review board (Fachkollegiat) Materials science and chair of the German Physical Society (DPG) division "Metals and Materials".

In the following, a brief overview of the activities and research highlights of the groups in the department is given.

## Research Groups

**Computational Phase Studies (T. Hickel)**

The group "Computational Phase Studies" is devoted to the physics of (meta)stable thermodynamic phases in metals as well as transitions between them. Its major vision is an *ab initio* based prediction of thermodynamic bulk and defect phase diagrams, which are directly related to many technologically relevant properties and processes in metals. In this context, the group again made over the last three years substantial progress in developing methods and employing them for advanced material systems. This applies in particular to the following fields of research:

- The inclusion of new thermodynamic concepts to resolve, for example, the coupling of excitation processes, the lifetime of quasiparticles, or hitherto unclear features in experimental data.
- The prediction of phase stabilities near extended defects, such as grain boundaries, stacking faults and interfaces.
- The distribution of interstitials and solutes next to extended defects, including ordering, co-segregation and de-cohesion effects.
- The chemo-mechanical coupling during precipitate growth in structural materials, such as steels and Al alloys.
- The application of the developed thermodynamic methods to novel functional material systems (Fig. 3).

The research in the group is characterized more and more by **strong collaborations** with other groups, within the CM department, with other departments of the MPIE, as well as with academic and industrial partners in various research institutions. Out of more than 40 publications published by the group within the last three years, 95% resulted from such kind of collaborations, every second having a first author from a member of the group. Large scale net-working projects like those listed in pages 65 and 67 , but also a number of consortia consisting of 3-5 members were triggered by the multiple research interests of the group. The group was further active in co-organizing international meetings, like the above-mentioned series of ADIS workshops, as well as several symposia at conferences. This also helped the group to disseminate recent scientific achievements like the once discussed in the following:

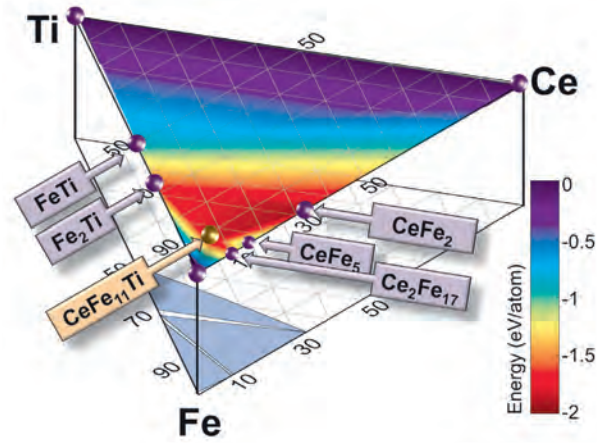


**Fig. 3:** *Ab initio calculated phase formation diagram for Ce-Fe-Ti alloys at 1500 K. Blue (red) color shows the energetically high (low) phases among the considered alloys.*

In the field of ***ab initio* thermodynamics** we were able to obtain several new insights. It was for example exciting to see that electron-phonon coupling is not only occurring at temperatures close to melting [6], but its explicit consideration is also required to understand experimental heat capacity data at temperatures below a few Kelvin [7] (A. Gupta). Similarly, the generalization of our methods for treating chemical disorder [8] (B. Dutta) and determining anharmonic lattice vibrations (A. Glensk) to phonon linewidths required intensive interactions with experimental colleagues. Only after unifying the physical concepts behind data evaluation, highly precise *ab initio* molecular dynamics has resulted into an amazing agreement with inelastic neutron scattering.

Recent efforts were spent on the interaction of magnetic excitations with lattice degrees of freedom. Close to the critical magnetic temperature, this interaction turned out to have a substantial impact on phonon linewidths [9]. Even the static relaxation of atomic positions next to a vacancy in paramagnetic iron was found to be highly non-trivial (see p. 197 ). Only the combination of the flexible IDE pyiron [2] (see above) to handle large sets of magnetic configurations, the recent implementation of constrained magnetic moments into our in-house DFT code SPHInX (see below) and the spin-space averaging approach developed in our group allowed us to handle this challenge (O. Hegde, O. Waseda). The success of this approach triggered its application to more complex materials such as Fe-based superconductors (F. Lochner).

The main purpose of these efforts remains to be the computation of phase stabilities and phase diagrams [10,11]. One of the promising strategies is to use our *ab initio* determined heat capacity as an input for Calphad assessments [12] (A. Zendegani). More interesting is, however, the consideration of Gibbs energies that are directly obtained by DFT. Our phase diagrams for magnetocaloric Heusler alloys computed in this way demonstrate that we can not only predict the chemical dependence of the martensitic transition temperature [13], but can also understand the origin of intramartensitic transitions between different twinned substructures (B. Dutta) [8,14]. To automatize such complex evaluations in the future, we develop algorithms that take the precision in the Gibbs energy as a convergence goal and automatically determine the convergence parameter to achieve it (J. Janßen).

The formation of **planar defects** such as twin boundaries and stacking faults [6,15] will give rise to structures, which are not part of bulk phase diagrams. We have identified such reconstructions, for example for twin boundaries in Mg [16], by mapping the gamma surface of all possible displacements of the neighbouring grains (Z. Pei, Fig. 4). Particularly fascinating, however, is the structure of defects in $Fe_2Nb$ Laves phases (see p. 173 ). Here, the formation of stacking faults is enhanced by the enrichment of Nb in the material. This phenomenon, analysed with high-resolution TEM in the SN department, could be explained thermodynamically (A. Zendegani), by generalizing bulk concepts of phase decomposition to defect structures.

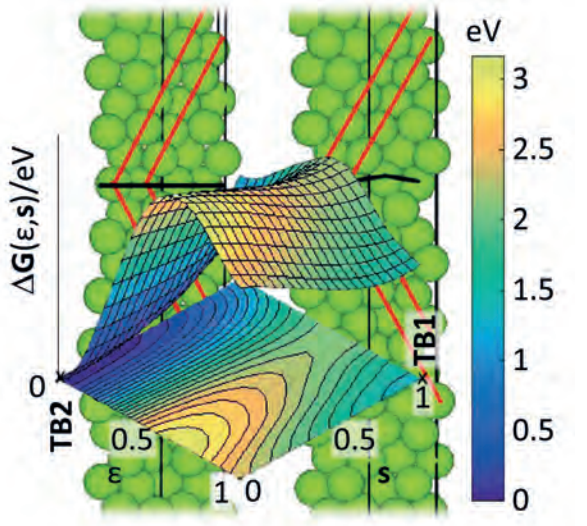


**Fig. 4:** *Gibbs energy gamma surface for {1011} compression twins in pure Mg [16].*

In this material, as in many other systems investigated within the group, the magnetic interactions add another level of complexity to the system. We often observe that structural stabilities depend on the magnetic state [17]. A careful analysis of this coupling in bulk materials gives occasionally the decisive clue for understanding also the reconstruction at the defects. In this way, we resolved for example a long-standing mystery about the thickness dependence of magnetism in Fe films grown on Cu(001) (X. Zhang) [18]. Nevertheless, the treatment of magnetism next to defects often requires its own methodological concepts, some of which we have developed for example

for the case of stacking faults in high-Mn steels (I. Bleskov) [19]. They are currently being generalized by machine learning techniques (O. Waseda). Altogether, the interplay of structure, chemistry and magnetism makes the thermo-dynamics of planar defects currently a comprehensive research topic of the group.

The **segregation of interstitials** next to planar defects is strongly linked to this topic. Interesting for steels is, for example, how C is redistributed if the phase boundary between austenite and martensite starts moving upon cooling. We realized that the path along which the structure transforms is decisive for the degree of Zener ordering in the virgin martensite (X. Zhang) [20].

Conversely, solutes such as H can have a decisive impact on the stability of planar defects in steels (see p. 177 ). We have extended our long-standing experience in investigating this detrimental effect (E. McEniry, S. Sreekala, A. Tehranchi) [21] by four major developments: (i) We have looked into co-segregation effects [22], including in particular the important competition between H and C [23]. (ii) We have performed tensile tests in order to study the decohesion and crack formation at a matrix-precipitate interface with and without H [24]. (iii) We have considered the impact of imperfections such as misfit dislocations in matrix-precipitate interfaces [25]. Finally, (iv) we have developed various coarse-grained and multiscale approaches to go beyond the scale accessible by *ab initio* calculations [26]. This spectrum of insights was beneficial for several industrial collaborations and further boosted our recognition in the community, e.g., by involving us in all major conferences in this field.

The **chemo-mechanical coupling** processes at the interface between precipitate and matrix have been further investigated (P. Dey) for kappa carbides $(Fe,Mn)_3AlC$, which form elaborate superstructures in high-Mn steels. We have explained the reduced C content observed experimentally with atom probe tomography in the MA department, to be mainly a result of the coherency strain in the carbide [27]. As we have shown, the C depletion has consequences for several other interesting phenomena, such as the change of anisotropy in the Young modulus and the resulting particle orientation in the superstructure [27], the formation of Mn antisites [28] as well as the reduction of the antiphase boundary energy and the resulting higher propensity for shearing by dislocations [29]. Interestingly, even the distribution of the C atoms that are consequently solved in the Fe matrix material is strongly influenced by the coherency strain, as resolved by a correlative APT-TEM-DFT study [30] (see p. 181).

To circumvent some of the challenges of steels, we used the prototype system of $Al_3Sc$ particles in Al alloys to study chemo-mechanical coupling during particle growth (A. Gupta). In combination with radio tracer diffusion experiments, we were able to proof that a solute atom approaching the growing precipitate will be influenced by the coherency strain and segregation effects of the latter (Fig. 5), reducing the effective diffusion rate of the solute [31]. This needs to be taken into account when performing kinetic simulations of TTT diagrams. Further, our multiscale simulations have shown that size-dependent concentration gradients in the matrix phase next to the precipitate can yield surprising phenomena like inverse ripening, where the smaller precipitates grow at the expense of the larger ones [32].

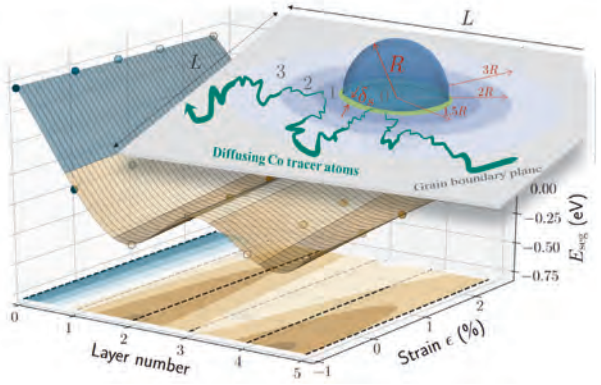


**Fig. 5:** *Schematic illustration of the employed diffusion model for Sc tracer particles (inset) together with the particle segregation energy surface in the misfit strain field of a $Al_3Sc$ nanoprecipitate [31].*

Many of the techniques and concepts discussed above have originally been developed for unary metals [33] or steels [34], but have been meanwhile transferred to a variety of further **functional materials** with high relevance for applications. For example, the incorporation of the interstitial element H into a crystal structure and the impact on its vibrational spectrum has been analysed for pentlandite ($Fe_{4.5}Ni_{4.5}S_8$) [35], which is a promising electro-catalyst for hydrogen evolution reactions (A. Zendegani). The interaction of structure and magnetism is important for magnetic shape-memory and magnetocaloric material systems [36]. Here, in particular magnetocrystalline anisotropies [37], concepts of disorder [38] and the impact of interfaces where martensitic transformations take place have been recently studied (B. Dutta, N. Shayanfar). One of the most recent developments is our (F. Lochner) application of these techniques to unconventional superconductors [39]. In particular, the methods developed for structural relaxations in a paramagnetic state have the potential to improve the performance of DFT for Fe-based superconductors substantially and to explain the nematic phase transitions observed there.

The various concepts of *ab initio* thermodynamics and in particular of treating magnetic excitations have been successfully applied to Ce-based hard magnetic materials (H. Sözen, Fig. 3). We were able

to show at which temperatures the promising hard-magnetic phase $CeFe_{11}Ti$ decomposes into pure Fe and the Laves phases $CeFe_2$ and $Fe_2Ti$, and how this detrimental effect can be influenced by changing the chemical composition. This example opens a new route of *ab initio* based materials design, which is currently extended to high-throughput and machine learning techniques.

**Adaptive Structural Materials (B. Grabowski)**

The general aim of the Adaptive Structural Materials (ASM) group is the design of advanced, next-generation structural materials based on innovative concepts driven by state-of-the-art simulation tools. To this end, the ASM group employs and further advances the methods developed in the CM department over the past years. The methods are rooted in accurate *ab initio* approaches and extend to large-scale molecular dynamics simulations based on empirical potentials and to analytical approaches based on continuum theory. The group has a strong collaborative network within the MPIE (e.g., Nano-/Micromechanics of Materials group in the SN department) and with external partners from academia (e.g., Imperial College London, KTH Stockholm, Linköping University, or Skoltech Moscow) and industry (Sandvik, Sweden). The projects investigated in the ASM group extend from simpler material systems, where the accuracy of the developed methods can be validated against experiment, to complex multiscale problems, where the focus is on understanding the atomistic mechanisms responsible for the experimental observations. The group activities are supported by the ERC Starting Grant TIME-BRIDGE (see p. 71 ).

A core effort of the ASM group is the development of efficient *ab initio* methods for a **highly accurate free energy determination at finite temperatures**. This work is carried out in close collaboration with the Complex Concentrated Alloys (CCA) and Computational Phase Studies (CPS) group. One example is the calculation of highly accurate stacking fault energies up to the melting temperature (X. Zhang) as required, e.g., for the design of Ni based superalloys for airplane turbines [6]. Another example is the thermodynamic description of dynamically unstable systems (Fig. 6; D. Korbmacher). In particular, we were recently able to develop a method that allows us to compute efficiently and accurately spectrally resolved quantities such as phonon frequencies (Fig. 9). Furthermore, a new method was developed for the accurate treatment of the coupling between vibrations and magnetic excitations [9] (I. Stockem, in collaboration with B. Alling from Linköping University). Further efforts have been directed to extend the methods to liquids (L. Zhu), which has enabled an accurate determination of melting properties from *ab initio* (TOR-TILD method; [49]). Recently, efforts have been undertaken to extend our methods also to kinetic properties, specifically temperature-dependent free energy barriers (L. Huber and R. Dsouza).

Many group activities have been focused on **large-scale simulations**. Within our SPP project on self-healing metals (SPP 1568), we have for example investigated the transformation behaviour of Ti-Ni shape-memory nanoparticles embedded in a Ni-Ti-V matrix [41] (S. Maisel). Our simulations allowed us to determine the transformation temperature as a function of particle size and matrix composition. This was crucial for our experimental colleagues (C. Tasan, MIT Boston), enabling them to optimize the microstructure. In another large scale simulation project we investigated the migration of general (twist and tilt component) grain boundaries [42] and [43] (S. Hadian). We could show that general grain boundaries relax into nano-facets and that their migration is determined by the nucleation and flow of steps (Fig. 7(a)). Based on a new detection method (Fig. 7(b)), we were able to break down the complex migration process into the elementary events (Fig. 7 (c)). Based on this we could set up a kinetic Monte Carlo simulation in order to access experimental time scales. Within this work, we also developed a software package that enables an easy to handle construction of general grain boundaries [44].

Several further method developments and investigations have been pursued in the group. We have developed a quantum mechanical/molecular

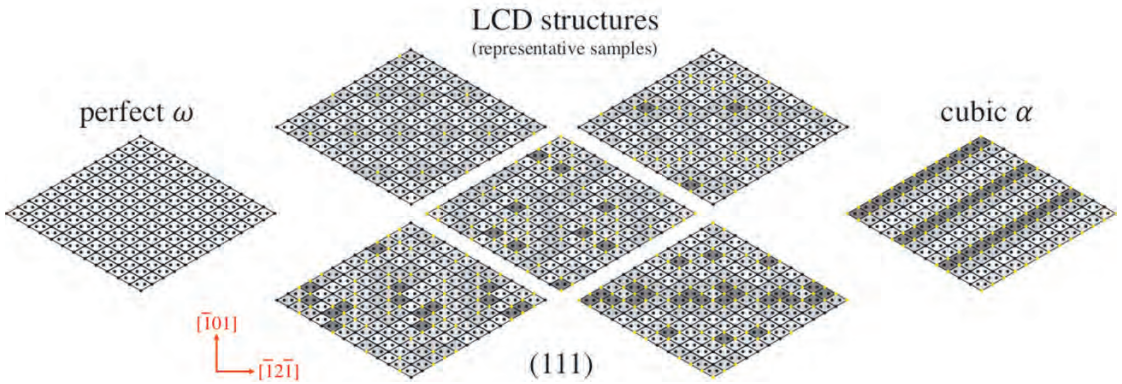


**Fig. 6:** *Representative examples of complex atomic structures discovered in Ti by finite temperature ab initio MD.*

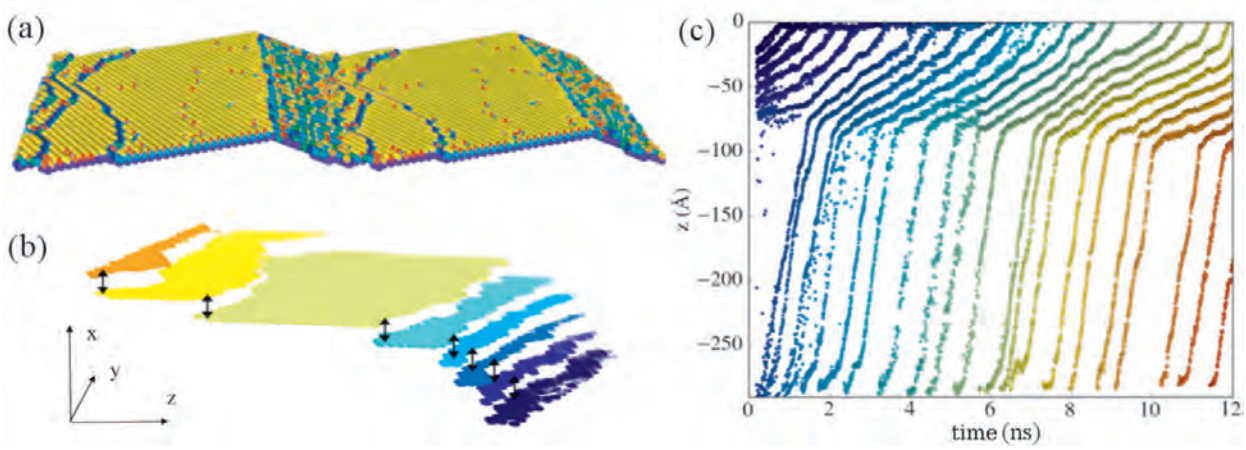


**Fig. 7:** *Molecular dynamics simulations of a general grain boundary (in the vicinity of a <111> Σ7 tilt boundary) in aluminum: (a) Snapshots of grain boundary atoms identified by an order parameter. (b) Representation of the grain boundary after applying the newly developed detection method. (c) Propagation of the steps as a function of time.*

mechanical (QM/MM) approach that is easily applicable to structures in which a defect (e.g., grain boundary) passes through the domain [45] (L. Huber). Moving towards larger scales, we also developed a molecular mechanical/finite element method (MM/FEM) coupling scheme (L. Huber; (see p. 71 )). In close collaboration with experimental colleagues (B. Gault MA department) we introduced a machine-learning based method to automatically detect atoms from field-ion microscopy data [46].

### Complex Concentrated Alloys (F. Körmann)

The key focus of the Complex Concentrated Alloys (CCA) project group is to develop the computational tools to satisfy the ongoing and increasing demands for the computational design and data-driven exploration of complex, multi-component alloys including the recent class of high entropy alloys (HEAs). To achieve this goal, the CCA group focuses in particular on advancing the approaches developed in the CM over the years towards complex multi-component alloys. The CCA group has a strong interdepartmental angle within the MPIE (e.g., via the SPP priority programme) and strongly collaborates with international groups (e.g., the Materials Science and Engineering Department, TU Delft, The Netherlands).

A main part of the simulation activities addresses the recently proposed class of HEAs, i.e. multicomponent solid solutions based on usually four to six main components (see p. 60). The large compositional space spanned by such alloys cannot be captured by experiments alone and *ab initio* techniques have emerged as a powerful complementary approach [47].

A crucial materials property is the mechanical performance. Recently most works on HEAs were based on investigations focusing on single phase solid solutions. In 2016 an alternative approach [48] was proposed based on experimental findings for a dual-phase (DP) HEA consisting of fcc and hcp phases. The $Co_{10}Cr_{10}Fe_{50}Mn_{30}$ alloy revealed a TRIP effect, as well as enhanced mechanical properties. The key ingredient to design such novel DP multicomponent alloys is to determine the fcc-hcp stability via tuning the alloy composition. This has been achieved in [44] by *ab initio* simulations in combination with thermodynamic concepts. $Co_{20}Cr_{20}Fe_{40-x}Mn_{20}Ni_x$ alloys with x=0-20 at.% were investigated. A critical value of ~6 at.% Ni was identified as a potential TRIP alloy and subsequent experiments validated the predictions. In the SPP 2006 (see p. 60) this direction is currently being extended towards the impact of interstitial impurities such as C or N, which promise enhanced interstitial solid solution strengthening but also impact the fcc-hcp stability and stacking fault energies. Further, the impact of local chemical fluctuations on stacking fault energies is investigated. A recent study combining the supercell approach with the coherent potential approximation revealed a strong impact of such fluctuations on the stacking fault energy. For prototype fcc CrCoNi and FeCoNiCrMn, compositional changes close to the stacking fault can induce variations of up to 100mJ/m$^2$, also suggesting a considerable driving force for chemical segregation, e.g., Mn segregation towards the fault plane or Ni depletion near the stacking fault [49].

Since a large class of HEAs and CCAs are magnetic, knowledge about the magnetic ordering in these alloys is crucial. Established approaches based on direct computations of magnetic interaction parameters and subsequent Monte Carlo simulations are computationally demanding and therefore only applicable to a limited set of alloys. The group has therefore developed an analytic mean field based approach utilising the coherent potential approximation and the disordered local moment model to predict magnetic Curie temperatures in a very efficient way [50]. This enabled high-throughput calculations for thousands of alloys and revealed the possibility to tune Curie temperatures by adjusting the composition.

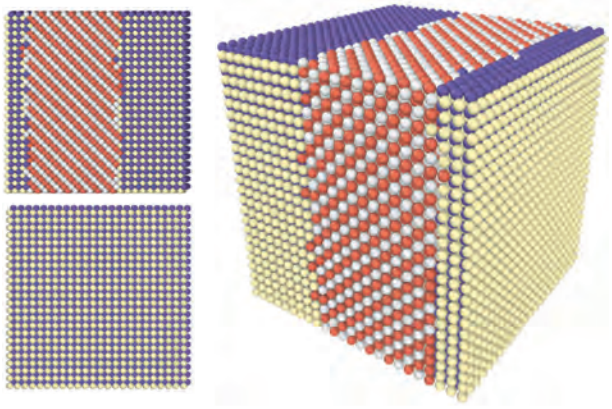

**Fig. 8:** *Predicted ground state of the bcc NbMoTaW HEA consisting of a B2(Mo;Ta) (blue and yellow) and a B32(Nb;W) (red and silver) decomposition [51].*

The chemical ordering is another critical ingredient for the design of CCAs. By compositional tuning based on *ab initio* calculations in collaboration with the ASM group, a new type of hcp Al-Hf-Sc-Ti-Zr HEA with an ordered superstructure was designed. This was achieved by tuning the Al concentration towards a $D0_{19}$ ordering on the hexagonal lattice. In general, however, the competing ordered configurations to be considered are not known in advance. At the same time, the established techniques such as cluster expansion quickly approach their limits for multicomponent alloys and require rather crude approximations such as, e.g., the limitation of nearest-neighbour pair interactions. By applying a perturbational approach based on the coherent potential approximation to extract pair interactions for a prototype bcc NbMoTaW HEA (see also Fig. 8) it was shown that the chemical interactions can be very long-ranged and can cause chemically frustrated configurations in the system, eventually stabilizing the solid solution [51]. Later supercell based calculations also revealed that local lattice distortions can further contribute to a stabilization of the alloy [52]. Lattice distortions are one of the so-called core effects of HEAs and were also shown to be significant in other, fcc-based HEAs such as FeCoNiCrMn [53]. The group currently works on extending these concepts by combining explicit supercell calculations with new generation of machine-learning potentials, which are capable of treating multicomponent alloys very efficiently, including the impact of lattice distortions and thermal vibrations.

For simulating lattice vibrations, a number of new tools were developed. In a recent study, *ab initio* calculations for twelve different refractory alloys were performed in combination with the band-unfolding technique to address the question in how far the inherent chemical complexity impacts phonons. The results revealed that both, the atomic mass as well as the force constants significantly contribute to the actual phonon energies and broadening of the

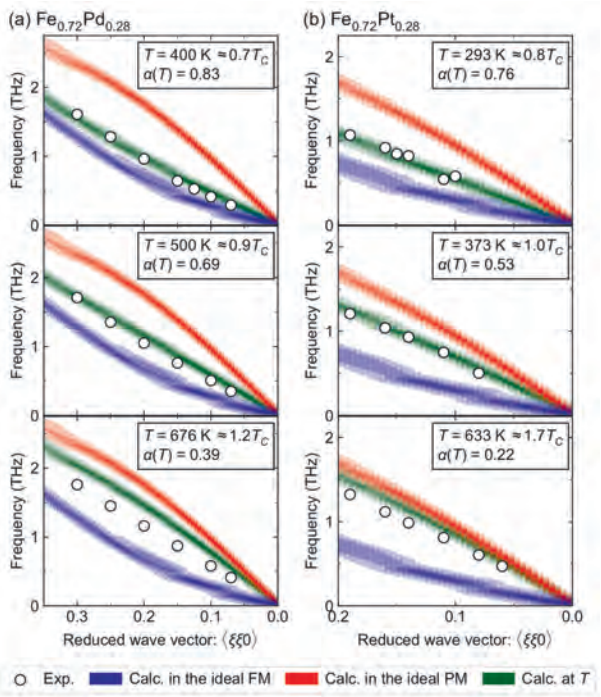


**Fig. 9:** *Temperature dependence of the phonon spectra along <110> direction for (a) $Fe_{72}Pd_{28}$ and (b) $Fe_{72}Pt_{28}$ Invar alloys. Blue and red lines are computed in the fully ordered and disordered magnetic state. The newly developed scheme also allows to compute intermediate temperatures (green lines). The magnetic fluctuations harden the phonon branches, which counteracts the usual thermal expansion and contributes to the Invar effect [55].*

spectral densities. This will enable future research to computationally design the phonon broadening for, e.g., thermoelectric applications, and opens the avenue towards tailored high temperature high entropy alloys.

As many high entropy alloys are magnetic, local magnetic fluctuations can affect other entropic contributions such as vibrations. Here, the group works on advancing the required simulation tools. A major advancement was the extension of the spin-space averaging (SSA) method [54] to magnetic random solid solutions [55]. In [49] a new scheme combining Quantum Monte Carlo simulations, SSA and band-unfolding approach was proposed. The approach was applied to the challenging magnetic Fe-based Invar alloys, for which the cause of their unusual low thermal expansion properties is, after half a century of research, still not fully understood. Based on the new computational scheme it was shown, that magnetic fluctuations strongly contribute to specific phonon branches (see Fig. 9) and thus contribute to the Invar effect [55]. The results reveal the strong interplay of atomic and magnetic fluctuations, which will be a critical factor in further exploring the physics of other complex alloys such as HEAs. An extension towards the inclusion of dynamic spin-lattice effects are currently being explored in collaboration with the

ASM and the CPS groups within the CM department. Application to a prototype CrN alloy revealed [9] a strong impact on phonon, as well as magnon, lifetimes. Currently the extension of such techniques towards more complex alloys is being explored in collaboration with A. Shapeev (Skoltech/ Moscow) by extending recently developed machine-learning potentials towards magnetic systems.

**Electrochemistry and Corrosion (M. Todorova)**

The Electrochemistry and Corrosion group aims at understanding how **interactions with the environment influence and modify materials and their properties**. With a strong focus on corrosion and, more generally, electrochemical processes the group is continuously extending existing methods, as well as, developing new methods to gain an in-depth atomistic understanding of the physical and chemical processes taking place at surfaces and (solid/ liquid) interfaces. To this end, the group also closely collaborates with different groups at the MPIE, in particular the "Defect Chemistry and Spectroscopy" group (CM) and the "Atomistic Modelling" group (GO).

The employed methodologies are firmly based on *ab initio* calculations. These calculations are often combined with thermodynamic approaches and/ or statistical mechanics enabling their extension to the macroscopic scale. The ensuing ability to compare computational findings with experimental observations is often invaluable, as exemplified for the following case of ZnO surfaces in aqueous environment. While it is generally accepted that knowledge about surface structures forming at solid surfaces immersed in an electrolyte is important to understand processes occurring in electro-chemical environment, little is known about the role the solvent plays towards their formation and stabilisation. The work of S. Yoo addressed this question, building on a methodological framework developed in the group [56,57]. Using two types of density functional theory (DFT) calculations, S. Yoo constructed *ab initio* derived surface Pourbaix diagrams, i.e. diagrams depicting regions of stability of surface reconstructions as a function of applied bias *U* and pH-value of the solution. In one case, the aqueous environment was neglected in the DFT calculations, except for water constituents (O, OH and H) specifically adsorbed on the surface. In this case, the impact of the aqueous environment is accounted for only implicitly by the thermodynamic model used to construct the surface Pourbaix diagram (Fig. 10, left). In a second set of calculations, the aqueous environment was explicitly included in the DFT calculations for the same set of surface structures. The effect of the aqueous environment is therefore explicitly accounted for in the resulting surface Pourbaix diagram (Fig. 10, middle). Comparison to experiments by M. Valtiner (GO) revealed that only the diagram constructed from DFT calculations with the explicitly included aqueous environment reproduces the experimental observations. The ensuing careful analysis of the electronic structure calculations revealed that solvation effects are highly selective. They revealed that due to the high propensity of metallic surfaces for screening unfavourable electrostatic interactions, solvation has little effect on surfaces with metallic character. In contrast, surfaces with semiconducting character, in particular those hampered by a high electrostatic

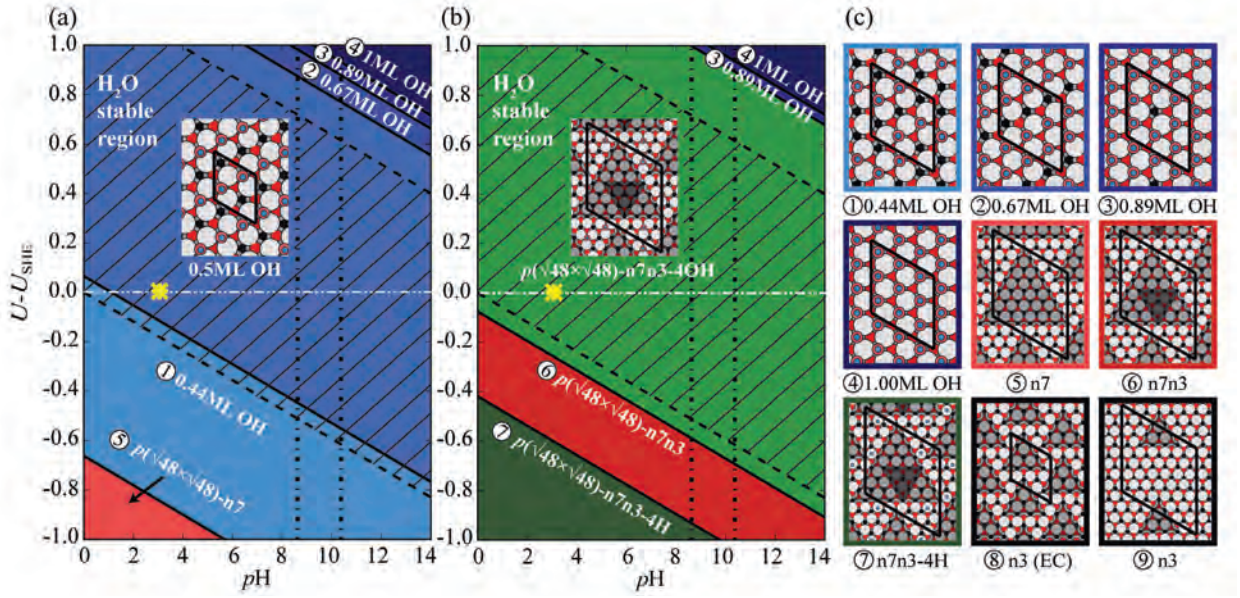


**Fig. 10:** *Surface Pourbaix diagram for the ZnO(0001) surface constructed using DFT calculations in which the aqueous environment (left) is not explicitly included and (middle) explicitly included in the calculations. The various surface reconstructions appearing in the phase diagram are shown as insets or to the right. The conditions at which a triangular surface reconstruction is observed experimentally are marked by a yellow star.*

penalty in vacuum, experience a strong stabilisation by the solvent and a high gain in solvation energy. This work was highlighted as an "Editors' suggestion" in Physical Review Letters [58].

Staying with the topic of stability of solid surface in contact with a liquid, the work of A. K. Vatti addressed the questions how ions other than $H^+$ or $OH^-$ affect the stability of surface reconstructions. Looking at clean and solvated Muscovite Mica (0001) surfaces, he was able to connect the surface stability to relevant $K^+$ ion concentrations, as well as explain the experimental observation of mica surfaces swelling in contact with water but not when immersed in ionic liquid [59].

A significant breakthrough in the modelling of electrochemical surfaces under realistic conditions is **the development of an "*ab initio* potentiostat"**, which enables *ab initio* calculations at solid/liquid interfaces under applied bias (S. Surendralal). Details about the method and the new insights it provided into the anomalous hydrogen evolution at anodically polarised magnesium surface in aqueous environment [60] are discussed on p. 199 .

Corroding surfaces may become amorphous. To address the question what are characteristic features of an **amorphous surface** and how do we build up representative models accessible to electronic structure calculations, which enable meaningful conclusions, M. Tautschnig recently ventured into the area of amorphous solids. Further activities in the group aim at understanding other fundamental properties of investigated materials, which affect their behaviour in solution or the correct way to model them. Examples are the (internal) polarisation of compound semiconductors (e.g. ZnO) or the energy level alignment (i.e. the relative position of energy levels with respect to each other), which become crucial in the context of surface reconstructions or reactions occurring at the interface.

To facilitate discussions with colleagues and aid these developments, the group is also active in co-organising international meetings, like the "High electric fields in electrochemistry and in atom probe tomography" workshop in March 2017.

### Defect Chemistry and Spectroscopy (C. Freysoldt)

The group "Defect Chemistry and Spectroscopy" focuses on **atomic-scale defects in non-metallic materials such as oxides, electrolytes, or semiconductors** by means of *ab initio* methods, and develops state-of-the-art methods and concepts for this purpose.

Point defects exert a critical influence on the electrical, chemical, transport, and other properties of real semiconducting and insulating materials. Computer simulations are a powerful tool to better understand the formation of point defects, their properties, and their role in modifying macroscopic material parameters [61]. Interestingly, the methodological developments of the past years have opened opportunities for new applications, notably in the area of **electrified-surface simulations**. Electrified surfaces carry a finite charge and are therefore associated with macroscopic electric fields. Understanding the location of the charge at the atomic scale and the impact of the fields on the energy landscape, geometry, and electronic structure of the surface is of great interest not only in electronic devices - that originally motivated the methodological efforts, - but also for electrochemistry (see p. 47 ), atom probe tomography (APT) and field ion microscopy (FIM). This gives **unique opportunities to generate novel theoretical insights into APT and FIM experiments** carried out in the MA department (B. Gault), and to improve their evaluation and interpretation.

The development of the multi-scale programme package SPHInX [5,62] is a continuous activity of the group. In addition to further improvements of the parallelization efficiency, recent in-house developments cover a novel geometry optimization scheme [63], Hubbard-U corrections for molecular orbitals [64], and a generalized dipole correction to account for surface calculations with large fields. An important aspect is making use of SPHInX in the pyiron framework and other simulation tools. For this, a pipe-based interface and a communication protocol was developed to control the program flow by external tools. For instance, the unique spin-constraint capabilities (M. Grabowski) of SPHInX have been used to rapidly devise spin-space algorithms in the Computational Phase Studies (T. Hickel) group, without the need to train scientists in DFT code development. Reversely, based on the same protocol, the new **powerful SPHInX geometry optimizer** [63] is made available to other programs. Both workflows have been successfully integrated into the pyiron framework. Extending the protocol to further features will accelerate the rapid prototyping of complex simulation protocols across traditional code boundaries beyond the current paradigm of generating input files and restarting the DFT code for each step.

The role of electrostatics for atomic-scale simulations at surfaces is of high interest for us. Surfaces are typically modelled in the repeated slab approach: the bulk material below the surface of interest is truncated, and – in order to take advantage of the highly efficient computer codes available for bulk crystalline materials – periodic boundary conditions are applied (with a certain amount of vacuum between the slabs). However, surface charges modify the macroscopic field along the surface normal, and hence are incompatible with periodic boundary conditions. Therefore, all such calculations contain implicit or explicit compensation charges, leading to artefacts in the field distribution and the energy. Much care is required to transfer raw simulation results to experimentally relevant situations. One approach is to produce more

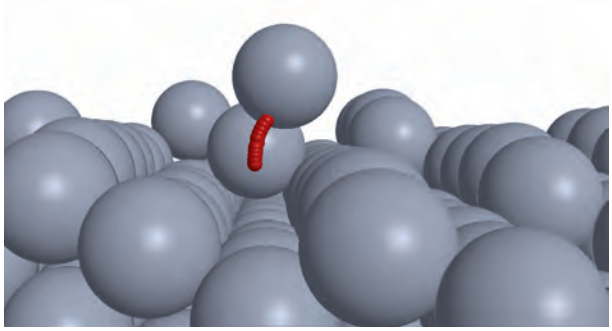

**Fig. 11:** *Field evaporation from a kinked Al surface: the trajectory (small red spheres) of the evaporating atom shows roll-over instead of a straight path due to bonding to neighbour atoms.*

realistic field distribution. For uncharged slabs with a permanent dipole, this is common practice: the "dipole correction" adjusts the potential in the vacuum to account for the vacuum potential shift induced by the slab's dipole, and avoid an artificial compensating field. For charged slabs, we generalized the dipole correction to adjust the field and the potential.

This new scheme enables us to address the **details of field evaporation and field-ion microscopy** by means of DFT calculations (A. Mishra, M. Ashton). This is driven by a collaboration with the experimental APT group (B. Gault) at the MPIE, and embedded in the BigMax network (see p. 53 ). DFT calculations for the elementary evaporation process yield not only element- and site-specific critical fields and barriers, but also show the source of trajectory aberrations by the roll-over effect, see Fig. 11. They also serve as input for meso-scale simulations of tip evolution (M. Ashton), which are required to develop and gauge improved reconstruction algorithms for APT.

In contrast to high-field applications, charges at semiconductor and insulator surfaces typically localize at surface defects at much lower densities than what can be feasibly simulated. In this case, correcting for the artificially high fields is the better choice. Along the lines of the Freysoldt-Neugebauer-van-de-Walle scheme for bulk defects, we had developed a preliminary correction scheme already in the previous reporting period. In this period, the scheme was further improved to also yield the field-dependence of formation energies and has now been finalized, published [65], and made available to the scientific community [5]. Ongoing work focuses on application of the scheme to **defects in 2D materials** in collaboration with R. Hennig (University of Florida, USA).

The modelling of disorder is another interest. Within a collaboration with the Max-Planck institutes for Solid State Research (Stuttgart) and for Chemical Physics of Solids (Dresden), we studied charge ordering in potassium sesquioxide ($K_4O_6$). This compound had evaded synthesis attempts for decades, but was recently realized by our experimental collaborators from a surprising disordered precursor that forms in equilibrium at elevated temperatures. The modelling of sesquioxides is challenging due to the presence of π-electron correlations between $O_2$ building blocks and the associated structural relaxation, giving rise to dynamic polaron hopping between distinguishable -2 and -1 molecular charge states. The DFT predictions using the newly developed Hubbard-U corrections for molecular orbitals, which are essential to include π-electron correlations in an efficient way, show excellent agreement with experimental results. The compound's thermodynamic stability was found to originate from polaron entropy as a novel stabilization mechanism, which may open a new understanding of mixed-valence compounds that exist, for instance, also in corrosion layers [64].

Disorder exists also in CuCr bcc alloys produced by molecular beam epitaxy. Cu does not usually exist in the bcc phase, but may precipitate from bcc alloys in the form of nanoparticles which are difficult to analyse. It is therefore of high interest to understand spectroscopic signatures from larger samples. In collaboration with C. Liebscher (SN), we simulated the electron-energy loss spectra (EELS) of Cu-Cr bcc alloys [66]. According to the calculations, random alloys show a clear composition-dependent feature in the Cu $L_{23}$ edge. Experiments for Cu-rich alloy (67%) showed the feature not at the expected position for the average composition, but at much higher Cu content. This is indicative of demixing at the nanoscale, in agreement with strong composition fluctuations detected by STEM.

### Growth Modelling (L. Lymperakis)

The growth modelling project group investigates the **epitaxial growth and the properties of compound semiconductors and nanostructures**. The research interests of the group focus on the thermodynamics and kinetics of epitaxial growth, the electronic properties and energetics of surfaces and interfaces as well as the growth and the properties of semiconductor nanostructures. Within the reporting period L. Lymperakis was and is involved in one EU and BMBF co-funded project (PowerBase) and in one DAAD (Deutscher Akademischer Austauschdienst) funded project **(Superlattices of ultrathin InGaN/GaN quantum wells for advanced optoelectronics and topological insulator applications, ULTIMAT)**.

Topics that were and are addressed by the growth modelling group include, but are not limited to:

III-Nitride alloys such as InN, GaN, and AlN dominate the optoelectronics industry with applications in light emitting devices (LED), laser diodes (LD), and power electronics. The growth, as well as the bulk and surface thermodynamics of InGaN alloys were investigated in collaboration with the Defect Chemistry and Spectroscopy group (C. Freysoldt) and the Institute for Crystal Growth in Berlin (M.

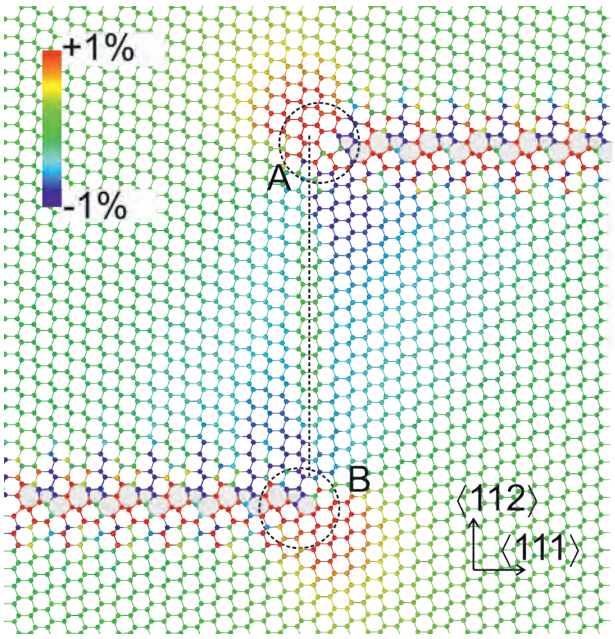


**Fig. 12:** *Local atomic strain at a Σ3{111} twin segment in Si (dashed line) embedded between two asymmetric Σ3{112} facets. The dashed circles denoted as A and B indicate the two junction cores. Blue and red regions denote compressive and tensile strain, respectively [72].*

Albrecht). An exhaustive ground-state search using DFT calculations was employed to set up a Cluster-Expansion (CE) Hamiltonian, which was used to perform canonical and grand canonical Monte Carlo simulations. The derived phase diagram of bulk InGaN alloys biaxially strained to GaN exhibits a rich set of hitherto unknown chemically ordered phases at various stoichiometries, in contrast to the wide-held belief that these alloys can be described by a simple regular solution model with a large miscibility gap.

A possible route to overcome key challenges related to high quality and high In content InGaN alloys is to employ **surface engineering**, i.e. to employ surface structures with compositions higher than the bulk solubility limit which are kinetically stable and do not change their composition when overgrown. We addressed this concept by combining *ab initio* simulations with advanced experimental characterization techniques (molecular beam epitaxy, MBE, high resolution transmission electron microscopy, HRTEM, and reflection high-energy electron diffraction, RHEED) to investigate the growth of single monolayer InGaN/GaN superlattices (SL). Specifically, we showed that the growth of the optically active InGaN films is self-limited with respect to thickness and chemical composition. Our calculations reveal that the **origin of the self-limitation is a novel surface stabilization mechanism**, elastically frustrated rehybridization [67]. In contrast to present understanding of surface stabilization mechanisms based on bond strength optimization, this mechanism prevents In atoms from occupying low-coordinated surface sites. The surface energetics indicate that this mechanism imposes strict upper limits in the order of 25% on the maximum In content that can be achieved at the surfaces. The new insight allows to surface-engineer growth to achieve alloys with contents that exceed the bulk solubility limits. Indeed, in a recent study we showed that surface rehybridization provides promising routes to grow B containing ternary nitride alloys with B contents exceeding the bulk solubility limits by almost one order of magnitude [68].

A common impurity, which is intentionally or unintentionally present during growth of III-Nitride surfaces, is hydrogen. The electronic and vibrational properties, the thermodynamics and kinetics of molecular and atomic hydrogen adsorption/desorption at/from non-polar GaN surfaces were investigated in a synergetic study with the Technical University of Ilmenau using DFT calculations and ultraviolet (UPS), X-ray (XPS) photoelectron and electron energy loss (EELS) spectroscopy experiments. Our results revealed that chemisorption in a gas exposure experiment is strongly dependent on the experimental conditions as well as on the energetics and kinetics of the dissociation/ adsorption reactions at the surface. In a series of ***ab initio* designed and driven experiments** we could confirm that hydrogen desorption requires elevated temperatures and is predominantly taking place as hydrogen molecules are desorbing from surface dimers [69].

Other topics related to the growth and properties of III-Nitride surfaces and nanostructures that have been addressed in the reporting period include the investigation of the electronic properties of non-polar AlInN(10$\underline{1}$0) surfaces [70] in collaboration with cross sectional scanning tunneling spectroscopy (Peter Grünberg Institut at Forschungszentrum Jülich), the selective-area growth of GaN nanowires on masked substrates (in collaboration with MBE experiments, Department of Physics, University of Crete, Greece) [71], as well as the energetics and electronic properties of fluorination of clean and oxidized GaN surfaces in collaboration with Infineon Technologies Austria AG. Fluorine adsorption and incorporation is employed to investigate and understand the electronic properties of the dielectric-barrier interface of metal-insulator-semiconductor high electron mobility transistor (MIS-HEMTs). The calculations revealed a strong tendency of fluorine to passivate cation dangling bonds even under extreme fluorine-poor conditions. Moreover, fluorine passivation induces considerable changes to the electronic properties of the surfaces/interfaces: Passivation of surfaces with oxide stoichiometry removes states from the gap. Nevertheless, passivation of surfaces that obey the electron counting rule shifts the surface states deeper into the gap.

The energetics as well as atomistic mechanisms underlying the **segregation of impurities at Si grain boundaries (GB) and GB junctions** were investigated in collaboration with the MA and SN departments

in a PhD project (M. Alam). Here, we employed DFT calculations to parametrize Si, C and Si-C modified embedded atom method (MEAM) interatomic potentials. Careful benchmarks showed that these potentials provide an accurate description of the atomic geometry, strain, and energetics of intrinsic Si GBs as well as of the C segregation at the aforementioned interfaces. Based on this new potential, we identified the preferential carbon segregation at faceted GBs at the experimentally relevant length scale. Using this insight, we were able to interpret the experimental findings showing an asymmetric line segregation of impurities along one particular type of facet junction core, instead of a homogeneous decoration of the facet planes. More specific, we showed that this **asymmetric segregation pattern** is a consequence of the interplay between the atomic arrangements at the core structure of the facet junction and the corresponding local strain state [72].

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# Research Projects in Progress

### Collaborative projects involving several groups

*Janßen, Surendralal, Huber, Waseda, Hickel, Grabowski, Todorova, Feysoldt, Neugebauer (in collaboration with Y. Lysogorski* and R. Drautz*, *ICAMS): Development of the pyiron platform*

*Zhang, Grabowski, Hickel, Körmann, Neugebauer (in collaboration with Y. Gong* and R. Reed*, *University of Oxford, UK): Temperature dependent stacking-fault-energies in Al, Cu, and Ni from ab initio*

*Stockem, Grabowski, Hickel, Körmann, Neugebauer (in collaboration with B. Alling*, *Linköping University, Sweden): Coupling of spin fluctuations and lattice vibrations*

*Grabowski, Hickel, Neugebauer (in collaboration with A. Glensk*, P. Neibecker** and M. Leitner** (*EPFL, Switzerland, **Technical University München)): Accurate determination of phonon linewidths*

*Grabowski, Körmann, Zhang (in collaboration with L. Rogal*, *Polish Academy of Sciences Krakow, Poland): Development of hcp based high entropy alloys*

*Ishibashi, Grabowski, Körmann: Thermo-dynamics of metastable Ti fcc*

*Grabowski, Freysoldt, Ikeda, Körmann (in collaboration with A. Shapeev*, A. Duff** (* Skolkovo Institute of Science and Technology, Russia, **Daresbury Laboratory, UK): Machine-learning potentials for computing anharmonic free energies of VMoNbTaW high entropy alloys*

*Ikeda, Grabowski, Körmann, Neugebauer (in collaboration with S. Ishibashi*, *AIST, Japan): Concept of atomic pressure and lattice distortions to characterize mechanical performance of bcc refractory high entropy alloys*

*Körmann, Hickel, Neugebauer (in collaboration with N. Wang*, T. Hammerschmidt*, R. Drautz*, *ICAMS, Bochum): Ab initio simulation of magnetic contributions to the thermodynamics of metals*

*Zendegani, Körmann, Hickel (in collaboration with A. Ladines*, T. Hammerschmidt*, R. Drautz*, *ICAMS, Bochum): Ab initio based calculation of the stability of selected TCP precipitates in steels: Temperature and interface effects*

### Adaptive Structural Materials (B. Grabowski)

*Korbmacher, Grabowski, Neugebauer: Highly accurate description of temperature driven phase transitions in Ti-alloys*

*Zhu, Grabowski, Neugebauer: Ab initio description of free energies of liquids*

*Hadian, Grabowski, Neugebauer: Molecular dynamics simulations of grain boundary migration*

*Hadian, Grabowski, Neugebauer: Development of a coincident site lattice software package for easy grain boundary creation*

*Huber, Grabowski, Neugebauer: Molecular mechanics/finite element method coupling*

*Zhang, Grabowski (in collaboration with S. Divinski*, *University Münster): Diffusion in high entropy alloys*

*Huber, Dsouza, Grabowski: Temperature dependent free energy barriers*

*Grabowski (in collaboration with A. Forslund* and A. Ruban*, *KTH Stockholm, Sweden): Anharmonic free energy calculations in TiN*

*Grabowski (in collaboration with F. Mouhib*, J. Guenole*, S. Korte-Kerzel*, *RWTH Aachen): Synchro-shear mechanism in Laves phases*

### Complex Concentrated Alloys (F. Körmann)

*Ikeda, Körmann, Neugebauer (in collaboration with X. Wu*, Z. Li*, D. Raabe*, *MA Department): Impact of interstitial alloying on stacking fault energies in FeCoNiMnCr high entropy alloys*

*Ikeda, Körmann, Neugebauer (in collaboration with S. Sohn*, D. Raabe* and S. Ishibashi** (*MA Department, **AIST, Japan)): Relation of local lattice distortions and atomic pressure on strength of VCoNi alloys*

*Körmann, Neugebauer (in collaboration with B. Dutta* and A. Shapeev** (*TU Delft, The Netherlands, **Skolkovo Institute of Science and Technology, Russia)): Development and application of machine learning potentials for magnetic systems*

*Körmann (in collaboration with B. Dutta*, *TU Delft, The Netherlands): Exploring $(Mn,Fe)_2(P,Si)$ magnetocaloric materials with ab initio*

*Körmann (in collaboration with Z. Rao*, Z. Li*, D. Raabe* and B. Dutta** (*MA Department, **TU Delft, The Netherlands)): Tuning magnetic properties and Curie temperatures in high entropy alloys*

*Körmann, Neugebauer (in collaboration with A. Shapeev*, *Skolkovo Institute of Science and Technology, Russia): Machine-learning potentials for exploring the phase stability and configurational ordering in MoNbTaW high entropy alloys*

### Computational Phase Studies (T. Hickel)

*Aslam, Waseda, Hickel: Improving empirical potentials by machine-learning techniques*

*Chakraborty, Hickel, Neugebauer (in collaboration with B. Gault*, *MA department): Hydrogen in aluminum alloys*

*Gajera, Janßen, Hickel, Neugebauer: Automatized determination of phase diagrams based on empirical potentials*

*Gupta, Hickel (in collaboration with B. Dutta*, S. Divinski** and G. Wilde** (*TU Delf, The Netherlands, **Universität Münster)): Mechano-chemical coupling during precipitate formation in Al-based alloys*

*Hegde, Waseda, Hickel, Neugebauer (in collaboration with C.C.Fu*, F. Soisson*, H. Amara**, V. Pierron-Bohnes***, S. Divinski**** and R. Drautz***** (*CEA Saclay, France, **LEM, France,***IPCMS Strasbourg, France, ****University of Münster, *****ICAMS, Bochum)): Magnetism in iron alloys: thermodynamics, kinetics and defects*

*Hickel (in collaboration with B. Dutta*, S. Ghosh**, B. Sanyal*** (*TU Delf, The Netherlands, **IIT Guwahati, India, ***Uppsala University, Sweden)): Ab initio study of lattice dynamics in systems with magnetic disorder*

*Janßen, Hickel, Neugebauer: Automatized determination of error bars of ab initio derived quantities using the pyiron workbench*

*Lochner, Hickel (in collaboration with I. Eremin*, *Ruhr University Bochum): Ab simulation of electronic and structural properties of iron-based superconductors*

*McEniry, Tehranchi, Hickel (in collaboration with B. Gehrmann*, J. Klöwer*, *VDM Metals GmbH, Research & Development): Ab initio study on the interaction of hydrogen and microstructure in the alloys system 718*

*Shayanfar, Hickel (in collaboration with A. Hütten*, A. Waske** (*University of Bielefeld, **IFW Dresden)): Coupling phenomena in magnetocaloric materials: From thin layers to composites*

*Sözen, Hickel, Neugebauer (in collaboration with O. Gutfleisch*, S. Biermann**, L. Pourovskii** (*TU Darmstadt, **Ecole Polytechnique, Paris, France)): Rare-earth-based alloys for hard magnetic applications: Temperature and pressure dependent phase stabilities*

*Sreekala, Hickel (in collaboration with Z. Georgeou*, F. Klose*, *Salzgitter Mannesmann Forschung GmbH): Impact of microstructure on hydrogen embrittlement in Cr-containing high-Mn steels*

*Tehranchi, Hickel, Neugebauer (in collaboration with C. Hüter*, R. Spatschek*, *FZ Jülich): Ab initio based mesoscale simulation of hydrogen embrittlement*

*Waseda, Hickel, Neugebauer, Raabe (in collaboration with R. Dronskowski*, B. Hallstedt*, *RWTH Aachen): Ab initio calculation of free energies, stacking-fault and grain-boundary energies at finite temperatures in Fe-Mn-C alloys*

**Defect Chemistry and Spectroscopy (C. Freysoldt)**

*Ashton, Freysoldt, Neugebauer (in collaboration with B. Gault*, *MA department): Machine-learning for reconstruction of atom-probe tomography data sets*

*Ashton, Freysoldt. Neugebauer: DFT calculations of field evaporation from metal surfaces*

*Freysoldt, Ashton, Neugebauer (in collaboration with S. Katnagallu*, I. Mouton*, L. Stevenson*, B. Gault*, D. Raabe*, *MA department): DFT calculations for Field Ion Microscopy*

*Freysoldt, Neugebauer (in collaboration with C. Liebscher*, A. Ziletti**, L. Ghiringhelli**, (*SN department, **Fritz-Haber-Institut, Berlin)): Automatic classification and feature extraction from multi-dimensional STEM data*

*Freysoldt, Waseda, Janßen: Method development across code boundaries via pipe-based inter-code communication protocols*

**Electrochemistry and Corrosion (M. Todorova)**

*Yoo, Todorova, Neugebauer (in collaboration with D. Marx*, *Ruhr-University Bochum): Impact of oxygen vacancies on Au nanoclusters supported on $TiO_2$(110).*

*Yoo, Todorova, Neugebauer (in collaboration with C.G. Van de Walle*, *University of California, Santa Barbara, CA, USA): Polarisation in semiconducting compounds.*

*Surendralal, Todorova, Neugebauer: The platinum-water interface in an electrolytic cell under open circuit conditions and under bias.*

*Surendralal, Todorova, Neugebauer: De-solvation of Mg-surfaces in aqueous environment*

*Tautschnig, Todorova, Neugebauer: Stability of low index surfaces of Anorthite in dry and wet/aqueous environment*

*Tautschnig, Todorova, Neugebauer (in collaboration with Schott AG): Modelling corrosion of glass surfaces*

*Surendralal, Janßen, Todorova, Neugebauer: VASP in pyiron*

*Tautschnig, Janßen, Todorova, Neugebauer: Phase diagrams in pyiron*

**Growth Modelling (L. Lymperakis)**

*Lymperakis, Neugebauer (in collaboration with T. Schultz*, M. Anikeeva*, and M. Albrecht*, *Leibniz Institute for Crystal Growth, Berlin): Recombination in (In,Ga)N quantum structures - role of hole localization.*

*Lymperakis (in collaboration with G. Dimitrakopoulos*, A. Georgakilas** and E. Dimakis*** (*Aristotle University, Thessaloniki, Greece, **University of Crete, Heraklion, Greece, ***Helmholtz-Zentrum Dresden-Rossendorf e.V., Dresden)): Superlattices of ultrathin InGaN/GaN quantum wells for advanced optoelectronics and topological insulator applications*

*Lymperakis, Neugebauer (in collaboration with B. Alling*, *Linköping University, Sweden): Thermodynamics of nitride alloys for piezoelectric applications*

*Lymperakis, Neugebauer (in collaboration with Ph. Ebert*, *Forschungszentrum Jülich): Electronic properties of non-polar AlGaN surfaces*

*Lymperakis, Alam, Neugebauer (in collaboration with the MA and SN departments), Thermodynamics of Si Grain Boundaries.*

*Lymperakis, Neugebauer (in collaboration with Ph. Vennégues*, *CNRS-CRHEA, Valbonne, France): Si incorporation at AlN surfaces*

# Department of Interface Chemistry and Surface Engineering

*M. Rohwerder, M. Stratmann (provisional head J. Neugebauer)*

## Introduction

The Department of Interface Chemistry and Surface Engineering (GO) is mainly focussing on corrosion and electrochemical energy conversion. It is internationally known to be one of the leading groups in the field of electrochemical sciences. Our mission is to combine both fundamental and applied sciences to tackle key-questions for a progress towards new or better, energy saving and efficient, cheaper and longer lasting materials for applications in structural (in particular steels and other alloys) and functional materials, e.g. for fuel cell catalysts, batteries, adhesives and smart coatings amongst others. The department currently hosts five research groups. The different groups focus on high-throughput methods and the development of combinatorial methods in adhesion science and electrochemistry, on characterization of electrified interfaces by complementary methods such as vibrational spectroscopy, *in situ* diffraction studies and scanning probe techniques, such as Scanning Flow Cell (SFC), Scanning Kelvin Probe (SKP), Atomic Force Microscopy (AFM) or Scanning Tunnelling Microscopy (STM), as well as on related *ab initio* simulation. We combine electrochemistry with a surface and interface science approach, and in most projects we complement both, experimental studies on atomically well-defined model systems as well as on technical systems with atomistic *ab initio* modelling. All groups in the department have their independent and strong research agenda, while collaborative research projects are synergistic and focus on major challenges and complex scientific questions that require the scale and interdisciplinarity.

In the last six years the department was subject to a number of advancements and adjustments: First of all, in June 2014 the head of the department, Martin Stratmann, took over as president of the Max Planck Society and is officially on leave from his position at the MPIE. Michael Rohwerder took over the coordination of the department and Jörg Neugebauer (head of the department "Computational Materials Design") acts as provisional head of the department. Also in 2014 Michael Rohwerder was offered the position as full professor in the MSE department at the Ohio State University, but could be successfully kept at the Institute. In December 2015 Andreas Erbe was appointed professor of Corrosion and Interface Chemistry at the NTNU Trondheim (Norway) and Karl Mayrhofer was appointed professor of Electrocatalysis at Friedrich-Alexander-Universität Erlangen-Nürnberg as well as director of the Forschungszentrum Jülich GmbH-Helmholtz Institute Erlangen-Nürnberg for Renewable Energy. And in May 2016 Markus Valtiner was appointed professor for Physical Chemistry "Colloid and Interface Science" at the TU Freiberg. The institute was successful, however, in securing the continuation of the corresponding groups by long term consultancy contracts with these group leaders. At the current stage the groups of Andreas Erbe and Karl Mayrhofer will continue at least until middle of 2019. The department is actively participating in various collaborative research efforts with internal and external partners. An important example is the German Research Foundation (DFG) Cluster of Excellence "Ruhr Explores Solvation" (RESOLV),

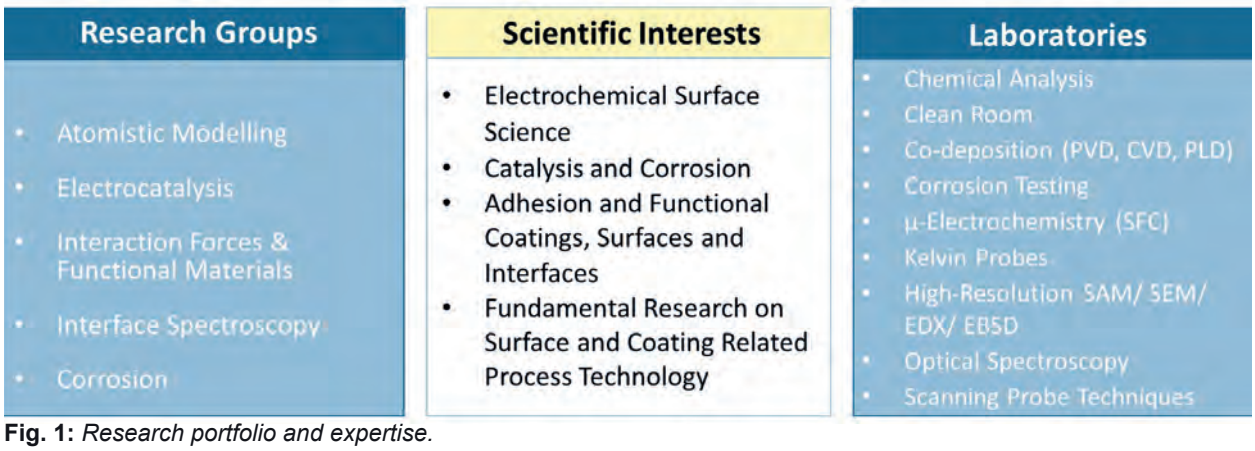


**Fig. 1:** *Research portfolio and expertise.*


**Fig. 2:** *Part of the GO department 2018.*

which is centred at Ruhr-Universität Bochum's (RUB) Faculty of Chemistry and Biochemistry. Our contributions to solvation science in RESOLV focus on the role of solvents in electrochemical reactions, and solvation of interfaces.

With its versatile experimental and theoretical expertise (Fig. 1) the GO is in the unique position to assist and promote diverse industrial research by its profound expertise in investigating the underlying fundamental electrochemical reaction mechanisms and kinetics. For instance, electrochemical oxygen reduction reaction (ORR) - a key process in corrosion as well as energy conversion - has been the focus of several joint research projects in the department aiming at a fundamental understanding of its mechanism for better control in corrosion protection as well as improved catalysis in fuel cells and air batteries. These research projects combine both advanced electrochemical as well as *in situ* and in operando spectroscopic experiments with theoretical modelling. In the reporting period besides ORR also the oxygen evolution reaction (OER) has become object of intense research activities and in this context also research on transpassivity of electrode materials under OER conditions. The knowledge obtained in the fundamental research on electrochemical key reactions such as oxygen reduction and oxygen evolution plays a crucial role in helping us to unravel practical problems met in industrial applications or processes such as in corrosion, batteries and fuel cells.

Several research projects focus on industrial processes such as electrophoretic coating, phosphating, alternative surface treatments. A special collaborative interest of the institute is hydrogen in steel. The activities in this field have been further enhanced, complementing experimental and theoretical methods in cooperation between the departments play an important role. In the GO in particular the Scanning Kelvin Probe and Scanning Kelvin Probe Force Microscopy were further developed in combination with complementing techniques to uniquely and directly detect hydrogen in steel and also hydrogen originating form corrosion by through-sample detection with high spatial resolution (see p.45).

## Scientific Concepts and Broader Impact

All our research groups are synergistically working on common areas of interest and we are strongly dedicated to collaborative work with external partners. Our scientific concept comprises diverse fundamental and industrial fields:

### Electrochemical sciences

Fundamental research on electrochemical interfaces is a key activity within the GO department as an in depth characterisation of these interfaces or interphases is of indispensable importance for a full mechanistic description of electrochemical processes in the key areas corrosion and electrocatalysis. In the recent years extensive collaborative experimental and theoretical work focussed especially on the electrochemical oxygen reduction reaction (ORR), a fundamental electrochemical reaction relevant in both corrosion as well as energy conversion processes. At metal surfaces the ORR is the cathodic partial reaction driving many corrosion processes. On the other hand, the electrocatalysis of the ORR in fuel cells and air batteries is intensely studied with the aim of improving the kinetics and reducing the over-potential that limits the energy efficiency. One important approach for advancing our understanding of this reaction is to make progress in according *ab initio* simulations. This is, however, difficult, because reliable experimental *in situ* data for instance of reaction products are difficult to obtain and thus experimental feedback is more or less missing. To overcome this problem dedicated model experiments were designed. By combining electrochemical experiments with attenuated total reflection infrared absorption spectroscopy and DFT based simulation, the mechanism of the electrochemical oxygen reduction reaction on n-Ge(100) as a model semiconductor has been investigated, providing deep insight into the reaction mechanisms [1-4]. Especially in acidic

solution, the onset of the oxygen reduction is closely linked to a change in surface termination to an H-terminated surface at negative electrode potentials. On the basis of several experimental datasets, a catalytic cycle for the ORR on Ge(100) was suggested [1]. Details of the transformation mechanism have been revealed by *in situ* IR spectroscopy [5]. During this surface transformation, water is effectively displaced from the interface, the interfacial hydrogen bond network is weakened, and a "hydrophobic gap" of few Å thickness develops [6,7]. Both interfacial desolvation and interfacial IR absorption spectra have been reproduced by *ab initio* molecular dynamics calculations [6]. Details of the desolvation process have been extracted from the IR spectra by a novel analysis technique, combining a transition model with a principle component analysis based spectrum decomposition [7]. These IR results follow a previous study of desolvation by *in situ* ellipsometry, where also a layer of low refractive index at the interface between hydrophobic organic layers and aqueous electrolytes [8].Ongoing activities center around the stabilisation of oxide-free silicon in contact with aqueous solutions, and the extraction of potential dependent IR spectra. A parallel computational project has been carried out in the Atomistic Modelling Group. Extending previous experimental approaches first attempts have been made to derive depth-dependent IR spectra from the inversion of angle dependent internal reflection data [9].

The molecular structure of the electrode/electrolyte interface is essential in electrochemical and natural processes. In the recent years, we started to use force probe experiments as workhorse to directly probe structural forces at solid/liquid interfaces. For instance, electric double layers in static and dynamically changing systems were studied in a close collaboration with the cluster of excellence RESOLV at Ruhr-Universität Bochum. It was e.g. shown how specific ion adsorption can strongly influence charge compensation in the electric double layer on model ceramic surfaces [10]. Also, anion hydration layers were investigated using force probe experiments, and similar effects were observed [11]. Work was also extended into non-aqueous electrolytes such as ionic liquids and battery fluids. Influence of trace molecules on structuring of ionic liquids at electrified and charged interfaces. It was shown how water and other impurities alter the interfacial structuring and charging characteristics of ionic liquids on dielectric surfaces and electrified interfaces, and electric double layer screening in high salt solutions was shown to proceed via an unexpected long-range mechanism [12-15]. This work was very well received and triggered a rethinking of how force probe experiments in IL liquids should be conducted and interpreted, and how charge compensation works in high salt environments, which was recently reviewed [16].

Of increasing importance is our surface science approach for fundamental investigation of electrode surfaces. For this we have developed a novel methodology that allows to fully control not only the potential of electrodes covered by just ultrathin electrolyte layers, but also to measure the full current density-potential correlation (I(U) curves) for electrochemical reactions such as oxygen reduction on that same electrode. This methodology is based on combining Kelvin probe with a hydrogen permeation experiment, which allows for the first time direct measurement of e.g. the oxygen reduction kinetics at the buried interface, first performed and proven to work in a modified Devanathan-Stachurski set-up where at the exit side the potential was measured instead an oxidation current density [17,18] (see p. 116 and p. 45). This approach is denoted by us as the permeation based potentiometry method (ppm).

This is a breakthrough of highest importance for the field. It will allow us

- to measure current-potential (I(U)) curves on electrodes covered by ultrathin electrolyte layers, even down to the submonolayer range (see p. 45)
- to use analytical surface science tools without any restrictions, as well as other spectroscopic techniques such as infrared spectroscopy (without need of attenuated total reflectance)
- to characterize the full electrode, as the electrolyte layer is very thin and controllable, from clusters over monolayers to nanometres

These electrodes are just covered by ultrathin electrolyte layers denoted by us as "electrodes in the dry". The humidity of the environment can be adjusted to different partial pressures of water, thus adjusting the exact thickness of the electrolyte layers. This novel approach enables us to control the structure of the double layer in a so far unimaginable way. For instance, under full potential control electrodes with double layers containing water in the sub-monolayer range can be realized and still the full current-potential dependence for electrochemical reactions such as oxygen reduction can be obtained. For the first time this should make a fully controllable electrode accessible for analytical techniques for in operando investigation without any restrictions, such as surface analytical tools like NAP-XPS and infrared spectroscopy.

In accordance with the importance of the oxygen reduction reaction for the department the main activities of the current research focus on this reaction. So far ORR on "dry" palladium and iron membranes have been investigated.

This novel approach has also great potential in fundamental research on electrocatalysis. For in-

stance, an interfacial descriptor of the electrocatalytic activity for the hydrogen evolution reaction, analogue to the adsorption energy of $H_{ad}$ intermediate, has been identified by measuring the potential change during nitrogen/hydrogen gas change. The derived activity trends give clear indication that the electrocatalytic activity for hydrogen evolution reaction is a consequence of an interplay between metal-hydrogen and metal-water interactions [19].

Many of the research projects allocated in the field of electrochemical sciences are closely related to the DFG-funded Cluster of Excellence RESOLV with the RUB. More specific current research within RESOLV is, among other activities, focussed on electrochemistry in the "dry" (see further below) and on *in situ* vibrational spectroscopy, with the aim on the understanding of the electrode-potential dependent solvation of electrodes [20]. Main aim is again to link experimental results to first principles calculations.

**Corrosion**

The aim of the department is to obtain fundamental insight into corrosion mechanisms with the aim to develop advanced countermeasures.

During the last six years the corrosion research of the department covered a wide range of topics in the areas of aqueous, atmospheric and bio-corrosion processes and their inhibition, covering both fundamental and applied aspects. In the latter mainly microbially influenced corrosion (MIC) by marine sulfate-reducing bacteria was investigated [21], and information on related direct electron transfer processes at the electrode/bacteria interface was obtained [22,23,24]. One important focus of work on aqueous corrosion was transpassivity. A combination of Raman, PL and ellipsometric *in situ* spectroscopy was used to study surface changes on copper and manganese, initially while forming surface oxides, and subsequently when entering the potential range of the oxygen evolution and transpassive dissolution [25-27]. Also understanding the working mechanisms of corrosion inhibitors is of importance. For instance, the same combination of *in situ* techniques, complemented by IR spectroscopy was used to investigate the mechanism of action of the well-known corrosion inhibitor 2-mercaptobenzothiazole (MBT) with copper. As a result it was e.g. shown that in contrast to current literature opinion, MBT can adsorb to oxide-free copper [28,29].

A key technique for corrosion research is the Scanning Flow Cell (SFC). Using the SFC system with downstream analytics such as mass spectroscopy or UV-vis analysis allows electrochemical high-throughput screening and characterization of corrosion properties of material samples. This method, which was developed in the GO, has become a routine technique for corrosion research and was applied on a wide range of materials including magnesium, where it provided important insights, including the much disputed negative difference effect [30,31], zinc alloy coatings [32], and noble metal catalysts. In contrast to the plain activity evaluation of catalyst materials that dominate the literature in the field, we focus on the overall performance including stability and selectivity, as operation over extended times is crucial for the success of fuel cells and electrolysers. Namely, the conditions during the reactions in these devices are often quite harsh and lead to corrosion of the catalyst material, even though they typically consist of noble metals. Pt, which is among the most active materials for the ORR, for instance dissolves significantly during transient operation when the surface alternates between reduced and oxidized condition [33-37]. Au instead dissolves continuously and to a major extent during steady-state operation at positive potentials close to the oxygen evolution, since it does not form a passivating oxide layer as Pt [38-41].

The investigations by SFC are mainly focused on the fundamental active dissolution kinetics. Atmosphere change experiments in the Kelvin Probe, on the other hand, are providing information primarily about the reactivity of the surface oxides of the as prepared samples and to some extent the initial stages of long term performance, depending on the exact exposure conditions and the duration of the experiments. One example is the performance of zinc alloy coatings. The effect of changes from oxygen free to oxygen containing atmospheres and back on the potential measured by Kelvin probe on the surface of such a coating are taken as an indicator for the reactivity of the corresponding surface oxide, which was indeed found to correlate well with observed corrosion behaviour. The potentials obtained by standard Kelvin Probe are averaged over a macroscopic scale of a several thousands of square micrometres, which is much larger than the underlying microstructure. For this reason high resolution studies by Scanning Kelvin Probe Force Microscopy (SKPFM) play a crucial role in unravelling the origin of the observed potential changes. We are currently trying to establish according measurement routines that are expected to make Kelvin Probe based techniques for corrosion research of similar importance as they have already gained for the investigation of coating performance or hydrogen detection. Many problems have to be solved and are addressed in our activities in further developing the Scanning Kelvin Probe methodology (see p. 45). This includes research on how to obtain reliable calibration of potentials measured by Kelvin Probe under different atmospheric conditions [42] as well as how to achieve calibration in SKPFM. Longterm corrosion performance is mainly determined by the corrosion product layers forming over time. These were in focus of research, too, from initial stages to long term. Important information on the effect of environmental factors and the role of

the micro-structure could be elaborated [43-46] and is still ongoing research (see p. 116).

Within the reporting period work was performed to adapt also the surface force apparatus (SFA) for fundamental investigation of corrosion in confined zones. For this, the electrochemical surface forces apparatus, developed partly at the MPIE, was modified to utilize white light interferometry (WLI) for a direct visualization of corrosion processes in real-time, *in situ* in confined (i.e. buried) geometries [47]. This is a unique experiment that allows to *in situ* study e.g. of crevice corrosion (CC) with unprecedented resolution in time and space. In a first case study, we investigated in detail how pure aluminium corrodes in crevice geometries and how vanadate ions can effectively inhibit CC of aluminium [48]. This work was then extended into studying Nickel and its alloys that are prone to CC [47]. This work confirmed at the nanoscale that there is a strong interplay between migration kinetics of chlorides, bulk chloride concentrations, and the related IR drop (voltage drop), which leads to pronounced qualitative changes in the location (at the rim or center) at which pits form, and their subsequent kinetics. Importantly, local fast corrosion was found to play a crucial role in the initial development of a crevice corrosion site within the crevice that drives local pit growth and propagation, suggesting that understanding and controlling surface chemistry, surface defects and morphology are essential to prevent the onset of corrosion in the tested systems. With the EC-SFA it was also possible to uniquely measure local pit-current densities ranging from ≥5 A/cm$^2$ for swiftly arresting noncritical pits, and ~25 A/cm$^2$ for critical pits. This constituted the first *in situ* and real-time measurement of a local current density of a single corroding pit site with nanometer resolution [47].

**High temperature oxidation** is another topic that is investigated within the GO. Special focus are short term high temperature treatments that are crucial in many industrial processing steps in steel making, such as hot rolling and recrystallization annealing before hot dip galvanizing. These relatively short processing steps are generally not much investigated yet and are determined by kinetics of oxygen uptake, nucleation and growth of oxides [49] and only to limited extent by diffusion, usually considered of key importance in high temperature oxidation, which leads to final morphologies that are still far from equilibrium. This research was originally part of the Christian Doppler Laboratory for Diffusion and Segregation during the Production of High Strength Steel Sheet. A more recent example is the investigation of selective oxidation at grain boundaries in noble metal anti-adhesion coatings applied on hard metal molds for hot stamping of high precision glass lenses. Indications for an interaction between chromium stemming from the interlayer between the anti-adhesion layer and the hard metal and oxygen was found that promotes chromium segregation at the GBs below the stage where oxidation occurs (see [50,51], and p. 56). Such interactions may play also an important role in enhanced grain boundary oxidation phenomena observed e.g. during cooling of certain hot rolled steel grades, which is object of current research.

**Adhesion, thin films and friction**

Organic coatings play an important role in the research within the GO. One important aspect is understanding coating adhesion. Unravelling the complexity of modern adhesives acting in the macroscopic world relies on understanding the scaling of single molecular interactions towards integral macroscopic interactions. A new and unique approach was developed to demonstrate how it is possible to directly extrapolate a macroscopic work of adhesion based on single molecule Atomic Force Microscopy (SM-AFM) measurements [52,53]. Utilizing specifically end-functionalized poly-ethylenglycol (PEG) tethers extending from lipid bilayers (PEGylated bilayers) and SAM covered AFM tips as model system, dynamic forces-versus-distance characteristics of unbinding a specifically bound single tethered functionality from an apposing chemically well-defined surface were measured. Using non-equilibrium thermodynamics it was then possible to extract equilibrium interaction free energies ($\Delta G0$) from non-equilibrium single molecule adhesion measurements, together with dynamic free energy landscape parameters such as transition state barrier heights and rates of desorption. However, there are significant issues concerning reliability, as it was found that certain arrangements work excellent while others are not useful [54], in a sense that data cannot reliably be converged in the analysis.

**Functional surfaces, interfaces and coatings**

Our research on coatings is mainly focused on understanding their corrosion driven degradation and how to improve their performance. Organic coatings are commonly employed to protect materials surfaces against corrosion. On steel, including galvanised steel, cathodic delamination is the main mechanism of failure of these coatings. In this delamination mode oxygen reduction at the buried interface and especially the radicals produced as intermediates or side products play a crucial role in destroying the adhesion at the interface. In order to improve the delamination resistance the standard strategy is to use pretreatments prior to application of the organic coating that effectively inhibit electron transfer reactions at the interface and thus also oxygen reduction. Examples are chromatation and phosphatation, where the first is more or less fully banned now and on the latter there is strong pressure to replace or even skip it. GO is involved in corresponding research. The main

problem, however, is that any development of novel pre-treatments and coating concept is slowed down by the required long term evaluations. Unfortunately, up to now no real break-through has been made in a simulation of the delamination process and long-term prognosis. An important requirement for such simulation is of course a deep insight into the underlying mechanisms and knowledge about the key processes. Hence, for this fundamental investigations of the interfacial (electrochemical-)reactions at buried interfaces are of utmost importance and are hence a key research topic within the department. Further efforts have been made towards understanding details of chemical processes during cathodic delamination through preparation of model polymer systems and an investigation of their delamination rates. For instance, thin polyacrylate films had been prepared on zinc by a co-polymerisation in the presence of zinc surface-modified with covalently bound vinyl-terminated silanes, and their delamination behaviour was studied [55-57] . Also surface bound polymers on iron were prepared by surface initiated atom transfer radical polymerisation. In these polymers, the initiator precursor state is crucial for the final delamination rate [58]. An interesting side observation in these studies was the detection of chemical oscillations and pattern formation during cathodic delamination [59,60].

Up to now one unsolved hindrance for a detailed study of cathodic delamination was that the oxygen reduction rate at the buried interface was not directly accessible. Based on the new methodology of combining Kelvin probe with a hydrogen permeation experiment, a novel methodology was developed which allows for the first time direct measurement of the oxygen reduction kinetics at the buried interface (see p. 45). Also of interest and of crucial importance for understanding delamination is the role of surface oxide terminations and studying its effect on the properties of the resulting interface with polymers [61]. This also affects the mobility of charges along the buried interface. Hence, the study of charge mobility and of its dependence on crucial surface parameters such as OH termination is of great importance [62].

The development of intelligent coatings for corrosion protection within the department focuses to a significant extent on the application of conducting polymers and particle modified zinc coatings. We have a leading expertise about the problems involved with the use of conducting polymers for corrosion protection which we have analysed in depth and solutions how to solve them were developed. One main success in the last six years was the development of polyaniline capsules that can be loaded with inhibitors or other self-healing agents (together with partners from the Max Planck Institute for Polymer Research in Mainz) and first successful applications [63,64]. Another major break-through was the successful combination of an intelligent organic coating containing smart capsules loaded with monomer with a zinc coating containing capsules that were loaded with a catalyst [65]. For the first time a coating system could be demonstrated to case-sensitively release active agents upon onset of corrosion that closed a macroscopic defects site by formation of a new polymer coating.

A general problem with these intelligent self-healing coatings, however, is that the release of active self-healing agents towards the defect is a limiting factor concerning the time to self-healing and the maximum size of the defect that can still be healed. We have found that this can be only improved by ensuring a much faster release rate. Hence, an important research topic was the effect of trigger signal spreading and mobility of the released active agents on the overall self-healing performance. This work was carried out mainly within the framework of SPP “Self-Healing Materials” funded by the DFG. It is found that the performance indeed can be significantly improved by especially enhancing the trigger signal spreading (see below).

**Industrial processes**

The expertise of the department is of great relevance for the investigation of fundamental aspects of industrial processes. Especially noteworthy is the potential of the SFC for fast through-put measurement. For instance it can be applied to increase our understanding of the impact of the electrolyte components on the fundamental corrosion mechanism and kinetics of Zn based systems [32]. The fully automated SFC has been also extended for the analysis of real, high surface-area electrocatalysts, which are important in electrochemical energy conversion devices such as fuel cells and electrolysers. This has been highly beneficial in the collaborations with industry, as the wide parameter-space for material composition and structure as well as operation conditions require also fast screening techniques to obtain reliable information within a reasonable timeframe. The SFC has been shown to reliably acquire the activity and the stability of noble metal catalysts with high-throughput [66], and is currently employed for a wide range of different types of porous materials including exciting non-noble catalysts for oxygen reduction [67].

Also work on conversion coatings, e.g on high-strength steels [68,69] and Al-SI coated steels [70], as well as on nanoceramic coatings was carried out. In collaboration with a pretreatment manufacturer different *in situ* spectroscopic techniques have been used to study the effect of cathodic polarisation, such as experienced during cathodic electrodeposition coating, on the structure of a nanoceramic, $ZrO_2$-based conversion coating on several industrially relevant substrates. No significant structural changes after po-

larisation were found [71]. These conversion coatings have earlier been shown to work by passivating grain boundaries and cathodic intermetallic particles [72].

Joining different materials by welding is an important industrial process, but some material combinations are not accessible in the classic welding processes that involve melting. In collaboration with the Institute of Production Engineering and Forming Machines of TU Darmstadt headed by P. Groche within the DFG-funded priority programme SPP1640 "Joining by forming", the role of the interface chemistry on cold welding of steels and aluminium alloys is being investigated. The department is here mainly involved with chemical and electrochemical surface treatment and *ex situ* investigation of prepared structures [73,74]. Current research mainly focusses on the potential of metallic coatings for enhancing the joining process.

Using a systematic variation of alloy composition and *in situ* spectroscopic analysis has advanced the understanding of sour gas corrosion, the corrosion of steels in the presence of $H_2S$ [75], in a joint project with a steel manufacturer. *In situ* Raman spectroscopy showed the phase evolution of oxide- and sulfide-containing corrosion products in different drying stages [76]. On the example of a Mo-containing model alloy, the interrelation was explored of long term integral corrosion rate as measured by mass loss, and the instantaneous corrosion rate measured by electrochemical experiments [77]. State of the art in this field was also summarised in a book chapter presenting an overview over sour gas corrosion [78].

Fundamental problems of oxidation and hydrogen uptake during industrial production steps of high strength steel sheet have been the focus of the Christian Doppler Laboratory of Michael Rohwerder and many of the current activities on these topics are based on that earlier work. A high performing high temperature lab is available for fundamental investigations of according industrial processes [79,80], where also our NAP-XPs might be of interest [49].

## Scientific Groups

**Electrocatalysis (K. J. J. Mayrhofer)**

The research interests of the electrocatalysis group are related to electrochemical reactions at the solid-liquid interface, both for corrosion processes and electrochemical energy conversion. The main focus of the group is placed on the concerted investigation of the activity, stability and selectivity of electrode materials for such heterogeneous electron-transfer reactions. Thereby the behaviour of well-defined and real material surfaces is investigated and compared in order to achieve a fundamental understanding of the decisive processes and structural effects. This is achieved by a unique combination of electrochemistry with complementary techniques for surface characterization and time-resolved reaction product determination.

The new electrochemical methods, which have been developed in the group over the last years [81] are utilized to investigate a wide range of scientific challenges. High-throughput combinatorial screening tools combined with sophisticated automation and advanced methods for data evaluation and processing are central for the more systematic and reliable investigation of a large number of samples. In addition, coupling electrochemistry with online reaction product determination by Inductively Coupled Plasma Mass Spectrometry and Differential Electrochemical Mass Spectrometry [82] increases the information depth significantly.

These advanced techniques have provided new exciting insights into processes at the solid-liquid interface particularly of materials for electrochemical energy conversion. The key reactions studied in our laboratory include the oxygen reduction reaction (ORR) and evolution (OER), as well as the utilization of $CO_2$ by electrochemical means for the production of so-called solar fuels [83]. The overall performance including selectivity and also stability, as operation over extended times, is crucial for the success of fuel cells and electrolysers, and is investigated [33-35,38-41,84,85]. All noble metals have in common that they dissolve to a certain extent, but clearly there is no inverse relationship between activity and stability as commonly believed [86]. When noble metals are alloyed with transition metals to enhance the intrinsic activity the dissolution becomes more complex, yet still the performance can be resolved with our special techniques. The full potential of our combinatorial approach in resolving complex scientific challenges is enabled when electrochemical screening is combined with material library development, which we perform in a long-standing collaboration with the group of Alfred Ludwig from the RUB [87,88]. Activity-stability studies have been further extended to the investigation of different catalyst materials like the promising Ru and Ir oxides for the OER [89,90]. Exciting insights have been generated that helped to resolve the difference in performance and reaction mechanism of amorphous Ir (hydroxy-)oxides and rutile Ir oxides [91-94]. Moreover, the structural evolution of the near-surface oxide layers of Ir-based catalysts was monitored on the atomic scale utilizing a combined electrochemical atom probe tomography (APT) approach for the first time [95]. Combined with the introduction of the Stability-number as a quantitative

descriptor for dissolution during reactions, the behaviour of several different Ir-perovskite structure could be efficiently assessed, leading to potential pathways for improved electrolysis catalyst development [96].

Besides these studies on rather model like electrode surfaces, we are also highly interested in high surface area catalysts as typically employed in real electrochemical reactors. The aim is to additionally enhance the fundamental understanding of the structural effects on performance, in order to derive catalyst design principles and achieve optimal operation in applications [97]. In joint efforts with various expert material science groups we therefore contribute to the development of new catalysts, eventually with lower content of scarce noble metals. For instance, together with the department of Ferdi Schüth from the Max-Planck-Institut für Kohlenforschung the concept of "confined space alloying" has been introduced, providing alloy catalysts with unprecedented structural and chemical stability [36,98,99]. Furthermore, in collaboration with the National Institute for Chemistry in Slovenia we have demonstrated the beneficial effect of ordered alloy nanoparticle catalysts as well as specific surface doping [100-102], while with the TU Berlin we could show general performance trends of nanoporous alloys for ORR and OER [103-105]. Also non-noble metal catalysts have been majorly improved in joint efforts with Frederic Jaouen and his team from the University of Montpellier, unravelling the active sites and resolving stability challenges using operando investigation during ORR [106-109]. Significant contributions could be also achieved in understanding particularly stability aspects of non-noble electrocatalysts during hydrogen evolution reaction, important for low-temperature water electrolysis [110-112]. Within MaxNET-Energy a strong collaboration with the group of Graham Hutchings from Cardiff University has been established, addressing selectivity and stability challenges of the electrochemical production of hydrogen peroxide in fuel cells (see p. 54) [113-116]. Besides catalyst material challenges, several fundamental aspects of support material, reactor operation strategy and accelerated degradation testing are in the focus of our research [117-119]. Overall, the parallel and time-resolved study of activity, selectivity and stability in electrocatalysis utilizing our unique portfolio of advanced methodologies has led to major enhancement of the understanding of key reactions for electrochemical energy conversion.

**Atomistic Modelling (S. Wippermann)**

Since 2013, the Atomistic Modelling group is working in three directions: (i) charge density waves and electron/phonon coupling in one-dimensional electronic systems, (ii) interfaces, defects, optical and electronic properties of complex nanostructured materials, e. g., assemblies of nanoparticles and (iii) development of *ab initio* molecular dynamics techniques with finite electric fields to describe electrode/electrolyte interfaces.

Topic (i) is motivated by the exploration of fundamental excitations in one-dimensional charge density waves with topological properties and how to use them as information carriers in new types of information processing. These activities are embedded into the DFG research group FOR 1700 (http://www.atomicwires.de) (see p. 64) [120-123].

For topic (ii), S. Wippermann was awarded an independent junior research group within the "NanoMatFutur" programme of the German Federal Ministry of Education and Research (BMBF). The group No. 13N12972 received 1.8 Mio € from 01/2014 – 12/2019. Group activities cover topics from optical and electronic properties of individual nanoparticles, surface functionalization and defects to colloidal assembly into nanoparticle solids with targeted properties for solar energy conversion [124-128]. Experimental collaborations exist with the groups of Dmitri Talapin at the University of Chicago (synthesis of nanocrystals and nanocrystal solids, EXAFS) and Gerd Bacher at the University of Duisburg-Essen (single quantum dot absorption spectroscopy and time-resolved photoluminescence). It is hoped to understand in detail (a) nucleation and growth processes of nanocrystals, (b) light-induced charge carrier dynamics in general and multi-exciton generation in particular, (c) anomalous temperature dependences of optical properties that are often observed in nanocrystals and (d) colloidal assembly processes into nanocrystal solids as a function of synthesis conditions (see p. 193).

In the context of topic (iii), insights at the atomistic scale into electrochemical and electrocatalytic processes require robust *ab initio* methods to perform molecular dynamics simulations of interfaces between solid electrodes and liquid electrolytes. The groups of C. Freysoldt, M. Todorova in the department Computational Materials Design (CM) and the group of S. Wippermann are optimally suited to develop the required methods ( see p. 47). Further collaborations exist with the groups of Giulia Galli at the University of Chicago and Francois Gygi at the University of Davis. In the Atomistic Modelling group, the Modern Theory of Polarization in conjunction with a basis set of maximally localized Wannier functions is used to apply electric fields in *ab initio* molecular dynamics (MD) simulations for solid/liquid interfaces. A first approach to perform MD simulations at constant electrode potential was implemented into the open source density functional theory package Quantum Espresso. Interfaces between elemental semiconductors, such as, e.g., Si and Ge, with liquid water are employed as model systems for corrosion processes and electrode potential-dependent surface structures. The newly developed methods are validated against spectroelectrochemical experiments

performed in the Interface Spectroscopy group of A. Erbe, (see p. 165).

**Interface Spectroscopy (A. Erbe)**

Activities in the interface spectroscopy group continued also after the move of the group leader Andreas Erbe to NTNU, the Norwegian University of Science and Technology, Trondheim, Norway. The group has a strong focus on using the combination of different *in situ* and operando spectroscopic techniques, such as IR absorption spectroscopy, Raman spectroscopy, photoluminescence (PL) spectroscopy and spectroscopic ellipsometry, to study fundamentals of corrosion processes [129]. *In situ* techniques were often complemented by the necessary *ex situ* experiments.

A combination of Raman, PL and ellipsometric *in situ* spectroscopy was used to study surface changes on copper and manganese, initially while forming surface oxides, and subsequently when entering the potential range of the oxygen evolution and transpassive dissolution. On copper, the importance of the mixed oxide $Cu_4O_3$ was realised at intermediate potentials [25]. Interestingly, when polarising copper to more and more positive potentials, onset of the oxygen evolution and breakdown of the oxide film coincides with a sudden appearance of a defect luminescence typically attributed to a singly charged oxygen vacancy in $Cu_2O$. This observations is a hint that oxides may become unstable towards defect formation above certain potentials, which may trigger oxide breakdown [26]. In buffered chloride solution, oxide breakdown occurs at much lower potentials under formation of soluble copper(II) chloro complexes [27] (see p. 167). The latter result is important for the antibacterial action of copper, which was studied earlier [130]. Within the BMBF-funded cluster project MANGAN, aimed at advancing manganese-based oxygen evolution catalysts, similar experiments were done for manganese. Data interpretation is significantly more challenging in this system, due to the many possible oxidation states and different phases of individual oxides, and is hence still ongoing.

Also research on pretreatments [71,72,70,131] and the working mechanism of inhibitors was carried out, namely MBT [29]. Furthermore, in many repeats, the effect of post-preparation aging on the formation of the inhibitor film was shown to be tremendous, highlighting the importance of appropriate pretreatments [28].

The fruitful, long-lasting collaboration with M. Krzywiecki, Silesian University of Technology, Gliwice, Poland, was extended. In a systematic development of photoemission based analysis approaches detailed insight into electronic structure such as band-bending and defect levels at semiconducting oxide / organic interfaces was obtained. Initially, an approach was developed to analyse angular dependent photoemission data with quantitative depth information at surfaces [132], defect levels were characterised and large stoichiometry deviations detected in thin films of ZnO [133], and morphology – local thermal property correlations were established [133]. Especially the analysis of ZnO defect levels advanced the understanding of previous works on which defects can form in electrochemically grown ZnO [134]. More recently, the degradation was investigated of thin layer of the organic semiconductor copper phthalocyanine (CuPc) [135]. Combining angular dependent x-ray photoelectron spectroscopy and photoemission yield spectroscopy, the band structure across a tin oxide/CuPc interface was characterised in detail (see Fig. 3). Significant stoichiometry deviations in the tin oxide was found, and a charge transfer across this interface [136]. Depending on transfer conditions, this charge transfer could be completely blocked, creating different electronic structures across chemically nominally identical interfaces [137]. The peculiar behaviour of the tin oxide lead to a detailed follow up study, disentangling defect formation vs. changes in oxidation state of tin [138].

The detailed analysis of interfacial electronic structure was crucial in the understanding of the behaviour of the cyclic oligosaccharide β-cyclodextrin (CD), which acts as corrosion inhibitor against zinc corrosion. β-CD does so by destabilising point defect formation in zinc oxide, hence rendering the oxide mode intrinsic and less defect rich than usually found [139]. β-CD can also function as a carrier for hydrophobic corrosion inhibitors, amongst others MBT, and stop corrosion-driven cathodic delamination of coatings in which such inhibitor-CD complexes were incorporated [140]. Other water-soluble polysaccharides [141] and polypeptides [56] have been deposited on metallic zinc as films of 10s of nm thickness, and delamination rates of deposited model top coating were significantly reduced even though these polymers can easily take up water. Reason for the reduction is presumably a decrease in the ion transport rate along the interface [141].

Following up from previous attempts on zinc to exploit a cathodic delamination for the preparation of nanorods [142] by using delamination, it was found that the resulting rods have different optical properties on both ends, due to their different defect structure. This behaviour offers interesting applications for corrosion processes as synthesis method in nanotechnology [143]. Ongoing activities in a Marie Skłodowska-Curie project investigate the possibility to create peptide-based switchable interfaces on metal or semiconductor surfaces.

In collaboration with Academia Sinica, Taipei, Taiwan, nanofluidic channels have been fabricated on a germanium internal reflection element and have

been used to detect proteins, were the total amount of protein need is only in the femtomolar range [144]. Earlier collaboration work with the same partners included the fabrication of an electrode nanogap, trapping of proteins in this gap, and protein detection with Raman spectroscopy [145].

### Corrosion (M. Rohwerder)

The main scope of this group is to address fundamental questions of corrosion, surface and coating technology by isolating the crucial problems behind them and designing model experiments and model samples for their systematic investigation. During the last six years three major research projects in the group were carried out in the highly competitive programmes of the Christian Doppler Society (namely the CD lab for Diffusion and Segregation

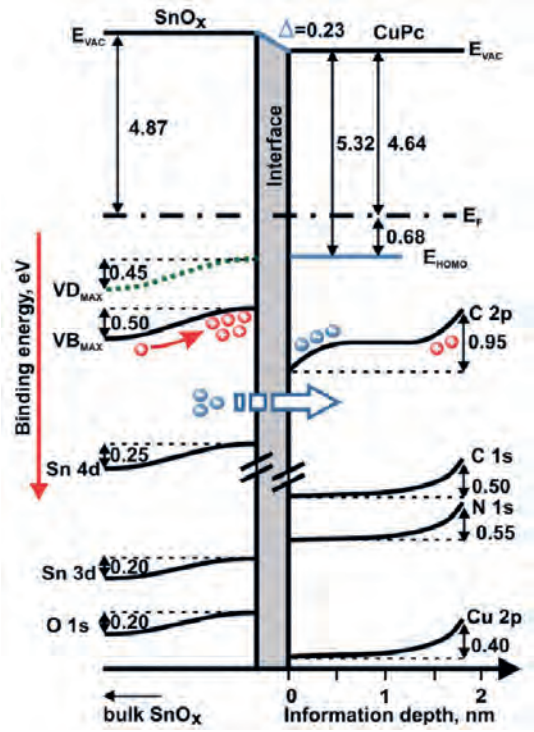


**Fig. 3:** *Band structure at tin oxide/CuPc interface.*

during Production of High Strength Steel Sheet) and the collaborative project framework of Fraunhofer Society (FHG) and Max Planck Society (MPG), namely the projects “Active coatings for corrosion protection (ASKORR)” and “Initial wear”. All three projects were very successful and had a lasting effect on the group´s research. The CD lab especially initiated our research on hydrogen in metals and ASKORR on intelligent self-healing coatings. Initial Wear (2014-2017) refuelled our interest in selective grain boundary research (see p. 56) that was originally started in the CD lab. In detail the main activities on the research interests in the Corrosion group can be summarized as follows:

1. *Elementary steps of electrochemically driven de-adhesion of organic coatings*

Fundamental research on coating delamination is of paramount interest for the department. This is, however, very challenging, because coating delamination is extremely complex and the buried interface is difficult to investigate, as it is inaccessible for most analytical tools. A huge breakthrough was the new approach based on a potentiometric measurement of the equilibrium potential of the oxygen reduction and oxidation of hydrogen permeating from the backside of the sample to the buried interfaces, denoted by us as permeation based potentiometric method (ppm). This approach overcomes the main obstacle preventing electrochemical measurements at the buried interface, the high resistance of the organic coating against ionic current that makes a controllable polarization of the interface by standard three electrode set-up impossible. From the hydrogen uptake on the entry side thus a full current-potential relationship curve (I(U)) can be constructed [17,18]. The investigations focus on two sets of samples: one are well defined samples based on inert noble metal, which allow well controllable structuring of the buried interface and integration of functional groups e.g. by use of self-assembled molecular films at the interface [146-149], the others are research in progress first on adapting the methodology also on technically more relevant samples, such as coated iron/steel and zinc. Concerning the latter we could show that one possible way to make them accessible by the ppm approach is to apply thin layers onto a Pd membrane. As long as the investigated current densities remain low, this was found not to violate the prerequisite that really about 100% of the hydrogen formed at the entry side is entering the palladium and permeating through it. For instance 100 nm iron at the exit side do not impede the permeation up to current densities of about 100 µA/cm$^2$ [18]. But this also shows that it is important to investigate the limits of this approach. The other way that is investigated and seems to be very promising is to adapt the ppm approach directly to e.g. iron samples. In this case not 100% of the hydrogen formed at the entry side is taken up, but the according relation was successfully established and was proven to work even up to much higher current densities than the thin film approach on palladium (see p. 45).

However, studies on delamination at buried interfaces are still extremely challenging, because oxygen reduction causes degradation already at very low current densities, i.e. it is nearly impossible to investigate the one independently of the other. This is one key topic of current and very exciting research, which has already yielded highly interesting results, such as an at least partial re-establishment of interfacial bonding

when polarization is stopped for a while and thus the formation of radicals and the correlated attack by radicals pauses (see p. 68). This will be relevant for understanding delamination under real atmospheric conditions, where e.g. humidity change will cause active/passive transitions at the defect site and hence will also cause phases of ongoing cathodic delamination and according breaks. Concerning the effect of the environmental conditions, an important topic of research was the role of $CO_2$ on the delamination behaviour. Strong indications were obtained that $CO_2$ is affecting the interfacial ion migration at the interface organic coating/zinc, the initial step inducing the delamination process. A crucial role of ion migration at the coating/metal interface was up to now not recognized and hence is widely neglected. We will accordingly intensify our research in interfacial ion mobility [61,62], also especially with a focus on the effect of $CO_2$. The effect of different pre-treatments on the interface with different coatings and their effect on ion mobility was studied in detail for aluminium [61, 62].

2. *Electrochemistry in the "dry"*

Electrodes covered by just ultra-thin electrolyte layers are another important topic within the corrosion group. This is of practical importance e.g. for our fundamental studies on atmospheric corrosion, where we take the potential change upon gas changes as an indicator for their reactivity. But electrodes in the dry are of general importance. Many phenomena in corrosion and electrochemistry are still not well understood. For instance, it is known that oxygen reduction of electrode covered by thin electrolyte layers shows a limiting current that does not increase when the film thickness decreases below about 5 microns. Then the maximum current densities are not any longer determined by diffusion, but by the uptake process at the surface. Typical values that are reached lie in the range of a few mA/cm$^2$. In experiments where we make use of the ppm technique we could show that this is indeed valid at least even down to the range of 500 nm electrolyte thickness. However, when we investigate ORR on a surface just exposed to high humidity and where the electrolyte layer is in the range of 1 nm we could not find a limiting current density up to about 1000 mA/cm$^2$, which was our experimental limit. It is an interesting question what exactly makes the difference for the $O_2$ uptake between 1nm and 500 nm electrolyte layer thickness. This is also interesting when seeing results obtained in the electrocatalysis group with a so-called floating cell set-up, where current densities for ORR of several hundreds of mA/cm$^2$ are readily obtained. Is the high current density achieved there mainly stemming from the outer, very thin fringes of the 3-phase region at the border of the wetted electrode surface? Another example are differences in the I(U) curves e.g. of ORR on palladium and iron(oxide) between dry and humid conditions where, however, the thickness of electrolyte layer varies less than 1 nm. On iron (oxide) polarization of the surface additionally leads to partial reduction of the oxide which complicates the investigation of ORR on such electrodes, but which can directly be followed by use of the Near Ambient Pressure – X-ray Photoelectron Spectroscopy (NAP-XPS). The NAP-XPS, combined with attached electrochemical cell and Kelvin Probe, is now gaining increasing importance as investigation tool for our studies of electrodes in the dry. Currently, we are complementing this set-up also with integrated infrared spectroscopy in order to obtain also information about ordering in the water layer.

Quite a number of projects have now been started on the topic of electrodes in the dry, including besides the mentioned research, fundamental investigation of so called "frozen" double layers, where we transfer polarized electrodes e.g. to the Kelvin Probe and the NAP-XPS for characterization. Regarding the hydrogen electrode in the dry on Pd [150] the main focus is currently to understand why the pH remains so stable. This is the reason why the potential measured by Kelvin Probe on Pd in nitrogen atmosphere can be used as a direct measure for the hydrogen content. However, in principle, since the equilibrium reaction is $H_{ab} \leftrightarrow H^{ad} \leftrightarrow H^+ + e^-$ an increase in H in the metal should lead to an increase in $H^+$ in the nanoscopic layer, because the layer in contrast to bulk electrolyte has no buffering capability. However, the observed behaviour is in accordance only with a pinned pH. First results obtained by in operando study of such hydrogen electrode on the dry on palladium indicate that adsorbed $CO_2$ contamination might play a role in the pH buffering. This research on electrodes in the dry will also play a role in the GO part within the continuation of the excellence cluster RESOLV.

3. *Measurements of hydrogen distribution and effect on embrittlement*

The novel SKP and SKPFM based method for hydrogen mapping by making use of the hydrogen electrode in the dry has by now become an established tool for our research on hydrogen related topics, in close cooperation with other departments (see [151-156] and see p. 177).

Especially noteworthy is a fundamental research project where we try to evaluate the importance of the full 3D-parameter range of mechanical strain, hydrogen activity and exposure time on hydrogen induced material failure. We found that exposure time is an important factor, i.e. at a certain mechanical load and hydrogen activity, we observed that exposure time plays a role whether hydrogen induced degradation of the mechanical properties occurs or not. Since the experiments where performed with a ferritic model alloy, where the samples are quickly fully loaded by hydrogen, the effect of time is not simply due to

increase of the loading level. We found that under combined mechanical load and exposure to hydrogen activity vacancy formation occurs [151] that, most likely as hydrogen-vacancy pairs, leads to the observed failure. The formation of these vacancies is a slow process that leads to the observed time dependence. The microstructure, such as e.g. oxide inclusions play an important role here.

4. *Semiconducting properties of surface oxide films*

The semiconducting properties of surface oxides play a crucial role especially in atmospheric corrosion and coating delamination. One huge research field are zinc alloy coatings, where alloying with magnesium and aluminium can result to significantly enhanced performance [43-46]. Galvanic coupling between different phases can significantly modify the activity of the resulting surface oxides. Of special importance are the cathodic sites. We found that for Zn-Mg-Al alloys the finer the microstructure the smaller is the potential change upon changes between oxygen free and oxygen containing atmosphere. This is currently mainly investigated within the framework of an RFCS project (MicroCorr), where a combined SKP and SKPFM approach is applied. Of huge current interest is also the conductivity of the surface oxide of bipolar plates. In projects with industry as well as with the research centre Jülich we have started to investigate passivity and conductivity of different stainless steels in order to understand how to optimize their performance. One key technique we are establishing for that is current sensing AFM.

5. *Intelligent self-healing concepts for corrosion protection*

In the last years the main activities on self-healing have been carried out within the framework of the DFG SPP "Self-Healing Materials" Within the reporting period, we succeeded to synergistically combine capsule loaded zinc coatings with capsule loaded organic coatings for superior intelligent self-healing [65]. Other important results were the development of polyaniline PANI based capsules for intelligent release and their modification for use on zinc and first successful application of intelligent corrosion protection [63,64]. Of special importance is the interfacial stability between conducting polymer and the metal surface [157,158]. A remaining challenge is how the coating design has to be modified in order to be able to routinely self-heal defects of macroscopic size, such as 1-2 mm broad scratches, with coatings just a 10-20 microns thick. We found that embedding PANI capsules loaded with active agents into a matrix of conducting polymer (polypyrrole) is a promising way to achieve this. In principle we have shown in earlier works that continuous films of conducting polymer must not be used for corrosion protection. Although they can provide excellent protection when there is no large defect, i.e. only small pinholes which can be easily passivated by the conducting polymer, they disastrously fail in presence of larger defects, by fast reduction and subsequent coating breakdown. Exactly this fast reduction can be made use of as fast spreading of a trigger for release. The self-healing induced by the released agents in turn stops corrosion and coating reduction and delamination, the reduced conducting coating being re-oxidised by atmospheric oxygen.

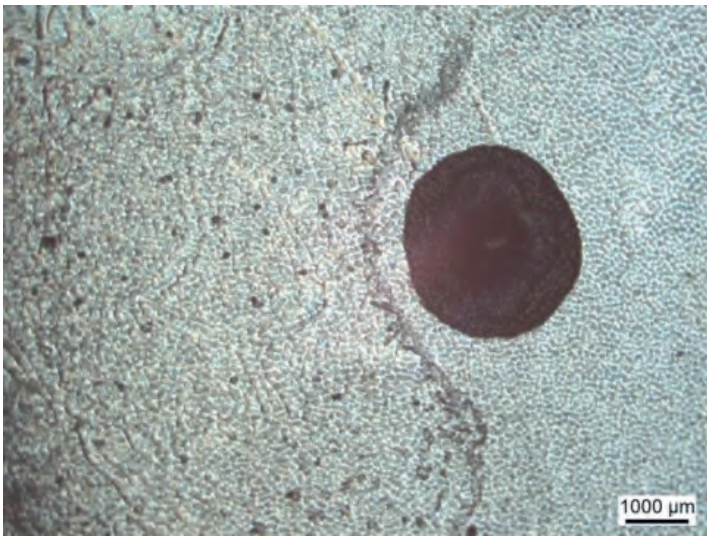


**Fig. 4:** *Photo of a partially delaminated clear coating on iron: around the black spot of PANI there is a clearly visible protection zone (delaminated area appears dark).*

Discontinuous patterns of conducting polymers are also topic of research. Here we are interested in understanding the working mechanisms behind what we call protection zone surrounding deposits of conducting polymers (see Fig.4). These protection zones are several hundreds of micrometres wide. The corrosion driven delamination process stops for a certain time and then proceeds slowly until the protection zone is delaminated, too. The results of our investigations so far indicate that polarization of the interface by the conducting polymer and thus suppression of interfacial oxygen reduction is responsible for this. Anion migration from the conducting polymer vs cation migration from the defect seem to play a determining role in how well the protection zone occurs: the protection zone surrounding PEDOT (is reduced solely by simultaneous cation uptake) provides significant longer protection than the ones surrounding PANI or polypyrrole (reduced mainly by simultaneous anion release).

6. *Novel developments with the Scanning Kelvin Probe*

Based on our world leading expertise of the Kelvin Probe also novel application fields are explored. The recent development of spatially resolved high-sensitivity hydrogen detection by Kelvin probe

(see p. 45; p. 167) has sparked new research on the possibilities to further extent the applicability of the Kelvin probe. In cooperation with NORCE Norwegian Research Centre AS a novel Kelvin probe for outdoor use and for through metal corrosion is currently being developed.

**Interaction Forces and Functional Materials (M. Valtiner)**

The Interaction Forces group was active at the MPIE from 2012 until end of 2018. The group leader Dr. M. Valtiner left the institute in May 2016. After receiving an ERC grant at the MPIE in 2015 he was offered a W2 professorship at the University of Technology in Freiberg, Germany, and soon after he accepted a full professorship at the Vienna University of Technology in Vienna, Austria. He finalized the relocation of his entire group to Vienna in 2018. His newly established team there collaborates closely with our department in many research projects, including corrosion in confined spaces, ionic liquids at interfaces and hydration at interfaces (Resolv).

In the last six years, the research interest of the Interaction Forces group was focused on the broad areas of (1) adhesion of single molecules in wet environments, (2) molecular structuring at solid/liquid interfaces and (3) crevice corrosion at confined areas of Nickel and Nickel alloys in aqueous chloride containing salt solutions. The broader scientific aims of the group were (1) to gain insight into the molecular interactions at equilibrated and dynamically changing reactive interfaces, on (2) how molecular interactions translate into macroscopic interactions (scaling and proportionality laws), and on (3) developing new interferometry-based approaches to study dynamic corrosion processes *in situ* at crevice interfaces. A particular focus was also to establish how molecular structuring of solvents and ions at electrified interfaces influences the mentioned processes.

The major activities and achievements of the group can be summarized as follows in the different areas mentioned.

1. *Adhesion science and single molecule interactions at solid/liquid interfaces*

In a collaboration with M. Scott Shell (University of California at Santa Barbara, U.S.A.) approach to extrapolate macroscopic work of adhesion from single molecule Atomic Force Microscopy [52,54] was further expanded into studying hydrophobic interactions on a molecular scale, and comparing experimental results directly with molecular dynamic simulations [159]. This work was supported within the framework of the exceptionally competitive “Materials world network” grant scheme which is funding collaborative bilateral projects through the German Research Society (DFG) and the National Science Foundation (NSF) of the United States of America. In the framework of this program, students and postdocs from the MPIE visited UCSB, and vice versa, for short (2 weeks) and extended (3 month) research stays multiple times between 2013 and 2016.

In addition, hydrophobic interactions between individual single molecules were tested [159] and hydrophobic interactions at extended scales were probed as a function of the ion concentration in solution [160] and as a function of the hydrophobic surface area [161].

Further, it was shown how the arrangement of individual bonds in an adhesive junction allows a tuning of adhesive strength even without changing the underlying adhesive bond. Using bifunctional designer peptides it was possible to manipulate the number of interacting bonds in parallel and in series [162] and to modulate adhesion at will. Interaction free energies of peptides could successfully be measured with various surfaces [163,164]. Specifically, marine animals such as mussels and barnacles e.g. use an optimized hierarchical structure and a large variety of functional peptides sequences in order to achieve unprecedented adhesion in high salt concentration environments. Also the adhesion of sequences of the barnacle proteins [165] and functional groups that are abundant in mussel foot proteins [166], were successfully tested at the single molecular level.

2. *Molecular structuring at solid/liquid interfaces*

Electric double layers in static and dynamically changing systems were studied in a close collaboration with the cluster of excellence RESOLV at Ruhr-Universität Bochum. White light interferometry in an electrochemical surface forces apparatus allowed to simultaneous decipher both sides of an electrochemical solid/liquid interface [167], with microsecond resolution under dynamically evolving reactive conditions that are inherent to technological systems in operando. Quantitative *in situ* analysis of the potentiodynamic electrochemical oxidation/reduction of noble metal surfaces showed that Angstrom thick oxides formed on Au and Pt are metallic or highly defect-rich semiconductors, while Pd forms a non-metallic oxide. On the solution side, previously unknown strong electrochemical reaction forces were observed, which are due to temporary charge imbalance in the electric double layer caused by depletion/generation of charged species. The real-time capability of our setups revealed significant time lags between electron transfer, oxide reduction/oxidation, and solution side reaction during a progressing electrode process. Comparing the kinetics of solution and metal side responses provides evidence that noble metal oxide reduction proceeds via a hydrogen adsorption and subsequent dissolution/re-deposition mechanism [167].

In collaboration with Frank Renner (University of Hasselt, Belgium) also battery fluids were intensively

studied [168]. Different wetting behaviour and wetting thicknesses of confined areas were observed, depending on the chemistry of the confining surfaces. This work suggests limits to effective wetting in battery devices and suggested that fluid transport along graphene pores is very effective compared to other materials. In a collaboration with the team of J. Maier (Max Planck Institute Stuttgart) glyme-based battery electrolytes were studied using the surface forces apparatus [169]. Based on comparing with interfacial spectroscopy data a model for the interfacial structure of triglyme electrolytes on muscovite mica was proposed. A surprising result of great fundamental significance is that the effective screening length measured by surface force apparatus at considerable lithium triflate concentrations (above 0.2 M) is substantially higher than expected from the Debye-Huckel theory, which is in line with data found for ionic liquids.

3. *Crevice corrosion, electrochemistry in confined spaces and high resolution imaging*

As already mentioned above the SFA was also utilized for corrosion studies in confined spaces [47, 170].

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## Research Projects in Progress

**Electrocatalysis (K. Mayrhofer)**

*Göhl, Mayrhofer, Ledendecker:* Investigations of PtTM@HGS catalysts for fuel cell applications

*Göhl, Mayrhofer, Ledendecker:* Development of core-shell catalysts with improved durability

*Kasian, Mayrhofer, Gault:* Atomic-scale insights into surface species of electrocatalysts in three dimensions

*Kasian, Mayrhofer:* Fundamental investigation of stability of electrocatalysts for oxygen evolution reaction

*Kulyk, Mayrhofer:* Modelling of noble metal dissolution

**Interface Spectroscopy (A. Erbe)**

*Chen, Kasian, Tecklenburg, Rabe, Mayrhofer, Erbe*: Mechanistic investigations of electrochemical oxygen evolution on manganese-based model electrodes

*Tecklenburg, Erbe*: Defect formation in ZnO formed during corrosion processes

*Pander, Tecklenburg, Wippermann, Erbe*: *In situ* spectroscopic characterisation of the oxide-free silicon/electrolyte interface

*Rabe, Erbe*: Designing novel smart sensor interfaces based on a biologically abundant peptide motif: coiled-coils

*Rechmann, Krzywiecki, Erbe*: Synthetic molecular models for passive films

*Ebbinghaus, Rabe, Erbe*: *In situ* chemical imaging of processes during cathodic delamination

**Corrosion (M. Rohwerder)**

*Beley, Palm, Rohwerder:* Fundamental investigation of hydrogen in iron-aluminium intermetallics

*Da Silva, Rohwerder*: investigation of oxygen uptake and its effect on short term internal oxidation

*Giesbrecht, Rohwerder*: Fundamental investigation of the emersed electrochemical double layer

*Kerger, Rohwerder*: *In situ* investigation of electrochemical reduction and oxidation processes by ambient ESCA

*Kim, Vogel, Rohwerder*: Investigation of surface oxides on bipolar plates of stainless steels

*Krieger, Springer, Zou, Rohwerder*: Fundamental investigation of role of microstructure on hydrogen embrittlement and effect of exposure time

*Merz, Rohwerder*: Investigation of optimal distribution of conducting polymer within an organic coating and at the interface with the metal for achieving optimal corrosion protection

*NN, Rohwerder*: Investigation of oxygen reduction at the interface between metal and organic coating by use of a novel permeation based technique

*Tran, Groche, Rohwerder*: Interface modification for optimized cold forging of aluminium-steel joints and their corrosion behaviour

*Tran, Rohwerder*: Investigation of the potential use of Kelvin Probe for detection of corrosion at the inside of tank and pipeline walls

*Uebel, Katsura, Rohwerder*: Role of microstructure in zinc alloy coatings on corrosion performance

*Uebel, Yin, Rohwerder*: Fundamental investigation of coating requirements for fast self-healing of large defect sites in organic coatings

*Wu, Krieger, Rohwerder*: spatially resolved and ultra-sensitive hydrogen detection in steels and investigation of hydrogen uptake

*Wu, Rohwerder:* SKP for the investigation of hydrogen in metals: further developing the technique

**Interaction Forces and Functional Materials (M. Valtiner)**

*Moreno-Ostertag, Spohr, Valtiner:* Fundamentals of molecular adhesion under electrochemical conditions

*Merola, Lorke, Valtine*r: In operando study of corrosion in confined spaces using white light interferometry

**Atomistic Modelling (S. Wippermann)**

*Adi Nugraha, Wippermann:* Point defects at SiC/$SiO_2$ interfaces

*Adi Nugraha, Wippermann:* Anomalous temperature-dependent band gap shift of CdSe nanocrystals

*Alaydrus, Wippermann:* Multi-exciton generation in core/shell nanocrystals

*Razzaq, Wippermann:* Solitonic excitations in one-dimensional charge density waves with topological properties

*Yang, Wippermann: Ab initio* description of solid/liquid interfaces with finite electric fields

*Khanifaev, Wippermann: Ab initio* molecular dynamics simulations at constant electrode potential

# Department of Microstructure Physics and Alloy Design

*D. Raabe*

## Scientific Mission and Department Structure

We work on the relationships between **synthesis, processing, microstructure and properties** of compositionally and structurally **complex metallic alloys** including steels, magnesium, aluminium, superalloys, titanium and high entropy alloys. Focus is placed on **phase transformations,** design of **metastable phases**, **micromechanics** and complex **defect substructures** as well as their effects on the **mechanical** and **functional properties** [1-16].

We pursue these goals by developing and applying **advanced characterization** methods from the atomic level up to the macroscopic scale. Examples are chemically sensitive Field Ion Microscopy (FIM) which is based on the integration of atom probe tomography (APT), FIM and machine learning as well as correlative APT and scanning transmission electron microscopy (STEM) in concert with a reaction chamber and an ultrahigh vacuum (UHV)-cryo transfer unit [17-30]; Electron Channeling Contrast imaging under controlled diffraction conditions (ECCI) [31-35]; 3D electron backscatter diffraction (EBSD) and cross-correlation EBSD [36-38]; *in situ* micromechanical experiments correlated to local strain and hydrogen mapping [39-51]; and standardized bulk high-throughput metallurgy and mechanical testing [52-56]. Several of these techniques are developed and operated in collaboration with the MPIE-groups of G. Dehm, C. Scheu, M. Rohwerder and with R. Dunin-Borkowski (Ernst Ruska Centre in Jülich), J. Schneider (RWTH Aachen) and G. Eggeler (Ruhr-Universität Bochum).

We design **experiments based on theory-guidance** and conduct them under well controlled boundary conditions: For example for better understanding, quantifying and improving our atomic scale APT and FIM probing methods we collaborate with the department of J. Neugebauer on the simulation of field evaporation and image gas ionization as well as on the use of machine learning for crystallographic pattern recognition in APT data sets. Regarding **thermodynamics** and **structure–property relations,** we also collaborate with in-house *ab initio* experts for instance on phase equilibria for bulk and confined states and the thermodynamics of high entropy alloys [57-61]. Concerning **constitutive simulations** we have developed further our in-house modular **freeware simulation package DAMASK** (Düsseldorf Advanced Material Simulation Kit). This is a hierarchically structured model of material point behaviour for the solution of elastoplastic boundary value problems along with damage and thermal effects [40,41,62-70].

As an example, one topic where many of these fields of interest overlap in the department, is the interplay of **local chemical composition**, **phase metastability** and **transformations in confined regions**, i.e. at decorated lattice defects [1-12]. Correlative atomic-scale probing and thermodynamic theory show that in many alloys segregation to lattice imperfections is an ubiquitous phenomenon, yet, it is typically acquired through trapping of atoms to defects during tempering rather than being engineered

**Fig. 1:** *The Microstructure Physics and Alloy Design team.*

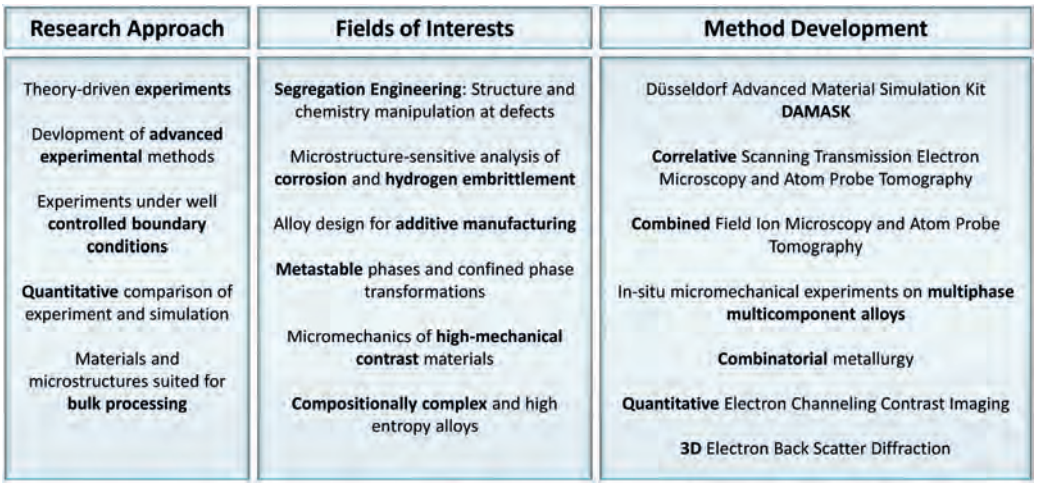


**Fig. 2:** *Research approach, interests and long-term method development in the Department of Microstructure Physics and Alloy Design.*

in a purposeful and property-directed manner. This has motivated us to conduct systematic **'Segregation Engineering'** experiments and develop from that corresponding alloy design and processing strategies where we utilize Gibbs and Fowler-Guggenheim – type decoration of lattice defects with the aim to turn these regions into chemo-structural entities that lead to beneficial mechanical and functional behaviour. This site specific manipulation of confined defect regions by chemistry has for example allowed us to tune lattice defects for improved local **cohesion**, **confined phase transformation**, **scattering**, **fracture toughness** and **impurity trapping**. Specific thermodynamic phenomena that we discovered in this context are composition-driven phase **transformations of dislocation cores** [1,5,9], confined **hydrides** [13,14], **stacking faults** [16,15], **spinodals** at grain boundaries and dislocations [1,5], and confined phase states and precursors phases preceding **nucleation** [1,5]. With these approaches and topics we conduct **materials engineering down to the atomic scale** (Fig. 2).

## Research Groups

The department is organized in scientific groups some of which are extramurally funded and non-permanent (Fig. 3).


**Fig. 3:** *Research groups in the Department of Microstructure Physics and Alloy Design. The upper 5 groups (bold) are permanently funded. The bottom 5 groups are temporary initiatives, which are funded by grants.*

### Mechanism-based Alloy Design (D. Ponge)

The group **'Mechanism-based Alloy Design'** works on the microstructure-oriented **design of advanced high strength steels**, **high entropy alloys** as well as on engineering **Al-, Ni- and Ti-alloys** [1-10,71-81]. Projects focus on multiple strain hardening mechanisms such as the interplay of dislocations, twins and deformation driven phase transformations. Of special interest are confined phase transformation phenomena at grain boundaries and dislocations. Projects in the group make intense use of the processing, mechanical testing and microstructure characterization facilities at the MPIE down to the atomic scale. Project are pursued in collaboration with partners from modelling, APT and microscopy. Theory-guided thermomechanical processing is a main pathway for optimizing the microstructures and mechanical properties of complex alloys. In this context a main objective of projects in this group lies in understanding and utilizing **elemental and mechanical partitioning** effects among neighbouring phases on the one hand and among the matrix and lattice defects on the other hand with the aim to adjust the (meta-)stability of local phase states. Depending on phase stability, deformation driven thermal transformations can be triggered such as spatially confined transformation-induced plasticity (**TRIP**) and transformation-inducted twinning (**TWIP**).

Main examples are the design of ultrafine grained, partially metastable, maraging, multiphase, medium-Manganese, martensite-to-austenite reversion and weight reduced steels for automotive, manufacturing and infrastructure applications.

### Atom Probe Tomography (B. Gault)

The group '**Atom Probe Tomography (APT)**' explores compositionally complex structural and functional materials based on the near-atomic scale information obtained from APT and FIM [13-30]. It operates three local electrode APT instruments (Cameca LEAP 3000X HR, LEAP 5000XS, LEAP 5000HR) and, for specimen preparation, three focused-ion beam microscopes, including one with a Xe-plasma source. A UHV-cryo transfer unit is used to transport sensitive materials between a glovebox with atmosphere control, and a reaction chamber. APT is a high-resolution characterization technique for 3D elemental mapping with near-atomic resolution. APT allows for studying nanoscale phenomena such as **precipitation**, solute **clustering**, **segregation** at defects, **complexions** and **partitioning** [1-11]. Important methodological progress lies in the use of correlative APT with scanning transmission electron microscopy and with FIM, as well as joint efforts with machine learning and *ab initio* simulations to aid the interpretation of the complex data. Projects are conducted in close collaboration with other groups and departments. On the metallurgical side, projects in this group are mainly concerned with Ni- and Co-based **superalloys, energy conversion materials, high- and medium Mn steels**, **stable hydrides**, **intermetallic**s, **Ti**-alloys and **high entropy alloys** [1-30,83-97], often in close collaboration with the group **Mechanism-based Alloy Design**.

### Combinatorial Metallurgy and Processing (H. Springer)

The group '**Combinatorial Metallurgy and Processing**' designs advanced structural materials along with suited synthesis and processing routes and techniques. The focus lies on steels with superior physical and mechanical properties. Projects explore novel pathways for the compositional and thermo-mechanical **high-throughput** bulk **combinatorial** investigation of structural alloy systems [52-56]. Innovative methods for the **accelerated synthesis**, processing and testing of bulk metallic structural materials are developed and applied, so that underlying metallurgical questions such as alloy- and processing-sensitive changes in strain hardening can be addressed more efficiently over a wide composition and processing range. The methods are thus referred to as '**Rapid Alloy Prototyping**' (RAP). This approach refers to semi-continuous high-throughput bulk casting, rolling, heat treatment and sample preparation, and allows for evaluating base alloys in up to 50 different bulk conditions within a week. The approach is applied to metal matrix steel composites with high elastic stiffness, martensite-to-austenite reversion steels, weight reduced FeMnAlC steels, and medium and high entropy alloys.

### Microscopy and Diffraction (S. Zaefferer)

The group '**Microscopy and Diffraction**' pursues two correlated tasks: on the one hand, its projects aim at understanding microstructure formation mechanisms and the relation between microstructures and properties of materials by investigations at the microscopic level. To this aim, several SEM-based microscopy and **electron diffraction techniques** (EBSD, 3D EBSD, XR (cross-correlation)-EBSD, ECCI) have been developed and advanced [39]. Imaging and diffraction in transmission electron microscopy (TEM) and x-ray diffraction is conducted as well. With respect to microstructures the focus is on deformation, recrystallization and phase transformations. Concerning properties corrosion, mechanical behaviour and electronic properties are studied. The spectrum of materials comprises DP (dual phase) steels, TRIP steels, complex phase steels, quench and partitioning steels, electrical steels, austenitic steels, superalloys, Mg-, Al- and Cu alloys, intermetallic compounds and photovoltaic materials. The group operates several instruments, e.g. a Zeiss Crossbeam XB1560 FIB-SEM for **3D EBSD** investigations, a JEOL JSM 6500 F SEM, and a JEOL JSM 840A SEM. These instruments are equipped with EBSD, *in situ* deformation and heating tools. For TEM a Phillips CM 20 is used. This instrument is equipped with the software **TOCA** for on-line crystallographic analysis.

### Theory and Simulation (F. Roters)

The group '**Theory and Simulation**' develops mechanism-based constitutive models [40,41,62-70] for a wide range of engineering alloy groups, focusing on crystal plasticity and multiphysics problems. Models range from phenomenological descriptions to physics-based formulations of **dislocation** slip, **twinning induced plasticity** (TWIP), **martensitic transformations** (TRIP), microstructural damage evolution and recrystallization effects as well as the associated temperature evolution. The models describe the evolution of lattice defects such as dislocations and twins under given mechanical or thermal boundary conditions. The predicted defect densities enter into kinetic structure-property relations that translate them into strength and deformation measures. Owing to the crystalline anisotropy of metallic alloys, the constitutive laws assume a tensorial form both in their elastic and plastic formulations, i.e. they

predict the defect evolutions on all crystallographic shear and twinning systems and their interactions. The resulting sets of nonlinear internal-variable differential equations are solved in a fully coupled way using either the **Finite Element Method** (FEM) or a **Spectral Method** (FFT). The models are accessible through the modular simulation framework DAMASK with multiple academic and industrial users worldwide (https://damask.mpie.de) (see p. 50).

### Alloys for Additive Manufacturing (E. A. Jägle)

The group '**Alloys for Additive Manufacturing**' was established in 2015 [82]. While particularly **Laser Additive Manufacturing** (LAM) is well-established to produce metallic parts, the design and further optimisation of alloy concepts tailored to match and utilize LAM requirements are still missing. Established alloys currently in use often do not exploit the opportunities inherent in this technique such as the rapid quenching, the intrinsic heat treatment coming from the next layers' deposition, and the metal-gas interaction during the process, leaving a gap for further development. Funding for the group comes from the joint Max Planck Society/ Fraunhofer Society research project "AProLAM" - **Advanced Alloys and Process Design for Laser Additive Manufacturing of Metals**. In this project, the two partners Max-Planck-Institut für Eisenforschung (MPIE) and Fraunhofer Institute for Laser Technology (ILT) work together on the development of alloys for the LAM process and at the same time on the adaptation of the LAM process for the synthesis of new alloys. The group operates an Aconity 3D SLM research size instrument and an in-house developed EIGA-type lab-scale atomizer for powder production. Projects examples are LAM of Fe-19Ni-xAl **maraging steels** with extremely high NiAl nanoprecipitation densities of $10^{25}$ NiAl precipitates per $m^3$, Al-Sc alloys and superalloys. Additional funding for the group comes from several projects of the German Research Foundation (DFG), including work on LAM of High Entropy Alloys.

### Hydrogen in Energy Materials (B. Gault)

Recently a new group on **'Hydrogen in Energy Materials'** was established, funded by an **ERC Consolidator Grant** awarded to B. Gault. It is concerned with the **3D mapping of hydrogen** at near-atomic scale in metallic alloys with the aim to better understand hydrogen storage materials and hydrogen embrittlement. His approach is based on using an ultrahigh vacuum cryogenic transfer unit which connects two state-of-the-art atom probe microscopes with a scanning electron microscope fitted with a xenon-plasma gun. Through a precise control of H-loading into the specimen, the quality of the data will be enhanced drastically while at the same time using data mining and machine learning techniques for data interpretation. More details on this new initiative are given on page (see p. 70).

### High-Entropy Alloys (Z. Li)

The new group on **'High-Entropy Alloys'** which is funded by a grant of the German Research Foundation (DFG) explores novel high- and medium entropy alloys with respect to the identification of promising composition and process routes for new compositionally complex metallic alloys with excellent combinations of mechanical, physical and chemical properties based on the understanding of their structure-properties relations [91-104]. Conventional alloy design over the past centuries has been constrained by the concept of one or two prevalent base elements. As a breakthrough of this restriction, the concept of HEAs opens a new realm of numerous opportunities for investigations in the huge unexplored compositional space of **multi-component alloys**. While conventional alloys use strengthening mechanisms such as grain boundaries, **dual-phase** structure, dislocation interactions, precipitates and solid solution, our recently developed novel **interstitial TWIP-TRIP-HEAs** concept combines all available strengthening effects, namely, interstitial and substitutional solid solution, TWIP, TRIP, multiple phases, precipitates, dislocations, stacking faults and grain boundaries. This leads to the exceptional strength-ductility combination of the novel HEAs, exceeding that of most metallic materials. Several groups of HEAs with specific property spectra are currently studied by the group: These are alloys with excellent **strength-ductility** combinations; enhanced **resistance to hydrogen-embrittlement**; reduced mass density and high-strength; high-temperature refractory properties; and with multifunctional features such as good **cryogenic toughness** combined with specific **magnetic** features and **invar** properties (see p. 60).

### Materials Science of Mechanical Contacts (M. Herbig)

The new **'Materials Science of Mechanical Contacts'** initiative is primarily funded by the federal ministry Bundesministerium für Bildung und Forschung. The group works on the metallurgical fundamentals of intense mechanical and environmental cyclic contact phenomena such as encountered in biomedical hip **implants**, **gears**, **bearings** and **railway** systems. In case of cyclic contact loading the microstructure never reaches a stable condition but evolves over time. Usually connecting liquid media such as lubricant or biofluids are involved leading to the formation of a reaction layer at the surface, the composition and structure of which can have an enormous influ-

ence on the overall lifetime of the part. The top layer of materials bearing such high cyclic contact loads for a longer time usually is comprised of a complex nanocrystalline multi-phase microstructure and thus understanding these phenomena requires joint crystallographic and chemical characterization from the micrometre down to the atomic scale. Details are given on p. 31.

**Advanced Functional Materials (O. Cojocaru-Mirédin)**

The group '**Advanced Functional Materials'** aims to understand the relationship between the chemical, electrical, and structural properties of microstructure-dominated functional materials such as solar cells and thermoelectrics. Focus is placed on **multicrystalline silicon** (m-Si) solar cells, and $Cu_2ZnSnSe_4$ (CZTS) and $Cu(In,Ga)Se_2$ (CIGS) **thin-film solar cells** and AgSbTe compounds for **thermoelectric applications**. To better understand these materials the group performs correlative studies using joint ECCI / EBSD / STEM, electron beam-induced current (**EBIC**) / **cathodoluminescence**, and **APT** [17]. The mission is to optimize the efficiency of solar cells and thermoelectrics based on the understanding of the interplay of local defect structures and 3D chemical analysis at the atomic-scale. The atomic redistribution of the impurities at the internal interfaces (grain boundaries and p-n junction) may affect the efficiency of a solar cell. For example, the efficiency of a CIGS solar cell has been improved by almost 50% only by Na doping (~ 0.1 at.%) inside the absorber layer. Furthermore, it was observed that this increase in the efficiency can be directly correlated with the Na segregation at the CIGS grain-boundaries. The group was originally financed by the NanoMatFutur competition awarded by the federal ministry Bundesministerium für Bildung und Forschung. The group leader has a joint appointment as group leader both at RWTH Aachen and at the MPIE.

## Main Research Interests

The objectives of the research groups and their core competences were described above. Here we present our **recent progress** in a number of **key interdisciplinary areas of interests** in the department which are **jointly pursued** by members of different groups including also members from other departments. More specific **scientific details** about some of these projects are given in the section **"Interdepartmental Research Activities - Selected Highlights".**

**Segregation Engineering: Structure and chemistry manipulation of lattice defects**

**Dislocations** and **interfaces** influence mechanical, functional, and kinetic properties of alloys. They can be manipulated via **solute decoration** enabling changes in energy, mobility, structure, cohesion and promote local phase transformation. In our approach termed **'segregation engineering**' solute decoration is not regarded as an undesired phenomenon

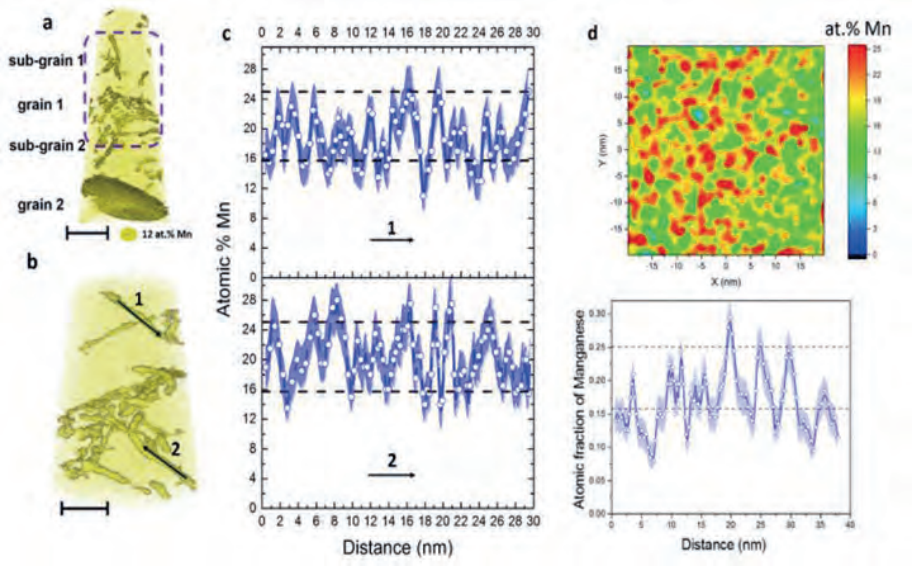


**Fig. 4:** *Locally confined spinodal decomposition states observed at lattice defects in a Fe-9 at. % Mn solid solution revealed by atom probe analysis. a) Dislocations decorated with Mn after 6h at 450 °C revealed by 12.5 at.% Mn iso-concentration surfaces to highlight the Mn-enriched regions showing a grain boundary and numerous dislocations decorated by Mn. Scale bar, 40 nm. b) Close-up on the middle section indicated by the dashed line showing decorated dislocations. Scale bar, 30 nm. c) 1D composition profiles along the two dislocations marked by the arrows in b). The points are the experimental values, which are connected by blue lines for better visualization. d) Spinodal decomposition viewed in the grain boundary plane and in form of a 1D profile through that plane [5].*

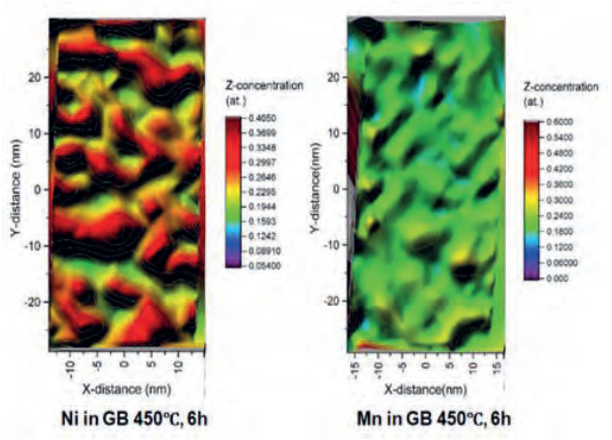


**Fig. 5:** *Spinodal decomposition viewed in the grain boundary plane in a FeMnCoNiCr Cantor High Entropy Alloy at 450°C after 6h acting as precursor state for intermetallic phase formation.*

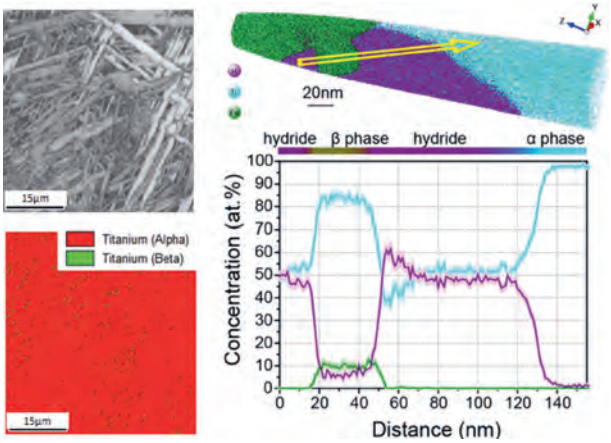


**Fig. 6:** *Multiscale characterization of solute H in a Ti-2wt%Fe matrix in the 950°C/45min-quenched state. Observation of hydrides on the α/β phase boundary.*

but it is instead utilized to manipulate specific defect structures and properties via composition change through Gibbsian decoration [1-10].

In that context we observed that **grain boundary (GB) segregation** and subsequent local austenite reversion of these decorated interface regions can turn interface embrittlement into toughness. In a Fe-9 wt.% Mn martensite we studied **grain boundary embrittlement** in the quenched and tempered state. While solute Mn directly embrittles martensite grain boundaries, reversion of martensite back to austenite at grain boundaries cleans the interfaces from solute Mn by partitioning the Mn into the newly formed austenite, hence restoring **impact toughness and fatigue resistance** [2]. Also, we discovered that Gibbs segregation to lattice defects, being a local equilibrium state, shifts the chemical working point from the material's bulk composition to a locally much higher composition. With this substantial shift in local equilibrium concentration at lattice defects compared to the bulk a number of thermodynamic phenomena can be observed at defects that do not occur in the adjacent bulk regions. Examples are spinodal decomposition, confined phase formation, complexion and confined phase transformation effects which are thermodynamically possible only at equilibrium doped lattice defects (see p. 169). Fig. 4 shows spinodal decomposition effects along dislocations and in grain boundary planes in the Fe-Mn system. The Fowler-Guggenheim segregation upon tempering shifts the decorated defects into a compositional range of the (local) phase diagram that is not readily accessible to the bulk. Similar interface **spinodal** decomposition effects were observed also on the grain boundaries of a FeMnCoNiCr Cantor high entropy alloy, where they act as precursor states for intermetallic phase formation (Fig. 5) (see p. 185).

### Microstructure-sensitive analysis of corrosion and hydrogen embrittlement

One of the main challenges in the field of **corrosion science** lies in identifying the relations between **microstructure features** and the associated electrochemical or physical reactions, respectively, such as **oxidation** [28,29,97] and **hydrogen embrittlement** [30,47-51]. In this context, measurements including sufficient spatial resolution of the associated phenomena down to the lattice defect scale are still hard to realize. Yet, the role of individual lattice defects and surface features together with a characterization of their individual structural and chemical state is essential for understanding corrosion and the resulting decay and failure mechanisms. Specifically **site-specific microstructure and composition characterization** is of great relevance. Instrumentation we use in this context are **correlative atom probe tomography**, **Scanning Kelvin Probe** mapping (together with M. Rohwerder) in conjunction with EBSD and ECCI as well as **nanoSIMS** maps. In the context of imaging hydrogen and deuterium at the atomic scale particularly the new atom probe laboratory which is equipped with a cryo-transfer unit and a charging glove box is essential. Its use allows charged samples to be exchanged and probed among different microscopes and atom probes without any exposure to air or elevated temperatures (see p. 34) (Fig. 6). More details on the latest instrumental progress at the MPIE are presented on p. 70 and 179. Atom probe analysis plays also an increasingly important role in electrocatalysis, where it serves in revealing oxides and intermediate products of the first few atomic layers of thermally and electrochemically grown iridium oxides (Fig. 7) (see p. 163).

### Alloy design for additive manufacturing

The **design of novel alloys** which are particularly suited to utilize the specific processing features associated with **Laser Additive Manufacturing** (LAM) is a key challenge in materials science. LAM processes allow production of small, custom-made parts directly from a Computer Aided Design model and metal powders. In the melt pool, the powder is completely melted. The resulting, dense

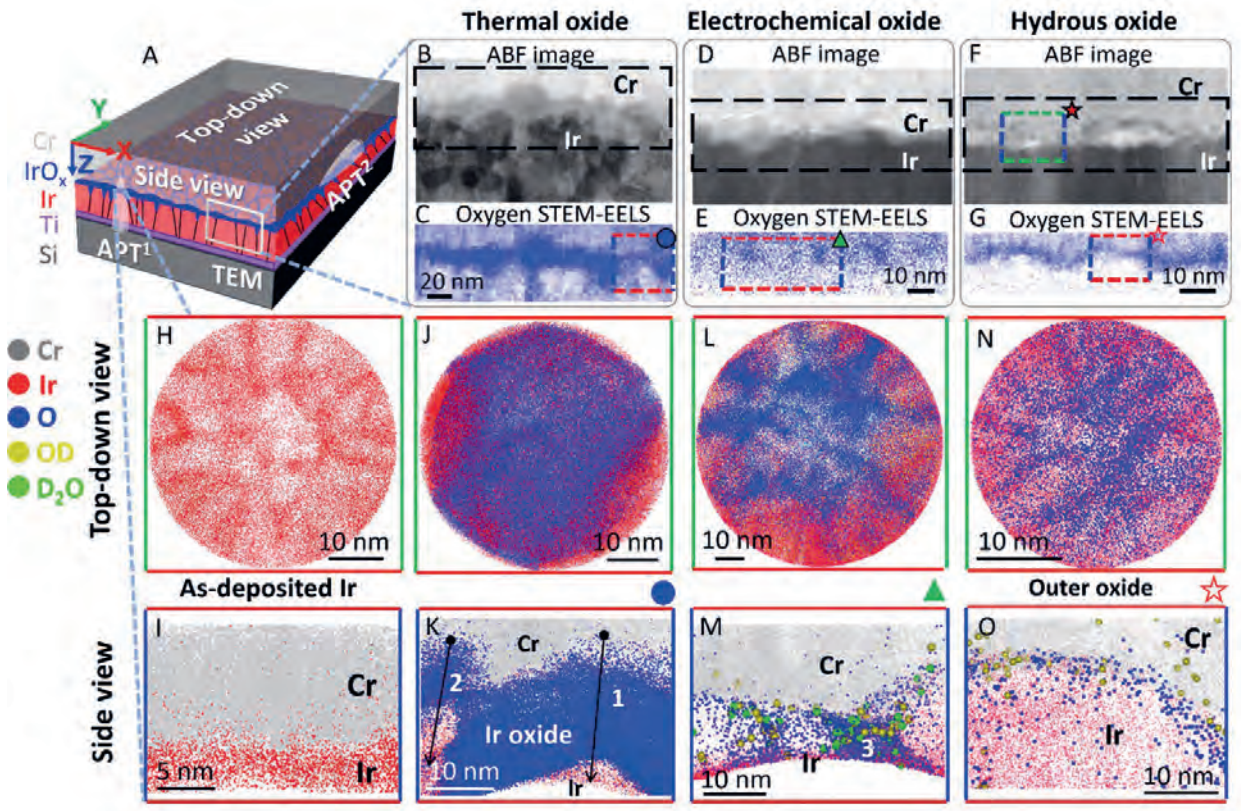


**Fig. 7:** *Multiscale characterization of the three-dimensional nanostructure of the first few atomic layers of thermally and electrochemically grown iridium oxides, efficient electrocatalysts for the oxygen evolution reaction. Atom probe analysis allows to image both the composition and its distribution of the metallic nanoparticles and also the oxides and some of the intermediate products which could be revealed by using heavy water, i.e. with deuterium [12]. This project is conducted in close collaboration with O. Kasian from the GO department, K. Mayrhofer from HGF Erlangen and T. Li from Ruhr-Universität Bochum.*

parts can have similar or even better mechanical properties than conventionally produced bulk metal. Two main aspects of the LAM process are particularly important in this context: Firstly, high cooling rates can be achieved during solidification (~$10^2$-$10^5$ $Ks^{-1}$) due to the small melt pool size and effective heat conduction into the underlying layers and the substrate. Secondly, as the laser passes by a previously deposited material volume during deposition of neighbouring tracks and subsequent layers, the material experiences cyclic reheating with gradually decaying temperature. This type of intrinsic heat treatment consists of sharp temperature pulses up to temperatures that may even be close to the melting point.

We work on several key material classes such as Ni-base **superalloys**, **tool steels** and **high strength Al-alloys** with the aim to design alloy variants which allow exploiting these processing features for manufacturing as-synthesized parts with improved properties.

One example is the successful combinatorial development of a model maraging steel consisting of Fe, Ni and Al, that shows a pronounced response to the intrinsic heat treatment imposed during the LAM process. Maraging steels belong to a class of Advanced High Strength Steels (AHSS) that combine ultra-high strength with good toughness and ductility. They are of great importance in tooling, aerospace and energy industries. Without any further heat treatment, it was possible to produce a maraging steel that is intrinsically precipitation strengthened by an extremely high number density of 1.2x$10^{25}$ $m^{-3}$ NiAl nanoparticles of 24 nm size. The high number density is related to the low lattice mismatch between the martensitic matrix and the NiAl phase (Fig. 8).

**Metastable phases and confined phase transformations**

Utilizing the **segregation engineering** approach presented above we developed a class of novel materials which we refer to as **Reversion Alloys**. These are ductile intrinsically structured **micro- and nano-laminate alloys** that are formed in a self-organized way by reheating as-quenched microstructures and phases such as martensite in steels or Ti alloys so that spatially confined segregation-driven reversion from martensite back to the high temperature phase such as austenite in steels occurs at the lattice defects that were first decorated by **equilibrium segregation** (Fig. 9). This reversion heat treatment can be conducted at modest temperatures and times to create very fine regions of metastable phase revision

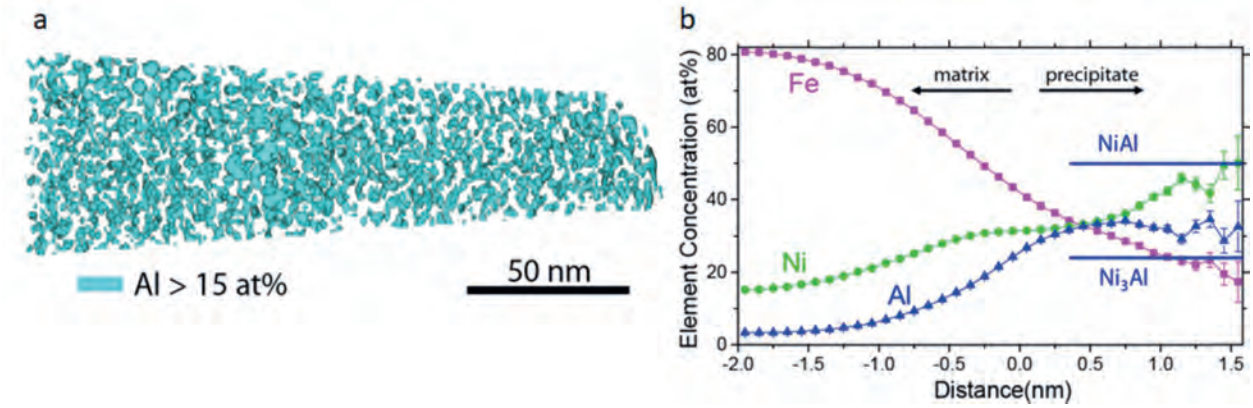


**Fig. 8:** *a) Precipitates in a lean Fe-Ni-Al LAM manufactured maraging steel visualized by drawing an isoconcentration surface at 15 at% Al. b) Corresponding proximity histogram plotting the chemical composition as a function of the distance to the isoconcentration surface. Expected Al concentrations for NiAl and Ni3Al are shown. The intrinsic heat treatment caused by the layer-by-layer build-up creates an extremely high number density of 1.2x10$^{25}$ m$^{-3}$ NiAl nanoparticles of 2.4 nm size and very high hardness. The work is conducted in collaboration with the Fraunhofer Institute for Laser Technology in Aachen.*

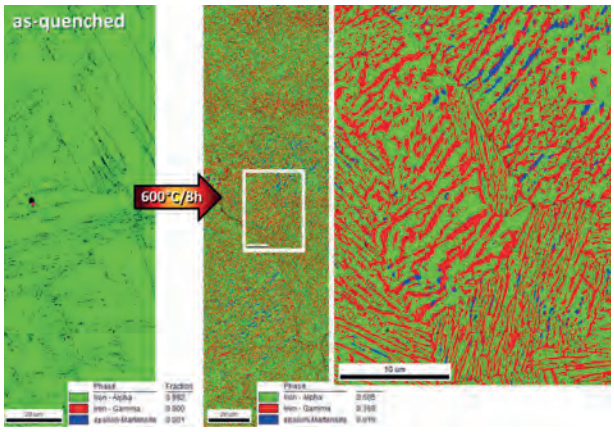


**Fig. 9:** *Grain boundary segregation followed by confined reversion transformation from as-quenched Fe-Mn martensite into metastable austenite enables the design of damask-type martensite-austenite nanolaminate steels where the solute decorated lath interfaces transform back to austenite.*

zones. This concept has proven particularly useful when designing nano-reversion steels with bone-like properties (Fig. 10). Such alloys unify **hierarchical nanostructures** consisting of a metastable nanolaminated morphology. Upon local mechanical loading due to the propagation of a crack the metastable reversed austenite laminate layers undergo a TRIP effect and transform locally. Such local TRIP effect leads to crack blunting and additional strain hardening and thus to excellent fatigue properties.

### Micromechanics of high-mechanical contrast materials

**Multiphase microstructures** containing phases with **high mechanical contrast** are the basis for many advanced alloys, particularly multiphase steels. As examples medium manganese-, quench-partitioning- and **dual-phase (DP) steels** take prominent positions in current efforts to quantitatively translate the

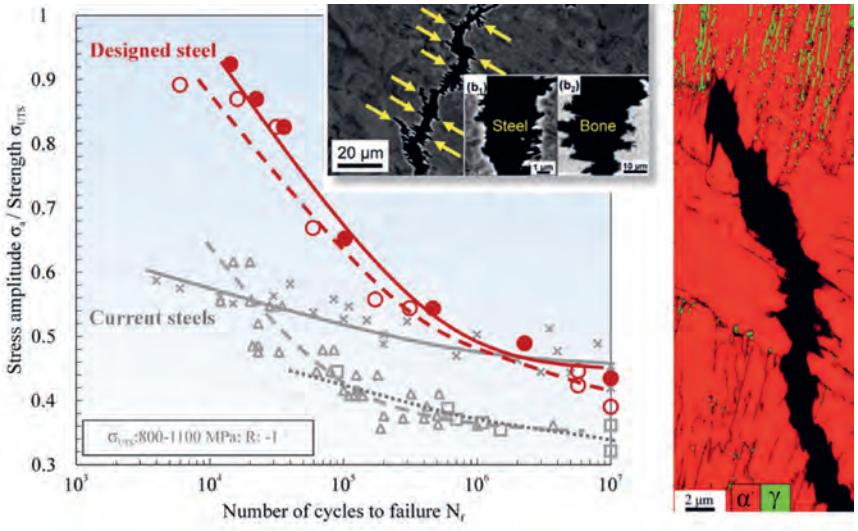


**Fig. 10:** *Microstructure and properties of a new nano-reversion steel with bone-like properties. The material unifies hierarchical nanostructures consisting of a metastable nanolaminated morphology. The EBSD map reveals that the metastable reversed austenite laminate layers undergo a TRIP effect and transform locally when exposed to the local stresses created by the crack. This effect leads to local crack blunting and additional strain hardening and thus to excellent fatigue properties [8]. The work was conducted in collaboration with C. Tasan from MIT and M. Koyama and K. Tsuzaki from Kyushu University.*

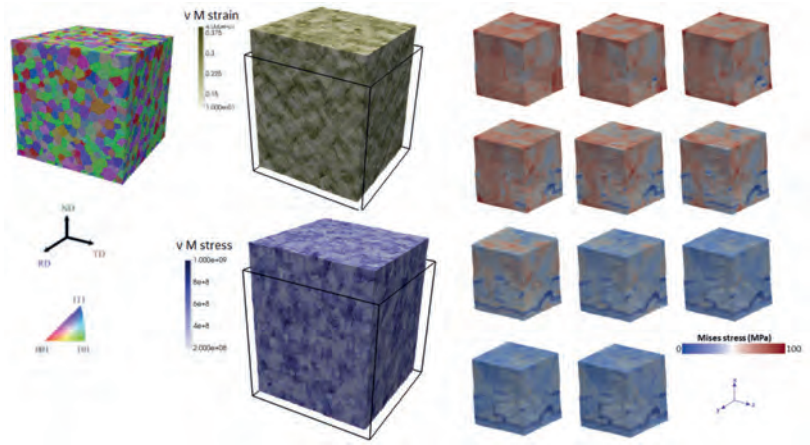


**Fig. 11:** *Representative volume element models of complex high-mechanical contrast microstructures such as encountered in multiphase steels or partially recrystallized materials (left). These simulations on artificial microstructural variants are used to systematically screen the influence of specific microstructural topologies, fractions as well as their strain hardening and damage parameters (middle). Particular efforts were recently placed on the development of advanced spectral solver methods for treating the associated boundary value problems more efficiently than the Finite Element method and on introducing damage models (right) into the simulations. All simulation tools are freely available under the umbrella of the DAMASK software package.*

features of complex microstructures into predictive models that can be used in processing and manufacturing. This is the core area of the micromechanical modelling activities in the department as described in more detail on page (see p. 50).

Handling the increased computational challenges associated with the underlying complex microstructures and the strong mechanical contrast among the phases requires not only improved **constitutive models** for strain hardening and damage but also an advanced numerical solution strategy that reaches beyond the established Finite Element solution approaches which are commonly used for solving corresponding **representative volume element models** [62-70]. These are simulations of artificial microstructural variants that are run routinely to systematically screen the influence of specific microstructural topologies, fractions as well as their strain hardening and damage parameters ( Fig. 11).

To this end, efforts in the department were particularly devoted to develop and improve **advanced spectral method** based approaches for solving the associated boundary value problems and to replace the much slower de facto standard Finite Element owing to its numerical inefficiency and mesh-dependence.

Additional efforts were likewise devoted to develop coupled *in situ* experimental approaches that can be coupled with the micromechanical simulations in the philosophy of an integrated computational materials engineering (ICME) approach (Fig. 12). All modelling features described here are freely accessible in

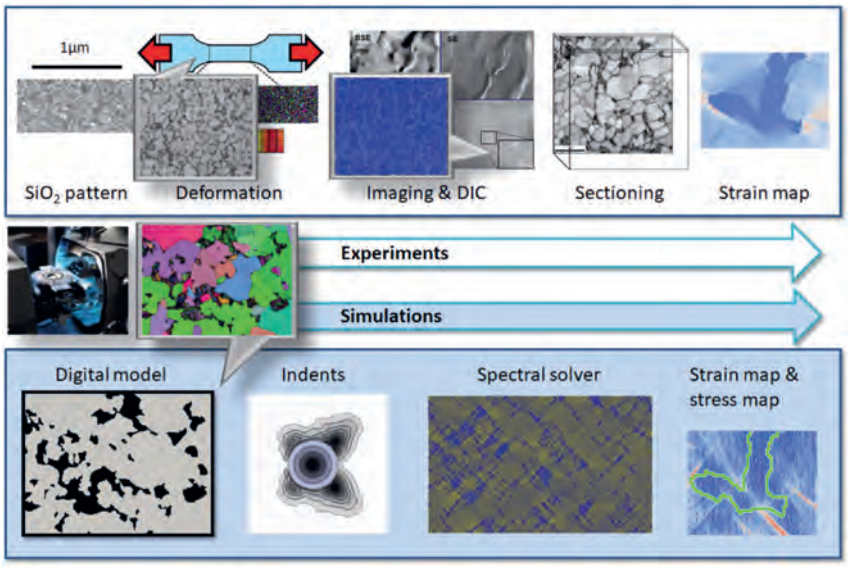


**Fig. 12:** *Example of an integrated computational materials engineering (ICME) approach applied to dual-phase (DP) steel: several types of in situ testing and parameter measurements are combined with micromechanical representative volume element models and full-field simulations using DAMASK.*

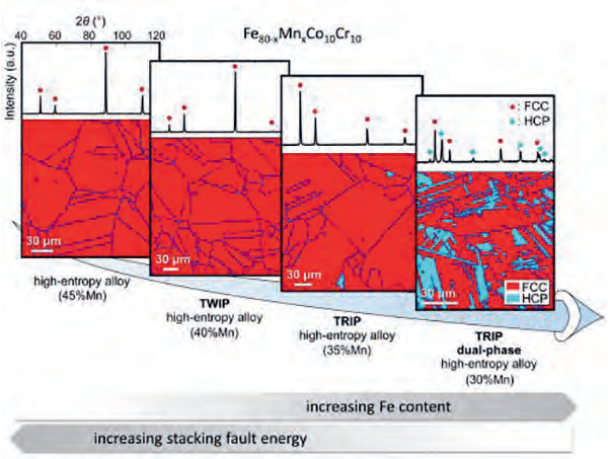


**Fig. 13:** *Change in the phase fractions (f.c.c.:red; h.c.p.: cyan) for the high entropy alloy system Fe(80-x)Mn(x) Co10Cr10 and the associated prevalent deformation mechanisms [94].*

our **Düsseldorf Advanced Materials Simulation Kit** (**DAMASK**) and can be downloaded at **https://damask.mpie.de.**

### Compositionally complex and high entropy alloys

Metallurgical alloying strategies have long been used to confer desirable properties on materials. Typically, it involves the addition of relatively small amounts of secondary elements to a primary element. A new alloying approach was recently introduced in which four, five, or more principal elements in high concentrations are combined to create novel materials called **high-entropy alloys** (HEAs). Some of these HEAs have already been shown to possess exceptional properties, exceeding those of conventional alloys (see p. 185).

Our specific approach to this field is a mechanism-based HEA design philosophy. This means that instead of conducting a systematic composition-screening of new HEAs we take a microstructurally- and **mechanistically-oriented design approach**. Traditional load carrying materials such as steels and aluminium alloys utilize specific strengthening mechanisms, considering also their dependence on temperature, stress and strain rate. Engineering such response over a more complex load path requires using not one effect alone but a sequence of mechanisms, including also their interplay and associated windows of operation. Examples are FeCrNi-based stainless or FeMnC-based TWIP steels, two alloy classes with some similarity to FCC HEAs [91-103]. These materials utilize marked **solid-solution** and **precipitation** strengthening, deformation **twinning**, ε-**martensite** and α-martensite, to name but a few characteristic mechanisms. The presence of solid solutions in these alloys not only strengthens the matrix but allows also for tuning of the stacking fault energy. Depending on its magnitude, its value affects the formation of partial dislocations and the occurrence of planar slip and double cross slip. This promotes the formation of rigid dislocation reaction products, dislocation storage rates, slip patterns and the evolving complex dislocation substructures. Reducing the stacking fault energy promotes the onset of twinning or martensite formation in the desired deformation, stress and strain rate window. The thermodynamic key-quantity for tuning all these features in these alloys is the **stacking fault energy** which can thus serve as one reliable governing alloy-design measure. In a mechanistic HEA design approach, the sequence of mechanism activation is also essential. For optimal strain hardening, dislocations alone are often not efficient since their multiplication can get

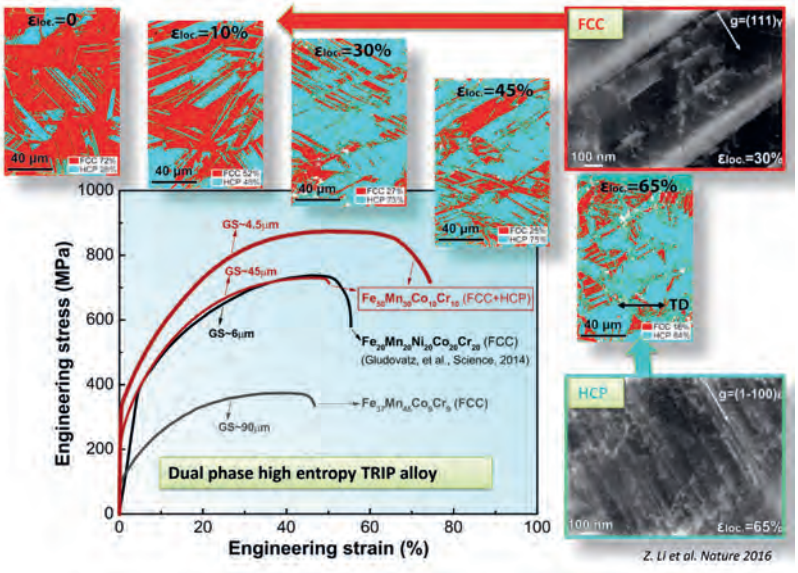


**Fig. 14:** *Engineering stress-strain curve, associated phase maps (red: f.c.c.; cyan: h.c.p.) and two exemplary dislocation substructures mapped by using Electron Channeling Contrast Imaging (ECCI) for the HEA Fe50Mn30Co10Cr10 (upper curve) for two different grain sizes (GS). The phase maps reveal the presence of the two phases prior to loading and the gradual martensitic transition from f.c.c. to h.c.p. at room temperature during tensile deformation. In the ECCIs, g is the diffraction vector [94].*

exhausted at early deformation stages, which is the result of the high initial strain hardening in common metals. Reducing the stacking fault energy enables mechanical twinning when the initial dislocation strain hardening gets weaker. When the additional strain hardening provided by mechanical **twinning** also gets exhausted, martensite formation could be activated if the stacking fault energy is sufficiently low (Fig. 13). We realize this alloy design strategy by developing for example non-equimolar and multi-phase derivatives of the Cantor alloy. Based on the equimolar Cantor alloy composition, several related variants with a smaller number of alloying components and non-equimolar compositions have been tested (Fig. 14).

## Main Recent Breakthroughs

In several cases we achieved breakthroughs over the past years. Some resulted from **unexpected and unplanned discoveries** [1,5,6,16-18], others were harvested from **long term and systematic developments** [19,20,22,27,30,33].

Regarding method development we have made substantial progress in conducting site-specific sample extraction in conjunction with **correlated ECCI-EBSD-(S)TEM-APT characterization, correlative time-of-flight FIM experiments**, i.e. the operation of joint FIM and APT experiments **and UHV cryo-transfer among different probes** and **charging devices** of sensitive samples. These approaches enable profound insights into the interrelationships between structure and composition in complex microstructures at atomic scale pertaining to the materials topics listed above.

Similar progress was enabled by rendering the **Electron Channelling Contrast Imaging** method quantitative by combining it with controlled diffraction conditions (cECCI). It allows the direct observation of crystal defects such as dislocations or stacking faults close to the surface of bulk samples. This technique, which has similarities to dark field TEM is applied in a SEM and allows probing the first 50–100 nm of material below the surface.

Substantial progress was also made in the field of **mapping hydrogen** with high spatial resolution, hence, correlating trapping sites and damage events with local microstructure features.

In the field of **simulation** substantial progress was made in the field of joint polycrystal and multiphysics modelling. The corresponding software package developed during the past 15 years was released to the public domain as **Düsseldorf Advanced MAterials Simulation Kit** (**DAMASK**) and can be downloaded at **https://damask.mpie.de**. It is used by a number of research groups worldwide. Regarding alloy design we have made substantial progress by introducing the concept of **non-equiatomic high entropy alloys in part with dual–phase microstructures** and the use of **interstitial alloying** in these materials.

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# Research Projects in Progress

Kürnsteiner, Jägle, Raabe: New high strength aluminium alloys for additive manufacturing (industry, DFG)

Jägle: Precipitation kinetics during non-linear heat treatment in Laser Additive Manufacturing (DFG)

Springer, Tasan: Self-Healing Materials (DFG)

Gault: Topological Engineering of Ultra-Strong Glasses (DFG)

Roters, Yang, Diehl, Kasemer: Through-process simulation of microstructure, recrystallization, texture and mechanical properties (industry, DFG)

Zaefferer, Shanthraj, Herbig: Electroplastic mechanisms in Mg-, Al-Cu and metallic glass alloys (DFG)

Kamachali, Shanthraj, Diehl: Strong coupling of thermo-chemical and thermo-mechanical states in engineering alloys and processes (DFG)

Ponge, Raabe, Li: OPTIBOS – New developments and optimization of high strength Boron treated steels through the application of advanced Boron monitoring techniques (RFCS)

Tasan, Grabowski, Raabe, Neugebauer: ERC-funded SMARTMET - Adaptive nanostructures in next generation metallic materials: Converting mechanically unstable structures into smart engineering alloys (ERC)

Raabe, Schneider, Dehm, Köhler, Schnabel: Topological Engineering of Ultra-Strong Glasses (DFG)

Sandlöbes, Nellessen: Constitutive modelling and microstructural validation for crystal plasticity finite element computation of cyclic plasticity in fatigue (DFG)

Zaefferer, Raabe, Sandlöbes, Ponge: Synthesis, Characterization and local texture analysis and crystalline anisotropy in Mn-steels (DFG)

Cojocaru-Mirédin, Choi, Schwarz, Raabe: Characterization of CIGS Solar Cells by Atom Probe Tomography (BMBF)

Choi, Tytko: Thermal stability of metal nitride superlattices studied by means of Atom Probe Tomography (DFG)

Li, Luo, Raabe: Hydrogen resistant high entropy alloys (AvH)

Sandlöbes, Friák, Raabe, Neugebauer: Fundamentals of the ductilization of Mg alloys

Shantraij, Roters, Eisenlohr, Svendsen, Raabe: Physically based approach for predicting and minimizing damage nucleation in metals (DFG, Industry)

Tarzimoghadam, Gault, Ponge: Hydrogen embrittlement in metallic alloys (Industry, ERC)

Wong, Roters: Constitutive modeling of joint TRIP and TWIP deformation of in advanced high strength steels (DFG, Industry)

Zaefferer, Ram: High resolution scanning electron back scatter diffraction experiments and local strain determination in Mn-based steels (DFG, Industry)

Springer, Belde, Baron: Combinatorial synthesis, alloy design and phase boundary mechanics in stiffness enhanced multiphase steels (DFG)

Roters, Diehl: Constitutive and RVE simulation of the mechanical response of complex steels (Industry)

Li, Choi, Goto, Kirchheim, Dehm, Neugebauer, Raabe: Fundamentals of the strength of pearlite (Industry, AvH, DFG)

Gault, Koantis, Makineni, Povstugar, Choi, Raabe: Atom probe tomography of the chemical composition of interfaces in Ni-base superalloys (DFG, AvH)

Gault: Direct observation of atomic hydrogen (ERC)

Herbig: Intense mechanical frictional contact and white etching layers (BMBF)

Jägle, Zaefferer, Raabe: Microstructure and Processing of FeSi soft magnetic alloys (Industry)

Zaefferer: Microstructure and texture of Nickel alloys (Industry)

# Department of Structure and Nano-/Micromechanics of Materials

*G. Dehm*

## Scientific Mission and Concepts

The department was founded in October 2012 with a research focus on **microstructure physics and mechanical properties** of structural and functional materials covering especially **small length scales down to the atomic dimensions**. Our mission is to advance the understanding of deformation processes and constraining effects on mechanical and tribological material properties for both bulk and miniaturized materials by developing and applying quantitative tools, which are suited for small dimensions and high spatial resolution. The experiments are complemented by simulation techniques to understand their limitations and constraints and to aid data interpretation. Our research embraces the variety of microstructure elements from point defects, alloying additions, dislocations, interfaces to second phases and employs advanced structural characterization techniques to shed new light on the interplay of mechanical properties and microstructure evolution. This research interest includes initiation of plasticity, fatigue, fracture, slip transmission across grain boundaries, and phase transformations of grain boundaries to name the most prominent examples. In this context, scale bridging characterization techniques such as atomic resolved scanning and transmission electron microscopy (STEM/TEM), scanning electron microscopy (SEM), focused ion beam microscopy (FIB), X-ray diffraction (XRD) and advanced synchrotron methods are utilized and further improved by in-house development. **Our specialty is the integration of imaging and/or diffraction methods with external stimulus** of the sample **to identify the underlying mechanisms *in situ* while heating** [1-8], **straining** [9-16] **or electro-chemically altering the material** [17,18] and **to extract quantitative data**. Several instruments have been designed and built in-house making use of the expertise of the engineers and scientists in the SN department supported by the mechanical and electronic workshops of the MPIE.

The installation of this new department at the MPIE with its 5 research groups required substantial reconstruction work of hall 8-9, especially to host the microscopy infrastructure for the **Advanced Transmission Electron Microscopy** (**Dr. C. Liebscher, since April 2015)** and **Nano- and Micromechanics of Materials (Dr. C. Kirchlechner, since March 2013) research groups.** The reconstruction work started in December 2014 concluding a ~2 year planning phase and finalized in March 2018. 4 high-tech cubes were constructed with 2 of them fitted with active and passive electro-magnetic shielding to allow operation of the aberration corrected electron microscopy equipment at its resolution limits (see p. 37). Additionally, new TEM sample preparation laboratories were built. The department hosts now 2 atomic resolution TEM/STEM instruments, one probe corrected STEM/TEM (since 2015) with analytical tools (electron energy-loss spectroscopy and energy dispersive X-ray spectroscopy), one image corrected TEM/STEM (since end of 2017), and a field emission gun TEM/STEM (since 2006) equipped in 2018 with a fast CMOS camera allowing dynamic experiments to be recorded at ~200 frames per second. A new high resolution field emission SEM (since 2017) and a focused ion beam machine (since 2013) complement the microscopy facilities. The research group **Nanotribology (Dr. S. Brinckmann, since December 2014)** installed a nanoindentation platform with self-designed electro-chemical cells. The research group **Intermetallic Materials (Dr. M. Palm & Dr. F. Stein)** moved to the SN department in October 2012 from its interimistic home at the department of Microstructure Physics and Alloy Design (MA) and operates a modern thermodynamic laboratory (see p. 38). The research group **Synthesis of Thin Films and Nanostructured Materials (Dr. M. Ghidelli, since November 2018)** just recently commenced its work completing the originally proposed structure of the SN department. All 5 research groups strongly interact within and across the departments to contribute to the overall mission of the MPIE by developing new high-performance materials for use as high-tech structural and functional components. Additionally, the research groups also pursue their own scientific agenda to tackle central scientific questions within their research themes, which are discussed in detail later.

Despite the lengthy and difficult reconstruction work of hall 8-9 and the successful installation of the new facilities, several major achievements have been accomplished over the last years. Focusing only on the last 3 years, we advanced the understanding

of **dislocation - grain boundary interactions** by combining micromechanical testing of individual grain boundaries with *in situ* SEM and synchrotron based µLaue diffraction studies [9-11,19-23]. Interestingly, twin boundaries in Cu permit dislocation transmission of mirrored glide systems with a common Burgers vector at stresses as low as those required for cross-slip in a single crystal, in contrast to predictions by molecular dynamics [24,25]. The experimental results are further supported by strain rate sensitivity measurements of twinned bicrystals. They match with the corresponding single crystals, while in contrast for a randomly oriented penetrable Cu grain boundary the strain rate sensitivity becomes substantially higher. This can be explained by dislocation climb as the rate controlling step for the dislocation transmission process subsequent to dislocation absorption in the grain boundary and prior to emission from the grain boundary [9,10]. Other cornerstones of our micromechanical research are toughening mechanisms of materials and miniaturized **fracture toughness** measurements. We recently advanced our small scale fracture experiments to elasto-plastic fracture mechanics by monitoring the crack propagation via the sample stiffness evolution and *in situ* imaging techniques. In collaboration with the Max Planck Fellow Group on *Self Reporting Materials* headed by Prof. Jochen Schneider we applied these tools to resolve possible ductility in metallic glasses and layered crystals with high hardness, like $Mo_2BC$, which reveal moderate ductility in accordance with atomistic predictions [26-30]. Interestingly, even superlattice structures of hard and brittle materials can improve both, the hardness and the fracture toughness with reducing layer spacing [31].

Our recent atomic resolved STEM/TEM studies of **grain boundaries** revealed a **novel segregation phenomenon** at faceted grain boundaries in multicrystalline silicon [32], and for the first time experimental evidence of a chemically triggered **nano-faceting transition** in an Ag-Cu alloy [33,34]. Furthermore, two substantially different atomistic structures were detected indicating the **coexistence of two structurally different grain boundary phases** for a symmetric high angle tilt boundary in pure Cu. Such grain boundary phases are believed to have a large impact on material properties and are the central theme of the ERC Advanced Grant *GB CORRELATE*, which started in August 2018 to explore grain boundary phase transformations and their impact on material properties like grain boundary mobility and grain boundary mechanics (see p. 69). These research topics benefit from the strong in-house collaborations with the MA department providing unprecedented chemical sensitivity by correlated STEM/TEM and atom probe tomography (APT) as well as the department of Computational Materials Design (CM) with their *ab initio* tools predicting grain boundary structures and energies.

**Materials development** in SN revolves around **nanocrystalline alloys** and **intermetallic materials**. Severe plastic deformation, rapid quenching from the melt (including additive manufacturing), diffusion couples and physical vapour deposition are methods which we use to synthesize materials with exceptional strength and thermal stability - in some cases far from thermodynamic equilibrium. The materials portfolio ranges from alloys like Cu-Cr,Zr,Ta [3,4,35-38], high entropy alloys (or chemically complex alloys) [39,40], steels [2,41-43] to iron aluminides [44-58], Laves phases [59-62], and ferritic superalloys [63-67]. In several cases, close collaborations with industrial partners provide a stimulating exchange between basic research and application demands. Our observation that decomposition of cementite in a pearlitic steel by severe wire drawing leads to a tetragonal distorted C-rich ferrite which corresponds to a strain induced martensite initiated further studies on the fracture behaviour [68] and **microstructure evolution under tribological contact**. Our studies on surface wear of pearlitic steel using a sliding micro-asperity contact reveal plasticity in the cementite phase. It can be speculated that the plasticity within the $Fe_3C$ lamellae of the pearlitic steel contributes to the decomposition process and C supersaturation of the Fe matrix.

The outcome of our research has led to several awards across all career stages; this includes a best poster award for young scientists at the Gordon Research Conference on Thin Films and Small Scale Mechanics (2016, N. Malyar), a best student talk award at the Nanobrücken conference (2017, W. Luo), a best paper award granted to F. Stein in 2016 by the International Commission of Alloy Phase Diagrams, the prestigious Heinz Maier Leibnitz award from the German Research Foundation (DFG) for early career researchers, which was granted to C. Kirchlechner in 2017 in “recognition of his outstanding achievements” [http://www.dfg.de/], and an ERC Advanced Grant in 2018 to G. Dehm - for which “the sole criterion for selection is scientific excellence” [https://erc.europa.eu/].

The recently founded SN department is already strongly connected within the MPIE, and with neighbouring universities and research institutes, like RWTH Aachen University, TU Dortmund, Research Center Jülich, and Ruhr Universität Bochum, where G. Dehm is appointed since 2012 as außerplanmäßiger Professor (adjunct Professor). The cooperations are well documented by joint publications, joint PhD students within the International Max Planck Research School SURMAT, and DFG funded research proposals like the Priority Programme (SPP 1594 Topological Engineering of Ultra-Strong Glasses, and SPP 2006 Compositionally Complex Alloys – High Entropy Alloys (CCA-HEA)) and Collaborative Research Centres / Transregio (TRR 188 Damage

**Fig. 1:** *2018 retreat at the Monastery Steinfeld.*

Controlled Forming Processes). The SN department hosts a Max Planck Partner Group in India on *Designing damage tolerant functional oxide nanostructures* (head: Ass. Prof. Dr. Nagamani Jaya Balila, Indian Institute of Technology Bombay) and the external research group *High Temperature Materials* headed by Prof. Gunther Eggeler, which continues the excellent interactions established during the preceding Max Planck Fellow group. Close research collaborations with France led to two DFG-ANR projects, one in the field of high entropy alloy thin film stability and fatigue, and the second focusing on the origin of fatigue damage in metals by developing and employing newest 3 dimensional µLaue techniques at the synchrotron facility ESRF in Grenoble. The large-scale collaborative EU research project HERCULES (http://www.hercules-2.com) develops within the FP7 long-term R&D Programme intermetallic materials for applications in large diesel ship engines with academic and industrial partners across Europe. The department hosts foreign guest researchers from abroad via the Erasmus programme, Alexander von Humboldt foundation, China Scholarship Council (CSC), Cambridge University summer student programme, and via secondments from institutes, universities, and industry.

Numerous conferences and workshops have been organized by members of the SN department. Recent examples are the 2018 Gordon Research Conference on Thin Films and Small Scale Mechanics (Lewiston, USA), the symposium Mechanical Properties and Adhesion at the International Conference on Metallurgical Coatings & Thin Films (ICMCTF) in 2017, 2018, and 2019 in San Diego, USA; the symposium Environmental, In-Situ and Time-Resolved Microscopy at the Microscopy Conference 2017, in Lausanne, Switzerland; symposia on Correlative Electron Microscopy & Atom Probe Tomography at the Materials Science and Engineering Congress - MSE 2018 in Darmstadt (C. Liebscher), on Experiments and Simulations towards understanding Tribology across Length-Scales at the MSE 2016 and at the MSE 2018 in Darmstadt (S. Brinckmann), on Mechanical Properties at Small Scales at the DPG meeting 2018 in Berlin, and on Experimental Nanomechanics at the 2018 European Mechanics of Material Conference in Nantes, France (C. Kirchlechner) as well as the biannual conference Intermetallics 2017 in Bad Staffelstein (M. Palm, F. Stein). In addition, several plenary, keynote and invited lectures were delivered at international conferences and institute colloquia by scientists from the SN department reflecting their high international visibility. A prestigious plenary talk at the European Mechanics of Materials Conference 2016, Brussels, Belgium; and keynote lectures at the Materials Science and Engineering Conference 2016 in Darmstadt and Israel Engineering Conference 2018 were delivered by G. Dehm, while invited talks were presented e.g. by C. Kirchlechner at the 2018 International Conference on Strength of Materials (ICSMA, Ohio, USA), C. Liebscher at Beijing University of Technology (2018), S. Brinckmann at the MRS 2017 Spring Meeting in Phoenix, M. Palm at the TMS 2017 Annual Meeting in San Diego, and F. Stein at the Thermodynamics of Alloys (TOFA) conference 2018 in Seoul. Our community services range from memberships in various selection committees (e.g. for the Allocation of Humboldt Research Fellowships, and for Independent Max-Planck-Research Groups), and in the Board of Governors of Acta Materialia Inc., to leading technical committees (DGM Fachausschuss Materialographie: C. Kirchlechner) and acting as editorial board members, reviewers and advisors for journals, funding agencies, and promotions of faculties.

Teaching and career development are two important areas promoted by SN members. This includes

involvement in summer and winter schools (2017 C. Kirchlechner organization of a summer school on Experimental Nano- and Micromechanics, G. Dehm teaching Stresses and Plasticity in Thin films at the GDRi Mecano General School 2018, M. Palm and F. Stein giving lectures at the MSIT Winter School on Materials Chemistry, 2018), teaching courses for the International Max-Planck Research School SURMAT and for PhD students at the MPIE, and regular courses at the Ruhr-Universität Bochum (G. Dehm, C. Liebscher, S. Brinckmann) and Montanuniversität Leoben (C. Kirchlechner). C. Kirchlechner received his habilitation in 2018 from the Montanuniversität Leoben. G. Dehm launched in 2015 career talks at the MPIE where companies present their activities in informal talks often followed by on-site visits. Not only steel companies, but also chemical, and electronic industry showed interest in this successful format which is organized by the PhD representatives of the MPIE under mentorship of G. Dehm (see p. 80).

Retreats of the SN department (Fig. 1) together with the independent research group *Nanoanalytics and Interfaces (NG)* (Prof. Christina Scheu) and external scientific guests are performed annually to discuss the individual research topics and to strengthen interactions within the department. The weekly seminar is intended to report on challenges and recent progress in the research topics of Master students, PhD students, postdocs, guest researcher and senior scientists.

The next chapter reports in more detail on the scientific achievements of the research groups of the SN department.

## Scientific Groups

### Nano- and Micromechanics of Materials (C. Kirchlechner)

**The Nano- and Micromechanics Group: More than a mechanical microscope.** Aim of the Nano- and Micromechanics group of the MPIE is to quantitatively understand, predict and alter fundamental mechanisms governing plasticity, fatigue and fracture of materials. For this purpose, we are isolating individual mechanisms – such as slip transfer of dislocations across a grain-boundary – by performing small scale mechanical experiments on samples with hitherto unreached small dimensions. But our work surpasses the local measurement of strength and toughness by far: A central aspect of our research is to link the mechanical behaviour to the underlying and evolving defect structures (e.g. dislocation types and densities, length and density of cracks and crack networks, etc.) which requires an advanced characterization toolbox with *in situ* capabilities.

After founding the group in 2013 we have successively developed our toolbox which today comprises *in situ* loading experiments simultaneously applying scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), and synchrotron based X-ray Laue microdiffraction (µLaue) (see p. 41) while its three dimensional variant differential aperture X-ray microscopy (DAXM) is currently established. Today, this complementary toolbox permits to quantify topological changes of the sample during deformation, precisely measure the individual and collective density and type of dislocations, the local deviatoric strain tensor and track the grain-boundary character and orientations *in situ* under external stimulus.

A considerable part of our work focusses on the development of setups and analysis tools for extracting the relevant microstructural properties at the relevant length scale, which are often not available. One recent example is the development of DAXM with *in situ* capabilities, which is developed together with our partners at the ESRF in Grenoble, France (see p. 41). The tool allows for measuring the aforementioned microstructure parameters non-destructively with a voxel size clearly below 500 nm³ within unreached short experimental acquisition times. It is our vision to shed unprecedented light on the fundamentals of fatigue damage initiation and initiation of short fatigue cracks at grain- and phase boundaries in the upcoming years.

Our work is stimulated by key-questions concerning the mechanical properties of structural and functional materials. Structural materials of interest are various steels, high entropy alloys, intermetallics, and advanced magnesium alloys. In the field of functional materials we are focusing on conducting thin film materials and on advanced solder materials - often with a link to micro- and flexible electronics - and on tough hard coatings.

**Single crystal plasticity.** Our work on single crystalline materials was initially motivated by the “sample size effect”, where the strength of single crystalline tremendously increases by reaching the micron and submicron scale. Recently, we have analysed the size scaling in tin at 0.6 of its melting temperature [69] and in copper at 400 °C [70], which is both of outmost importance for the reliability of advanced solder joints. Today we apply single crystalline micromechanics to understand the deformation behaviour of complex systems. For instance, together with the Intermetallics group we are currently exploring the deformation mechanisms in cobalt-based Laves phases where the role of off-stoichiometry on the mechanical behaviour is not understood – neither at room – nor at service temperatures.

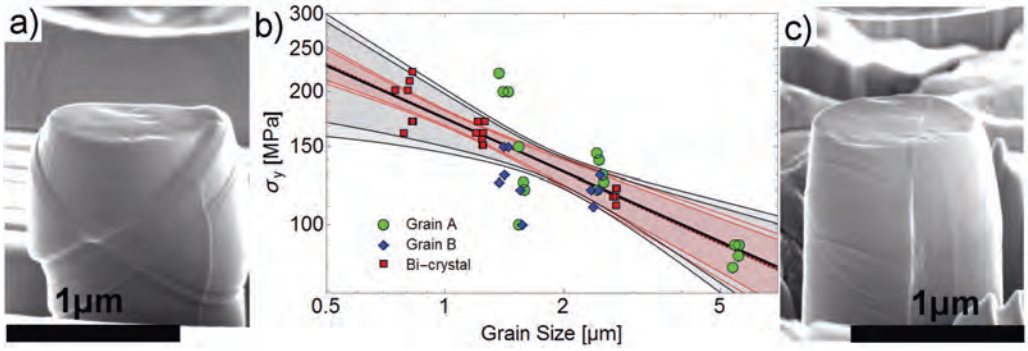


**Fig. 2:** *Micropillar compression on (a) single and (c) bi-crystalline pillars. (b) The yield stress of the bi-crystals is identical to the one of single crystals. The solid lines close to the straight fit following a Hall-Petch-like description indicate the 90, 95 and 99% confidence interval of the fit [72].*

A second set of projects on single crystals measures the anisotropy of the critical resolved shear stress (CRSS) in various materials. For instance, guided by the need of damage tolerant light-weight alloys, we are currently exploring the role of anisotropy of the CRSS on the formability of magnesium alloys. A second example is focused on the activation of anomalous slip in carbon containing ferrite in advanced dual phase steels, where we could show that the CRSS of {110}{112} and {123} slip is identical.

Finally, our group joined the worldwide efforts to understand the deformation behaviour of high entropy alloys (e.g. the Cantor alloy [40]), and, for the first time, reported on the micro-mechanical properties of hexagonal high entropy alloys [39]. In addition, together with the Advanced Transmission Electron Microscopy group we are currently exploring the role of atomic order, cross-slip and dislocation pile-ups on the critical resolved shear stress of the Cantor alloy.

**Fundamentals of plasticity at grain- and phase boundaries.** What stress is required to transmit a dislocation through a grain boundary? Is the transmission process strain-rate-dependent? What is the overall impact of dislocation slip-transfer to the strength of materials? Is there an impact of grain boundary structure and chemistry on the mechanical behaviour of bi-crystalline microsamples? These are the key questions motivating our grain boundary work with the ultimate goal to develop quantitative, mechanism-based material laws of dislocation slip transfer.

During the last 5 years we have extensively studied coherent Σ3 twin boundaries in copper. It was shown that the ideal slip transfer through such boundaries – which is possible only on 3 out of 12 slip systems – is similar to cross-slip. The slip transfer mechanism exhibits not only a similar activation volume [11], but also unexpected low transmission stresses of partly less than 20MPa further indicate the similarities of cross-slip and perfect dislocation slip-transfer [19]. Consequently, our early work was neither able to find dislocation pile-ups [15,16], nor revealed noticeable differences in the deformation behaviour of single crystalline and bi-crystalline copper [71].

Our work on penetrable [20] and impenetrable [72] high angle copper grain boundaries shows that general slip transfer through non-Σ3 twin boundaries requires non-conservative motion of dislocations in the grain-boundary plane. As a consequence, the slip transfer itself is a highly strain rate dependent process. A fact which is not well-captured in today´s literature on dislocation slip transfer. As consequence, at small strain rates dislocations can frequently overcome grain-boundaries while slip transfer can entirely be suppressed at high strain rates. We were able to identify the strain rate sensitivity of a high angle grain boundary for the first time [9].

Finally, irrespective of the grain-boundary character, our investigated grain boundaries indicate that the strengthening effect at the micron scale is rather governed by the grain size than the grain boundary type (Fig. 2) [72]. One exception here is the above mentioned coherent twin boundary, which allows transmission in a cross-slip-like mode and, therefore, behaves similar as a single crystal.

**Fracture at the micron scale.** Fracture ultimately limits the lifetime of engineering components. But, what is the influence of the local microstructure on crack growth? Can we accurately determine the fracture toughness of phases, which cannot be synthesized in macroscopic dimensions? What is the fracture toughness of an interface? The Nano- and Micromechanics group performs research at the forefront of international efforts to extract meaningful fracture properties at the micrometre length scale.

A significant share of our work is devoted to assure reliable fracture properties at the micron scale. Linear elastic fracture mechanics (LEFM), well suited for brittle materials, are nowadays well established, also in small dimensions. Our group has assessed and quantified the role of testing setup and geometry on the extracted fracture properties in the past 5 years in collaboration with the Nanotribology group [73-

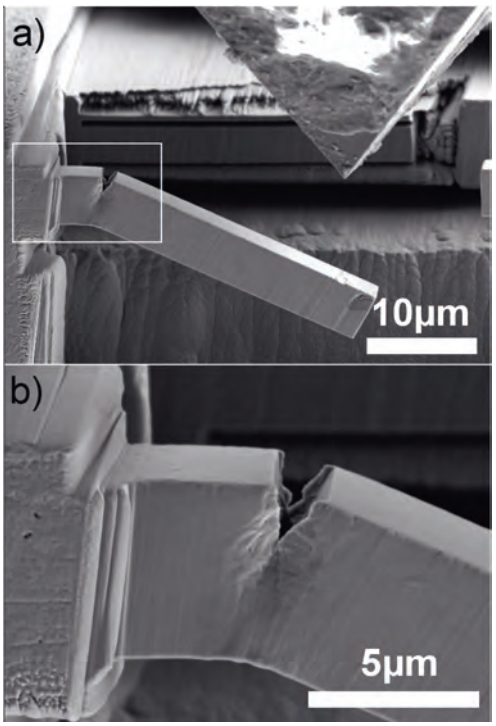


**Fig. 3:** *Microfracture experiment on a white etching layer (WEL). (a) The microbeam was bent by the diamond wedge visible at the top right. The zoom-in (b) shows the significant crack growth and ductile tearing of the nominally brittle WEL.*

75]. We further applied LEFM to identify toughening mechanisms based on super-lattice structures in hard coatings [31], to identify *ab initio*-based design criteria for damage tolerant metallic glasses [26,27] as well as hard coatings [28] and for identifying the Achilles´ heel of advanced solder materials [76,77].

Our current work heads towards reliable elasto-plastic fracture mechanics (EPFM) required to measure the fracture toughness of semi-brittle and ductile materials at the micrometre length scale. Essential ingredient to EPFM is the ability to track the crack tip *in situ*, for which we currently develop several different approaches based on the sample compliance as well as *in situ* imaging techniques. In parallel, we are applying this knowledge on the fracture toughness of white etching layers (see Fig. 3) in advanced railroad rails, on pearlitic steel wires with superior strength [68] and, together with the Nanotribology group on hydrogen embrittlement.

**Switchable structural materials.** Today's structural materials exhibit outstanding but predefined mechanical properties. To increase their adaptability e.g. for different crash scenarios in automotive applications we envision a new class of smart structural materials. Our key questions is if we can modify the strength of a material by an external stimulus in the required timescale of a few microseconds? While this question sounds like science fiction, it actually is currently brought into reality at the Micromechanics group. The concept of this high-risk, high-gain project funded by the German VolkswagenStiftung is to modify the acting shear stress by so-called eigenstrain causing materials. First promising multi-physics finite element modelling identified advantageous material combinations which are synthesized as next step.

### Advanced Transmission Electron Microscopy (C. Liebscher)

**Group Mission.** The Advanced Transmission Electron Microscopy (ATEM) group was established in 2015. The group develops, advances and employs methods in the transmission electron microscope (TEM) to unravel the fundamental atomistic aspects of complex materials and interfaces to establish a microstructure driven materials design. One of the key aspects is that **method development** is always targeted to solve a specific materials science related question [32,42,78]. For example, novel non-rigid image registration techniques are developed to enhance atomically resolved scanning TEM (STEM) towards fully quantitative imaging including atomic resolution strain mapping [42]. We are also **advancing** existing TEM and *in situ* TEM techniques [17] (seep. 40) to extend their limits and with this enable novel insights into the atomic structure of complex materials [38,78-82] and material defects [32,33,83]. The atomic scale correlation of aberration corrected STEM and atom probe tomography (APT) [32,42,78] is an example where we could uniquely establish the connection of the atomic structure of grain boundaries in Si and their solute segregation behaviour [32]. Furthermore, the advanced TEM methods are **employed** to design nanostructured materials based on their atomistic structure [35,42,81,84,85]. This culminates in the evolution of novel multicomponent materials with tailored nano-precipitates for advanced applications [86].

**Facilities.** The group utilizes four TEMs. The CM20 (Thermo Fisher Scientific) with $LaB_6$ emitter is used for conventional diffraction contrast imaging and electron diffraction experiments and serves as a training platform for TEM beginners. The JEM2200FS (JEOL) is equipped with a Schottky field emitter, an in-column omega energy-filter and an energy dispersive X-ray detector. The JEM2200FS is the main platform for *in situ* TEM experiments and was upgraded with a high-speed CMOS camera (TVIPS GmbH) in January 2018. This will also enable us to further advance *in situ* liquid cell experiments in collaboration with the department of Interface Chemistry and Surface Engineering (GO) and the Poseidon liquid cell holder (Protochips) [17]. Since April 2015, the probe-corrected Titan Themis 60-300 (Thermo Fisher Scientific) is one of the major microscopes for atomic structure observations and

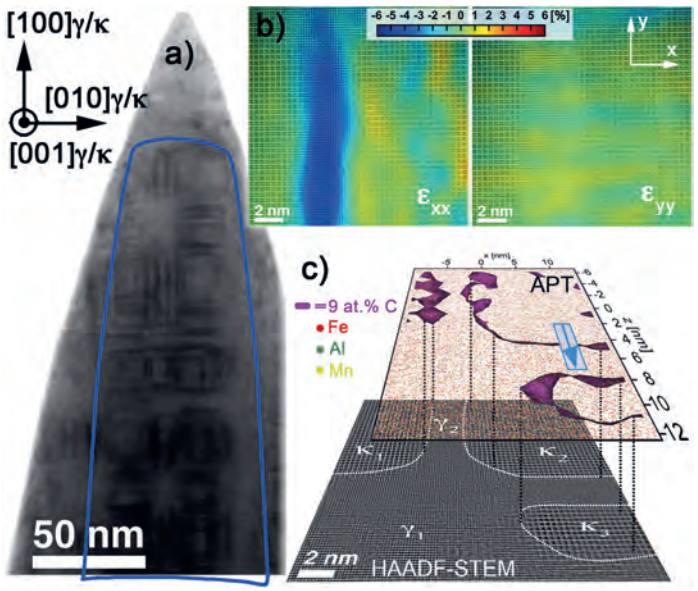


**Fig. 4:** *a) Overview annular bright field (ABF) STEM image of a needle shaped specimen. The volume of the APT reconstruction is outlined in blue. b) Atomic resolution strain maps obtained in the apex of the APT specimen. c) Direct correlation of STEM and APT resolving both the atomic lattice structure and composition [42].*

atomic scale analytics. The microscope was installed in an intermediate room in 2015 and moved to the microscopy laboratories by the end of 2017, where it was finally commissioned in April 2018. The last instrument completing the advanced TEM facilities is an image corrected Titan Themis 80-300 (Thermo Fisher Scientific). The instrument was commissioned in October 2017 (see p.37).

**Mechano-chemical coupling at coherent interfaces.** The aim of this research project was to extend the current limits of correlating TEM with APT by using aberration corrected STEM methods to unravel the intimate relation between the local strain state and composition at coherent interfaces [42]. An effective way of strengthening a solid solution is obtained by the dispersion of coherent, nanometre-sized precipitates. In low-density steels with high manganese (Mn) content, κ-carbide nano-precipitates, with a size in the range of 20 nm to 50 nm, are the major strengthening phases. These ordered $Fe_3AlC$ type precipitates exhibit a slightly larger lattice parameter than the face centred cubic (fcc) Fe matrix and hence complex internal strain states evolve. We developed a methodology to quantify local lattice strains by atomic resolution STEM in a needle-shaped specimen, as shown in Fig. 4a and b. The elemental distribution and composition in close proximity to the interfaces can then be probed with unprecedented elemental sensitivity in the same sample by APT illustrated in Fig. 4c. Atomic resolution strain mapping reveals that the lattice of 2-3 nm nanometre wide fcc-Fe matrix channels is tetragonally strained to compensate for the lattice mismatch. Atomistic simulation establishes that such a tetragonal lattice distortion has a strong effect on the C solubility and with this affects the growth kinetics of the precipitates as well as the interaction with dislocations during deformation.

**Unexpected segregation behaviour at faceted grain boundaries.** A major interest of the ATEM group is to unravel transitions and transformations at grain boundaries [32,33,83]. These planar defects are fundamentally determining the properties of advanced materials and the influence of grain boundary transitions on their properties is rarely explored. The aim of our work is to establish a generalized understanding of interfacial transitions across different types of grain boundaries and material systems. We are currently contrasting interfacial transitions in face centred cubic (fcc) Cu with controlled additions of Ag and S [33,83] with that in body centred cubic (bcc) Fe(Al) and Fe(Si) alloys. The atomic scale experimental observations are complemented by atomistic simulations in collaboration with Dr. Timofey Frolov (Lawrence Livermore National Laboratory, USA) and the CM department of the MPIE. In a more specific research highlight, we employed the previously described methodology correlating STEM with APT to discover the segregation of impurity elements C and Fe at nano-faceted grain boundaries in multicrystalline Si [32]. The majority of grain boundaries in this wafer material are large angle grain boundaries that often dissociate into nanoscale facets, whenever the overall grain boundary inclination deviates from

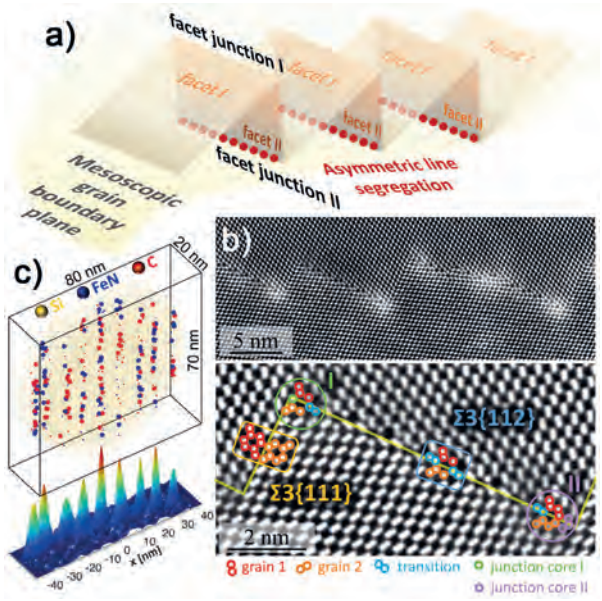


**Fig. 5:** *a) Schematic illustration of grain boundary faceting and its influence on solute segregation. b) Strain sensitive STEM images of a faceted Σ3 grain boundary and junction core structures. c) Corresponding APT reconstruction at the grain boundary highlighting the line segregation of Fe and C [32].*

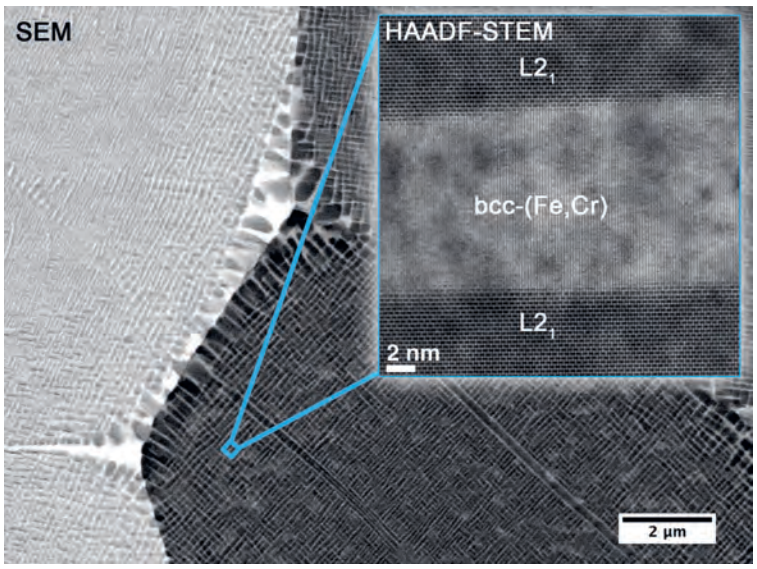


**Fig. 6:** *SEM and HAADF-STEM images of an $Al_{25}Cr_{15}Fe_{30}Ni_{20}Ti_{10}$ (at.%) compositionally complex alloy.*

the symmetric orientation. Hence, the grain boundary is composed of planar grain boundary facets that are separated by two different types of linear grain boundary facet junctions, as shown schematically in Fig. 5a. Atomic resolution STEM imaging shown in Fig. 5b reveals that the local atomic reconstruction in both facet junctions differs substantially and with this an asymmetric strain state develops. The low impurity concentrations in the lower ppm range require correlated APT measurements to uniquely locate the impurity atoms at these topologically complex interfaces. In contrast to the often assumed planar segregation, the impurity elements are forming segregation lines only within one particular type of facet junction, as seen in the APT reconstruction of Fig. 5c. With the aid of atomistic simulations performed by Dr. Liverios Lymperakis (CM), we were able to connect this unexpected segregation behaviour to the local strain state at the facet junctions. Both, the finite size of the grain boundary facets and the junction core structures leads to the evolution of an asymmetric strain state and segregation is favoured in facet junctions with largest compressive strains.

**Development of nanostructured compositionally complex alloys.** The method development and advancement of characterization techniques is utilized to design and understand the microstructure-property relationships in novel compositionally complex (CCA) [86] and high entropy alloys (HEA). In this alloy concept, an equal amount of at least five alloying elements is added to establish highly supersaturated solid solutions (HEA) or novel precipitate structures (CCA) that are otherwise not attainable with classical alloy design concepts. The compositional complexity strongly impacts the properties of these materials and by combining advanced TEM characterization with *in situ* TEM deformation, we are shedding new light on the atomic scale deformation behaviour in the Cantor alloy. We are particularly interested in resolving the effect of short-range order on the dislocation mobility, which is of utmost importance to decode the unique properties of HEA. Furthermore, two projects are focusing on the design of novel CCAs funded within the DFG priority programme 2006 Compositionally Complex Alloys - High Entropy Alloys (CCA - HEA). The first project is concerned with the development of precipitation hardened CCAs through selective laser melting of HEA powder samples. This work is in collaboration with Dr. Uhlenwinkel (University of Bremen) and Dr. Eric Jägle (MA), where, in a first step, we are focusing on the atomic scale characterization of phase separation processes in bcc-type CCA powders with an interconnected, nanoscale *B*2 network. The second project started in November 2017 and is a collaborative effort together with the department of Materials Chemistry at RWTH Aachen University. We are aiming to design novel alloys with tailored precipitate structures for advanced high temperature applications. The composition space investigated in the ATEM group is centred around the equimolar $Al_{20}Cr_{20}Fe_{20}Ni_{20}Ti_{20}$ (at.%) alloy. The goal is to establish materials that are comprised of abundant materials with low density and exhibit excellent mechanical properties up to temperatures of 900ºC. To achieve this, we allow the composition to be relaxed from the equimolar one, opening up an enormous phase space that is explored by combinatorial synthesis techniques coupled with advanced material characterization. A key point of the project is to design materials by optimizing their nano- and microstructure. Representative secondary electron microscopy (SEM) and high angle annular dark field (HAADF) STEM images of a promising alloy candidate with composition $Al_{25}Cr_{15}Fe_{30}Ni_{20}Ti_{10}$ (at.%) are illustrated in Fig. 6. The microstructure is composed of a high density of fully coherent $L2_1$-type precipitates embedded in a highly supersaturated body centred cubic (bcc) solid solution matrix of nearly 50 at.% Fe and 50 at.% Cr.

### Nanotribology (S. Brinckmann)

**Group mission.** The research group was established in December 2014 and focuses on the investigation of microstructure evolution during friction and wear. The projects study tribology using micrometre asperities that mimic single asperities of macroscale components, thereby aiming to understand fundamentally the irreversible mechanisms that result in energy and structural loss. The investigated evolution processes include grain refinement, plasticity,

phase formation and dissolution. Although we focus on the dry contact of metals with hard asperities, some projects probe the metal on metal contact in the presence and absence of lubricants.

Additionally, we use continuum simulations to further the insight into microscale fracture and toughness of brittle and ductile metals in collaboration with the Nano- and Micromechanics of Materials group. Moreover, we carry out experiments on hydrogen embrittlement of metals by developing procedures to quantify dislocation plasticity in the presence of hydrogen and evaluate the nucleation strength of dislocations.

**Tribology of steels.** Multiple parameters affect tribology: material properties of both materials in frictional contact, surface roughness, normal force, relative velocity, lubricant, temperature and duration of tribological loading. The influence of the parameters and their interaction are generally nearly impossible to decipher. It is our approach to decrease radically the number of parameters to simplify the tribological interaction with the aim to understand and analyse individual mechanisms. Therefore, we study the contact with a non-deforming (infinitely stiff and inert) diamond micrometre asperity. The room-temperature dry single stroke experiments use a low velocity, which does not heat the material. Therefore, only the normal force, contact radius and relative velocity are parameters in our experiments. The studies on an austenitic stainless steel (see Fig. 7c) [87,88] introduced the separation into elastic (that follows an adopted Hertzian model) and plastic deformation (that can be determined from the metal hardness). Moreover, that study showed asymmetric slip-pattern formation on the metal surface although the tribological loading is symmetric. The project revealed that the crystal orientation and the free-surface proximity introduce an asymmetry that result in the particular slip pattern. A study on Cu revealed that the slip steps in the wear track result also in the formation of surface cracks, which depend on the crystal orientation only. A DFG funded project (BR 3947/5) started in 2018 to investigate the crack formation in fcc and bcc steels during tribology.

In addition to the investigation of monolithic materials, we evaluate the microstructure evolution of pearlitic steel (see Fig. 7a), which consists of 200 nm thick cementite ($Fe_3C$) lamellae and a ductile ferrite matrix [89]. The project showed that the lamellae are bending plastically with strains up to 40% (Fig. 7b), which is atypical for $Fe_3C$. We found also that the bending strains depend on the distance from the wear track. Micromechanical specimens of $Fe_3C$ were used to quantify the fracture toughness and yield-strength. It was shown that $Fe_3C$ can deform by plastic slip at the microscale.

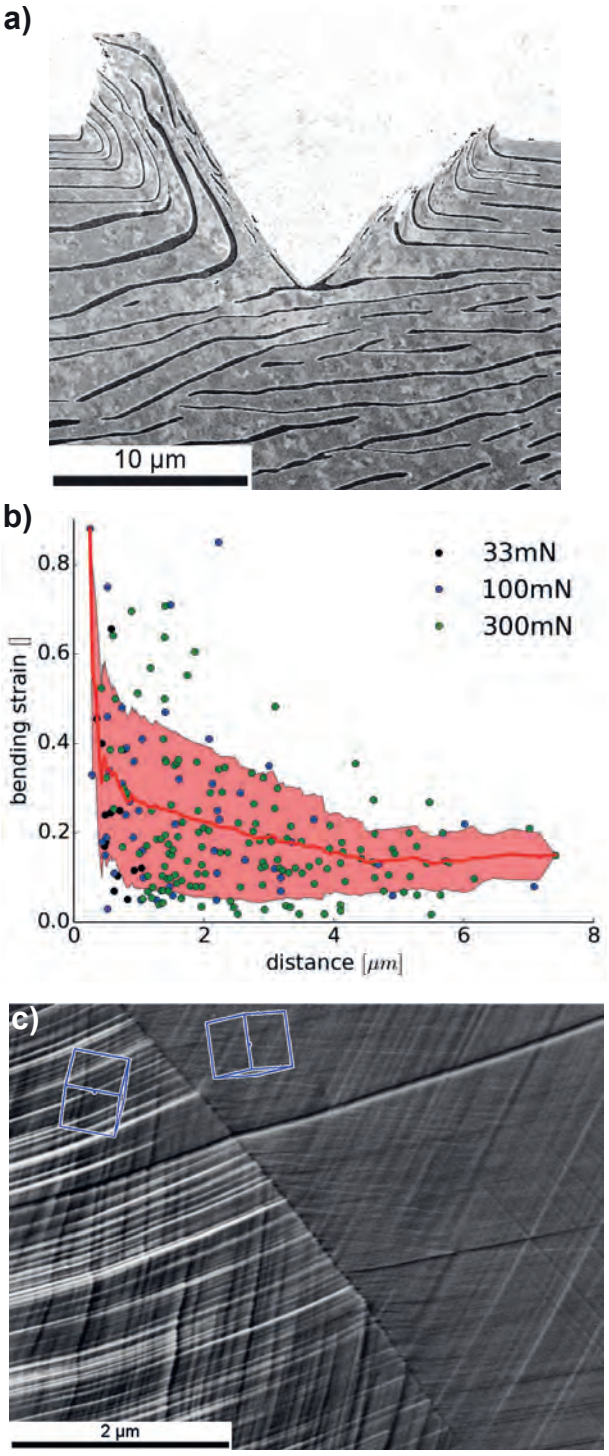


**Fig. 7:** *(a) Wear track in pearlitic steel, the cementite lamellae are plastically deforming. (b) Bending strains as a function of the distance from the wear track for different normal forces. (c) Tribology induced slip steps intersecting a grain boundary in an austenitic stainless steel.*

**Mechanochemistry of tribological surface layers.** Lubrication additives result in surface layers and in improved wear and friction properties. However, a number of parameters influence the surface layer formation and disagreement exists in the scientific literature on the influence of the parameters. In collaboration with the RWTH Aachen University, we

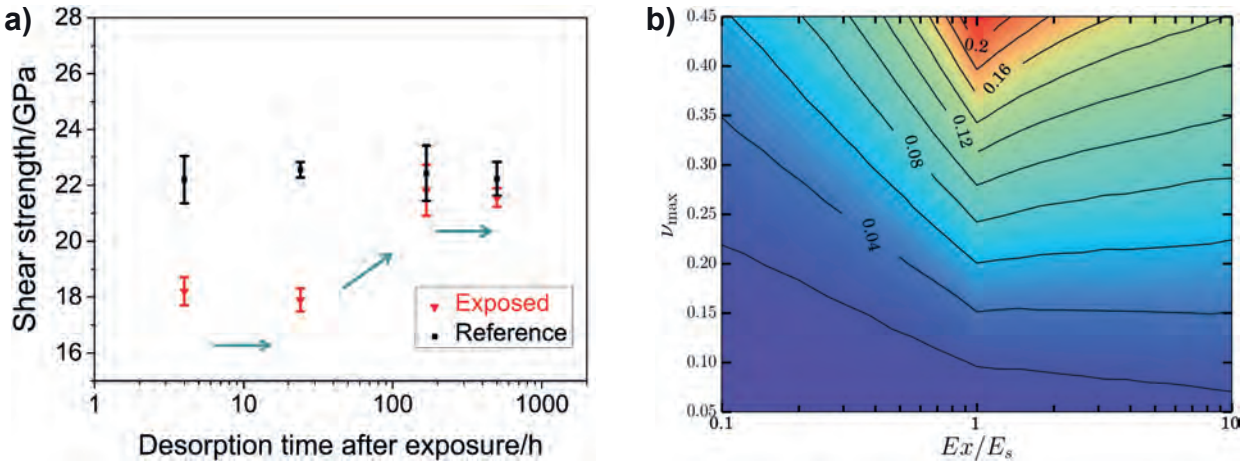


**Fig. 8:** *(a) Shear strength of tungsten as a function of the desorption of hydrogen, i.e. time after H exposure. The shear strength of dislocation nucleation was determined by nanoindentation. (b) 3D Fracture toughness evaluation for an anisotropic material (with a ratio of Elastic moduli in the axial and perpendicular direction $E_x/E_s$) and for different Poisson ratios: the fracture toughness is up to 20% larger in the centre of the crack path than at the surface.*

developed a novel experimental method that uses cyclic compression on the micro- and macroscale and that focuses on the mechanical properties in tribology. Following the steel on steel experiments with lubricant on the microscale, a number of characterization techniques identified a P, S and Zn rich layer of 100 nm thickness, which is similar to conventional tribolayers. Hence, the novel method is able to further the understanding of tribological surface layers [90].

**Hydrogen embrittlement of metals.** Hydrogen embrittlement of metals is of general importance in engineering applications. In tribology, it is of specific significance since hydrogen is linked to the growth of white-etching-areas, which result in catastrophic failure. This research group investigates the hydrogen-metal interaction using simplified loading conditions.

We perform nanomechanical testing while charging *in situ* the samples with hydrogen (see p. 42). The techniques use nanoindentation, nanoscratching, micropillar compression and microcantilever bending to study independently grain interiors, grain boundaries or precipitates. Two setups were designed in-house to charge electrochemically a sample and these setups were incorporated to the G200 nanoindenter for *in situ* testing [91]. In the "front-side" charging cell, the electrolyte is in contact with the sample surface allowing fast charging, while a "back-side" charging setup preserves the intact sample surface for additional post-deformation characterization. One example is the study of dislocation nucleation and hydrogen mediated plasticity in ferritic FeCr alloys, in which we found a decrease of the shear strength and an increased hardness as function of the hydrogen content. This work is funded by the DFG (DU 1628/1) since 2016.

In collaboration with the Forschungszentrum Jülich, we investigate the hydrogen-tungsten interaction using micromechanical experiments. After charging the metal with deuterium, we execute nanoindentation, pillar compression and microcantilever experiments. We investigate the effusion of deuterium and the recovery of mechanical material properties by executing experiments repeatedly after different waiting times following charging. For instance, our results have shown that the Young's modulus is not influenced by the hydrogen concentration while the hardness increases after the charging and then decreases as deuterium effuses from the metal (see Fig. 8a) [92,93]. On the other hand, the dislocation nucleation strength has the inverse relationship: the formation of new dislocations is eased in the presence of deuterium compared to the untreated and the effused sample. We investigate the dislocation avalanche probabilities in the presence and absence of hydrogen to understand thoroughly hydrogen mediated plasticity.

**Simulations of fracture at the microscale:** Fracture is the major process that occurs during three wear mechanisms: adhesion results in fracture from the host metal, abrasion leads to wear debris formation, surface fatigue brings about surface cracks. As such, the fundamental understanding of fracture at the microscale is essential for the solving tribology at all length scales. In collaboration with the Nano- and Micromechanics group, we execute continuum simulations to investigate the influence of the 3D stress-state on crack propagation in metals and material layer stacks. In one study [74], the influence of the elastic anisotropy and Poisson ratio on the fracture toughness along the crack front was quantified (see Fig. 8b). The experimental crack tip geometry was taken into account to determine accurately the fracture toughness and to answer fundamental questions regarding crack growth stability [75].

The delamination behaviour of metal layers is important in the integrated circuit industry, which uses four-point bending experiments to quantify the delamination strength. It had been previously observed

that these experiments are frequently unsuccessful [94,95]. Our study revealed the origin of the frequent experimental failure and the project gave design guidelines for successful experiments [96].

The project with the Boise State University, which was funded as part of the Materials-World-Network of NSF and DFG, was concluded. Our contribution investigated the conjugation boundary in hierarchical magnetic shape memory alloys and used disclination dynamics to simulate the growth of variants and material failure [94]. Our partner supported the microstructural evolution by using high-resolution TEM of a conjugation boundary and the variant evolution mechanisms.

We participated in the first and third Sandia Fracture Challenge, in which calibration experiments are used to identify the material and fracture model on the macroscale. After blind predictions are calculated for a custom 3D geometry, the experiments are used to verify the numerical predictions [97-100].

### Intermetallic Materials (M. Palm, F. Stein)

The mission of the group is the development of intermetallic materials including fundamental research on phase stability and phase transformations. Based on that, alloy concepts are established and employed for designing alloys with specific microstructures and optimized compositions. If - after evaluation of basic physical and mechanical properties and the corrosion behaviour - expectancy for a successful application exists, implementation is explored in cooperation with industrial partners. The majority of the research is performed within national and international collaborations and the application-oriented projects are collaborations with industries. Projects also often involve other groups at the MPIE.

**Fundamental research on phase stability and phase transformations.** Nb-based intermetallic alloys consisting of Nb solid solution and high-melting, strengthening intermetallic phases are of considerable interest for structural applications at very high temperatures. In a project a company for special metals, the high-temperature phase equilibria and solidification behaviour of Nb-based ternary alloys with Al and Fe were established yielding the liquidus surface in the Nb corner of the ternary system and isothermal sections at 1450 and 1600 °C [101]. The phase relations in the complete ternary Al-Fe-Nb were calculated by thermodynamic modelling using the Calphad approach within a cooperation with Nanning University [102], and a comprehensive assessment of the complete system was performed [103].

The precipitation of intermetallic phases from a supersaturated Co(Nb) solid solution is studied in a cooperation with the Hokkaido University of Science. These ongoing investigations show that the formation of metastable, coherent $L1_2$ $NbCo_3$ strongly affects the microstructural evolution and growth of the equilibrium phase $Nb_2Co_7$ [104].

Deviations from the ideal, stoichiometric composition of tcp (tetrahedrally close-packed) intermetallic phases as, e.g., Laves phases can be partially compensated by point defects like antisite atoms or vacancies, but also planar defects may offer an opportunity to accommodate excess atoms. In cooperation with the group Advanced Transmission Electron Microscopy, various types of such planar faults in a Nb-rich off-stoichiometric $NbFe_2$ Laves phase were investigated by high-resolution STEM and accompanied by *ab initio* calculations (performed by the CM department) [61,62,105]. Interestingly, all types of observed planar faults contain structural motifs, which are characteristic for the crystal structure of the

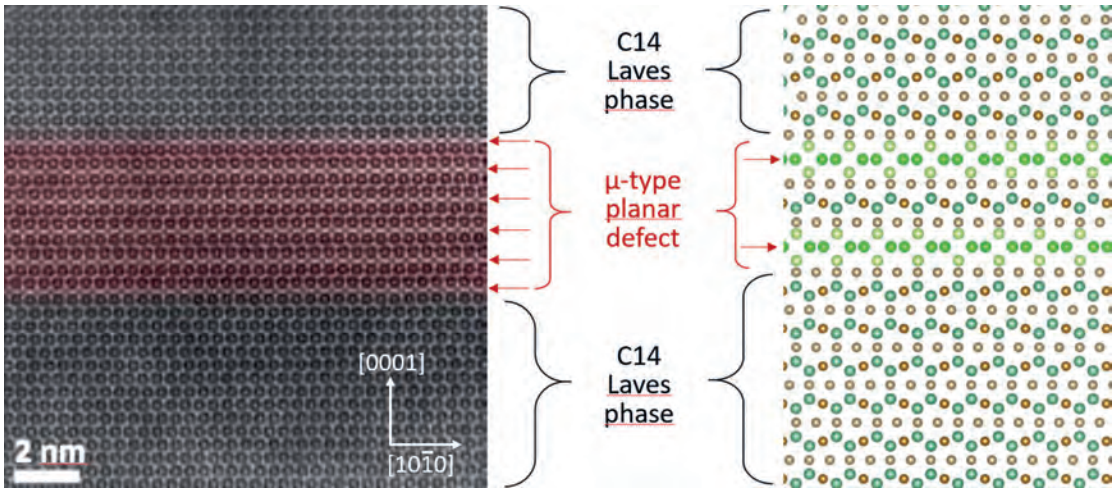


**Fig. 9:** *Atomically resolved STEM image of a C14-type, Nb-rich $NbFe_2$ Laves phase revealing an extended, coherent planar defect containing structural motifs marked by red arrows that are characteristic for the crystal structure of the Fe-Nb μ phase. For better visualization of the characteristic atomic arrangement in the planar defect, on the right side a magnified sketch of the structure is shown containing as an example a planar defect with two rows of the μ phase structural motifs.*

μ phase $Nb_6Fe_7$ that occurs at higher Nb contents in the binary system (see Fig. 9 for an example).

Multicomponent alloys with four or more principal elements in near-equiatomic ratios, commonly designated as high entropy alloys (HEAs), belong to the most discussed topics in materials science during the last years. The Intermetallic Materials group was involved in several projects dealing with various kinds of HEAs and focusing on questions related to stability and crystallographic structure of these alloys. Examples are the hexagonal HEA $Al_{15}Sc_{10}Ti_{25}Zr_{25}Hf_{25}$, where sublattice ordering resulting in a $D0_{19}$ superstructure was found below 900°C [106], and the equiatomic, hexagonal HEA YGdTbDyHo, where a hitherto unknown and still unsolved hexagonal superstructure with $P6_3$ symmetry was detected [39].

Prediction of the stability and properties of phases by *ab initio* methods is becoming more and more important for materials development. Within a cooperation with the Czech Academy of Sciences, Montanuniversität Leoben (MUL) in Austria and the SN department, thermodynamic, electronic, magnetic, structural and elastic properties of the $L2_1$ Heusler phase $Fe_2AlTi$ have been explored [67]. The phase is interesting for functional applications because of its unusual magnetic and electrical properties but also for strengthening Fe–Al alloys at high temperature. $Fe_2AlTi$ has an extended homogeneity range and the effect of off-stoichiometry on the magnetic states and thereby on the lattice parameter was investigated.

**Alloy design.** *Ab initio* results on various $L2_1$ Heusler phases contribute to the theory-guided design of novel Fe-Al-based superalloys. Such alloys have a coherent microstructure consisting of disordered *A*2 and intermetallic phases with *B*2 or $L2_1$ structure. Strength and stability of the microstructure of these alloys crucially depend on optimizing the coherency stresses between the phases. As actual alloys are developed in systems containing four or more elements, *ab initio* calculations for the prediction e.g. of the stability of $L2_1$ in such higher order systems and their lattice constants are fundamental for the design of these alloys [66].

In cooperation with the Montanuniversität Leoben and the group Advanced Transmission Electron Microscopy, we develop ferritic superalloys in the Fe-Al-Ni-Ti system [64,65]. The focus is placed on the evolution of the microstructure in dependence on different heat treatments. Specifically the coherence between the *A*2 α-(Fe,Ni,Al) matrix and the $L2_1$ $(Fe,Ni)_2AlTi$ precipitates and the formation of Fe-rich anti-phase domains (APDs) was studied by TEM.

Ferritic superalloys can also be generated within the Fe-Al-Ta system. However, in contrast to the Fe-Al-Ni-Ti system, where the coherent microstructures of the structural related phases *A*2 + $L2_1$ form within a miscibility gap, $L2_1$ $Fe_2AlTa$ forms metastably due to the kinetically retarded precipitation of the stable *C*14 Laves phase $(Fe,Al)_2Ta$. Within a cooperation with industry aimed at producing compressor blades strengthened by coherent *A*2 + $L2_1$ microstructures, possibilities to modify the microstructure by manipulating the metastable formation of $L2_1$ by doping with boron or by a thermomechanical pre-treatment have been explored [63].

Co-Ti based ternary γ/γ' superalloys containing 12 at.% Ti and 4 at.% Cr or Mo and heat-treated at 800 °C were investigated within a cooperation with the MA department. Mo and Cr were found to preferentially occupy Ti sites in the $L1_2$ γ' phase and to lead to an increase of the γ' volume fraction, a reduction of the lattice misfit, and an increase of the γ' solvus temperature that amounts to more than 100 °C in case of the Mo-containing alloy [107].

**Evaluation of basic properties.** Mechanical properties of intermetallic phases may be significantly affected by changes in composition what is most obvious for phases with extended homogeneity ranges. The $NbCo_2$ Laves phase is a perfectly well suited example to study this topic as the width of its homogeneity range is about 10 at.% and it additionally may exist with three different structure variants (cubic *C*15, hexagonal *C*14 and hexagonal *C*36). As the preparation of bulk single-phase Laves phase samples for classical mechanical testing is extremely difficult for such a brittle material, an alternative production route was employed. Diffusion couples were prepared containing a concentration gradient that covers the complete homogeneity range of the Laves phase. By performing various types of micromechanical testing methods along the concentration gradient, the mechanical properties were studied as function of composition and structure in cooperation with the Nano- and Micromechanics group [59,60].

Al-rich Fe-Al alloys were studied in a project with the Karlsruhe Institute of Technology (KIT). After a careful re-investigation of the phase diagram in the complete Al-rich part of the system [54], the investigations focused on the two-phase range FeAl + $FeAl_2$, where the microstructure consists of a fine-scaled, well-aligned lamellar arrangement of the two phases. The orientation relationship of cubic *B*2 FeAl and triclinic $FeAl_2$ was determined [55] and the coarsening kinetics of the lamellar microstructure were studied in detail [56]. In view of possible applications, creep experiments between 600 and 800 °C were performed on respective alloys [57] and the effect of ternary additions of up to 2 at.% B, Ti, Cr, Cu and Mo on the lamellar microstructure, their thermal stability and mechanical properties was investigated [58].

Coherent *A*2 + $D0_3$ ($L2_1$) microstructures as observed in the above-mentioned Fe-Al-Ni-Ti and Fe-Al-Ta systems also form in the Fe-Al-V system. The investigated alloys show appreciable mechanical properties, but their oxidation behaviour is imperfect due to the formation of porous and thick $Fe_2O_3$ +

$Al_2O_3$ scales [44]. Besides ferritic superalloys, iron aluminides with boride precipitates are of high interest in view of industrial applications. Fe-Al-Nb-B alloys with finely precipitated Laves phase show increased ductility after heat treating but only mediocre creep resistance [45].

Because systematic investigations on the variation of fundamental properties of iron aluminides in dependence on the Al content are missing, respective investigations have been performed over the years at the MPIE. Currently the oxidation [46] and the aqueous corrosion behaviour [47,48] are studied, the latter in cooperation with the GO department. X-ray photoemission spectroscopy (XPS) revealed that passivation during wet corrosion is due to the formation of an outer layer of mixed Al and Fe oxides and an inner layer of hydroxides enriched in Al.

**Implementation into industrial application.** Mechanical properties and corrosion behaviour of the Fe-Al-based alloys discussed above were evaluated in cooperation with industry partners. Besides optimizing or finding alternative intermetallic materials, these projects are aimed at producing and testing parts fabricated by various processing routes. Specifically, a number of different parts for ship diesel engines, industrial furnaces or steam turbines were cast or forged using boride containing iron aluminides and in several cases successfully tested under application conditions [49].

Additive manufacturing (AM) is a new technology by which near net-shape parts are generated by layer-wise melting of powders by a laser or electron beam. As intermetallic phases are highly wear resistant and therefore difficult to machine, AM is an interesting alternative for producing parts from intermetallic materials. Within a large-scale collaboration with research institutes and German industries, AM of advanced iron aluminides has been studied. Defect-free samples and parts were produced by different AM techniques and it was shown that basic alloy concepts developed for cast alloys can be transferred to AM [50-52]. Also, the possibility of generating chemically-graded samples by AM with a continuous variation of the composition between various stainless steels and iron aluminides could be demonstrated [53].

In recognition of the substantial research at the MPIE, invitations have been offered to write a review on iron aluminides [108] and a book chapter on Fe-based intermetallic phases [109]. The group is also active in co-organizing the bi-annual conference Intermetallics (https://www.intermetallics-conference.de/), the annual MSIT Winter School on Materials Chemistry dealing with heterogeneous equilibria (http://www.msiport.com/msit-school/) as well as the international workshop on Laves phases at the MPIE.

### Synthesis of Thin Films and Nanostructured Materials (G. Dehm, since Nov. 2018 M. Ghidelli)

This group was recently established with the aim to synthesize specific thin film microstructures and nanostructured thin film materials. The new group leader Dr. Matteo Ghidelli was attracted from Politecnico di Milano and complements with his expertise on physical vapour deposition techniques and microfabrication processes the research portfolio of the SN. While the head of this new research group started just recently, some studies in this research field had been already initiated earlier and were often performed jointly with the groups Nano- and Micromechanics of Materials, Advanced Transmission Electron Microscopy and/or the Max Planck Fellow group on Self Reporting Materials. Examples include new insights on solid state dewetting of thin films with oxide scale, which was studied in close collaboration with the independent research group Nanoanalytics and Interfaces (NG, head: Prof. C. Scheu). Epitaxial Al films on sapphire were dewetted in reducing and oxidizing atmospheres providing clear indication of the different diffusion paths being

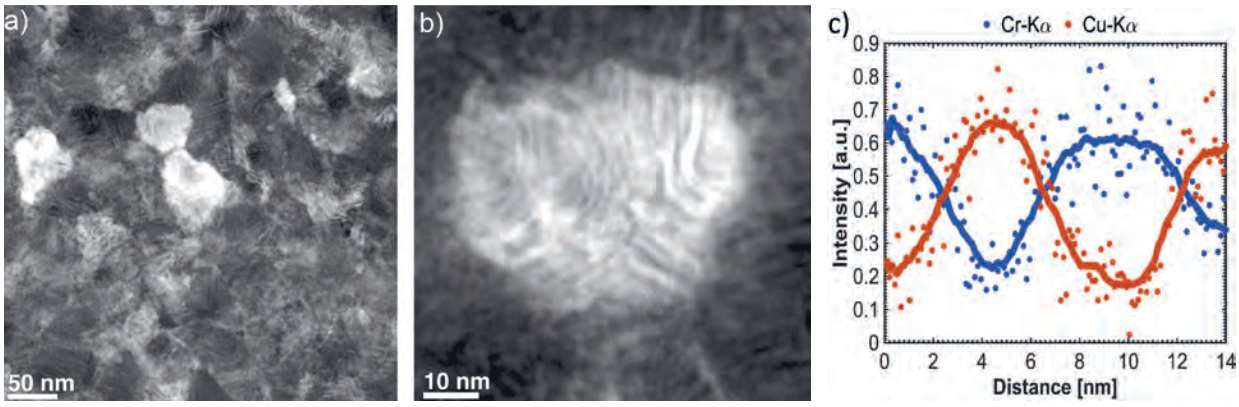


**Fig. 10:** *STEM Z-contrast images showing (a) the nanocrystalline structure of a bcc Cu-Cr alloy (67 at.% Cu, 33 at.% Cr) and (b) the chemical modulation within an individual grain (taken from [36]), (c) shows an EDX linescan within a single grain.*

activated [5,6,110]. Such studies are not only relevant for functional devices with their thin metallization layers but also for thin passivating coatings on alloys enduring long exposures to elevated temperatures. Another example of intensive research is the fabrication, structure evolution and thermal stability of alloy nanocomposites in form of thin films. Recent studies revolved mainly around the system Cu-Cr, where thin film structures [3,4,35-37] and severe plastically deformed bulk materials [1,7] were analysed. Thermal stability against grain growth with excellent strength is achieved in Cu supersaturated bcc Cu-Cr alloys, where spinodal decomposition via volume diffusions leads to a hierarchical nanostructure of chemically modulated layers within nanocrystalline grains (Fig. 10) [36,37]. These first studies indicate the potential of thin films to tailor nanostructures and to provide selection guidelines for upscaling to bulk materials via other synthesis techniques like rapid solidification or severe plastic deformation. This research path will be further explored for other material systems in the upcoming years.

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# Research Projects in Progress

**ERC Grant (G. Dehm)**

*Bishara, Meiners, Saba, Kirchlechner, Liebscher, Dehm:* Correlating the State and Properties of Grain Boundaries

**Nano- and Micromechanics of Materials (C. Kirchlechner)**

*Arigela, Kirchlechner, Dehm*: Setup of a microscale high-temperature loading rig

*Balijepalli, Kirchlechner*: StrengthSwitch: Can we design structural materials with switchable strength?

*Du, Kirchlechner, Dehm*: Micro-fracture of advanced solder joints

*Li, Kirchlechner*: Dislocation source activation at grain boundaries

*Kini, Kirchlechner, Dehm*: The role of microstructure constraints during slip transfer

*Kirchlechner, Fink, Kirchlechner, Dehm (in cooperation with J. Schneider, RWTH Aachen)*: Fracture behavior of metallic glass thin films

*Kumar, Brinckmann, Kirchlechner, Dehm*: Developing strategies for reliably assessing elasto-plastic fracture mechanics

*Kumar, Kirchlechner (in cooperation with A. Kumar and M. Herbig, MA-Department)*: Fracture toughness of a white etching layer

*Malyar, Hosseinabadi, Dehm, Kirchlechner*: Slip transfer through grain boundaries

*Molin, Renversade, Kirchlechner (in cooperation with J.S. Micha, CEA Grenoble)*: The first stages of fatigue

*Öllers, Arigela, Kirchlechner, Dehm (in cooperation with A. Ludwig, RUB Bochum)*: Combinatorial approach to tailor electrical and mechanical properties of alloyed thin film structures

*Seok, Kirchlechner, Dehm (in cooperation with S. Nandy, S. Zaefferer and D. Raabe, MA-Department)*: The anisotropy of the CRSS in Mg alloys

*Tian, Christiansen, Kirchlechner (in cooperation with D. Ponge, MA-Department)*: Damage initiation in DP800 at the micron scale

*Wenqi, Kirchlechner, Liebscher, Dehm*: The strain-rate-sensitivity of high-entropy alloys

**Advanced Transmission Electron Microscopy (C. Liebscher)**

*Ahmadian, Liebscher, Dehm (in cooperation with L. Romaner, Materials Center Leoben, Austria):* Atomic structure, transitions and segregation effects in bcc grain boundaries

*Devulapalli, Dehm, Liebscher:* Structural transitions and atomic scale segregation effects in Ti alloy grain boundaries

*Jeong, Brinckmann, Liebscher, Dehm: In situ* TEM nanotribology

*Jenko, Dehm, Liebscher*: *In situ* TEM observation of dynamics and growth characteristics in bi-metallic Fe-Au nanoparticles

*Lee, Duarte, Soler, Kirchlechner, Liebscher, Dehm (in cooperation with M. Feuerbacher, FZ Jülich, Germany and S. Ho Oh, Sungkyunkwan University, Republich of Korea)*: *In situ* TEM study on the dislocation plasticity in a single crystal FeCoCrMnNi high entropy alloy

*Lee, Meiners, Dehm, Liebscher:* Atomic scale *in situ* TEM investigations of dislocation grain boundary interactions

*Liebscher, Stein (in cooperation with A. Zendegani, T. Hickel, CM-Department; M. Šlapáková, Charles University in Prague, Czech Republic and S. Kumar, Brown University, USA):* Atomic scale transitions at planar defects in *C*14 $NbFe_2$ Laves phases

*Liebscher (in cooperation with A. Kauffmann and M. Heilmaier, Karlsruhe Institute of Technology, Germany):* Nanoscale phase separation and ordering tendencies in refractory MoCrTiAl high entropy alloys

*Liebscher, Dehm (in cooperation with C. Draxel and C. Koch, Humboldt University Berlin, Germany):* Development of data structures and metadata for big datasets in multidimensional scanning transmission electron microscopy

*Liebscher (in cooperation with C. Freysoldt, MA-Department; A. Ziletti and L. Ghiringelli, Fritz-Haber Institute Berlin, Germany):* Automatic classification and feature extraction from multi-dimensional TEM data

*Lu, Meiners, Liebscher, Dehm, Raabe (in cooperation with L. Morsdorf, M. Herbig, A. Breen, MA-Department; R.K.W. Marceau, Deakin University, Australia):* Phase decomposition in lenticular martensite during room temperature ageing

*Lu, Liebscher, Raabe, Dehm, Gault (in cooperation with Y. Chang, A. Breen, I. Mouton, D. Raabe, B. Gault, MA-Department):* Hydride formation mechanisms in Ti alloys

*Lu, Liebscher (in cooperation with A. Breen, I. Mouton, Z. Wang, A. Szczepaniak, P. Kontis, L. Stephenson, Y. Chang, A. Kwiatkowski da Silva, D. Raabe, M. Herbig, B. Gault, MA-Department; S. Wang and T. Britton, Imperial College, UK):* Atomic scale analysis of deuterides in Zircaloy-4

*Lu, Liebscher, Dehm (in cooperation with Z. Li, D. Raabe, MA-Department):* Atomistic deformation mechanisms and nanolaminate formation in dual-phase high-entropy alloys

*Lu, Liebscher, Dehm (in cooperation with Z. Li, D. Raabe, MA-Department):* Phase formation and deformation mechanisms in interstitial dual-phase high entropy alloys

*Meiners, Dehm, Liebscher (in cooperation with T. Frolov, Lawrence Livermore National Laboratory):* Atomic scale phase transitions at [111] tilt grain boundaries in Cu

*Peter, Kirchlechner, Liebscher, Dehm (in cooperation with T. Frolov, Lawrence Livermore National Laboratory, USA and C. Ophus, Lawrence Berkeley National Laboratory, USA):* Segregation induced nanofacet formation at asymmetric Cu grain boundaries

*Peter, Kirchlechner, Liebscher, Dehm:* Correlating the atomic structure of grain boundaries in Cu with their dislocation interaction behavior

*Wolff-Goodrich, Dehm, Liebscher (in cooperation with M. Amalraj, RWTH Aachen, Germany and K.G. Pradeep, IIT Madras, India):* Tailored, precipitation strengthened, compositionally complex FeAlCr (Mn, Co, Ni, Ti) alloys for high temperature applications

*Wu, Liebscher, Dehm (in cooperation with S.K. Makineni, P. Kontis, B. Gault, D. Raabe, MA-Department; G. Eggeler, Ruhr-University Bochum:* Segregation effects to dislocations and stacking faults in the γ'-phase of single crystal Ni-based superalloys

*Zavasnik, Dehm, Liebscher*: *In situ* TEM deformation of metastable Cu-Ag thin films

*Zavasnik, Dehm, Liebscher*: Atomic scale defect healing in acusto-optic $PbMoO_3$ single crystals

**Nanotribology (S. Brinckmann)**

*Brinckmann:* Blind predictions of plasticity and failure of additively manufactured metals (together with B. Boyce, Sandia National Labs)

*Brinckmann, Dehm:* Tribolayer formation during macro- and microscale cyclic contact (in collaboration with G. Jacobs, RWTH Aachen)

*Brinckmann, Dehm (in cooperation with C. Greiner, KIT and R. Chromik, McGill University):* Tribology of Cu on the macro- to microscale

*Brinckmann, Kirchlechner, Dehm (in cooperation with M. Bartosik and P. Mayrhofer, TU Wien):* Designing toughening concepts for future hard coatings

*Brinckmann, Soler, Dehm:* Shear experiments to determine the delamination strength of thin-films

*Duarte Correa, Dehm:* Crystallization kinetics and microstructural evolution of metallic glasses

*Duarte Correa, Dehm:* Corrosion and wear at the nanoscale

*Fang, Brinckmann, Dehm:* Hydrogen embrittlement of steels: environment-assisted *in situ* micromechanical tests

*Farzam, Brinckmann, Dehm:* Microstructure evolution in Cu and Al during friction

*Fink, Brinckmann, Dehm:* Microstructure evolution of pearlitic steel during nanotribology

*Patil, Brinckmann, Dehm:* Texture evolution during nanotribology in FCC and BCC steels

*Rao, Duarte Correa, Dehm:* Hydrogen-microstructure interactions in Ferritic alloys at small scale

*Xia, Brinckmann, Dehm:* Fracture initiation in FCC and BCC metals during tribology

**Intermetallic Materials (M. Palm, F. Stein)**

*Distl, Kahrobaee, Palm, Stein (in cooperation with Thermo-Calc Software AB, Sweden, Helmholtz-Zentrum Geesthacht Zentrum für Material- und Küstenforschung GmbH, Montanuniversität Leoben, Austria)*: ADVANCE – Sophisticated experiments and optimisation to advance an existing CALPHAD database for next generation TiAl alloys

*Jenko, Palm*: TEM investigation on boride precipitation in iron aluminides

*Liebscher, Stein (in cooperation with A. Zendegani, T. Hickel, CM-Department; M. Šlapáková, Charles University Prague, Czech Republic, S. Kumar, Brown University, RI, USA)*: Planar defects in off-stoichiometric, Nb-rich $NbFe_2$ Laves phase studied by HRTEM

*Luo, Kirchlechner, Dehm, Stein*: *In situ* micromechanical studies of intermetallic phases along concentration profiles in diffusion couple zones

*Merali, Stein*: Diffusion couple studies on the possibility of coexistence of hexagonal and cubic Laves phases in the Co-Ti system

*N.N., Palm, Stein (in cooperation with Siemens AG, Karlsruher Institute of Technology, Otto Junker GmbH, Rolls-Royce Deutschland Ltd & Co KG, Access e.V., Leistritz Turbinentechnik GmbH*): Pro-FeAl – Process development for economic and efficient iron aluminide turbine components

*Palm (in cooperation with P. Kratochvil, V. Sima, Dept. Physics of Materials, Charles University Prague; P. Hanus, M. Švec, Technical University Liberec, Czech Republic)*: Basic investigations of iron aluminide alloys including phase formation during infiltration

*Palm (in cooperation with I.G. Aviziotis, M. Armbrüster, Technical University Chemnitz)*: Synthesis and characterization of iron aluminide catalysts

*Palm, Stein, Liebscher (in cooperation with F. Godor, S. Mayer, H. Clemens, Montanuniversität Leoben)*: Development of Fe-Al materials with coherent microstructures (ferritic superalloys)

*Peng, Palm (in cooperation with Winterthur Gas & Diesel Ltd.; Wärtsila Finland Oy; Wärtsila Netherlands BV; Deloro Wear Solutions GmbH; ABB Turbo Systems AG)*: Intermetallics for engine applications (within HERCULES-2)

*Stein (in cooperation with S. Takajo, S. Vogel, Los Alamos National Lab, NM, USA)*: High-temperature phase transformation of Hume-Rothery-type phases in the Fe-Al-Mo system

*Stein (in cooperation with T. Horiuchi, Hokkaido University of Science, Japan)*: Discontinuous precipitation of intermetallic phases from Co solid solutions

*Stein (in cooperation with K. Yamada, T. Horiuchi, Hokkaido University of Science, Japan)*: Metastable $L1_2$ phase formation in Co-Nb alloys

*Stein (in cooperation with R. Sandt, University of Cologne, R. Spatschek, Forschungszentrum Jülich)*: Experiments and modelling on the reaction kinetics of the peritectoid decomposition of $Nb_2Co_7$

*Stein, Palm (in cooperation with R. Wartbichler, S. Mayer, H. Clemens, Montanuniversität Leoben, Austria)*: Experimental investigations of the effect of Mo-additions on microstructure, thermal stability and mechanical properties of Ti-60Al alloy

# PART III.

# INTER-DEPARTMENTAL RESEARCH ACTIVITIES – SELECTED HIGHLIGHTS

# Combining Identical Location Microscopy, Atom Probe Tomography and a Scanning-Flow Cell coupled with an Inductively Coupled Plasma Mass Spectrometer to Understand the Structure-Property of Catalysts

*O. Kasian [1], B. Gault [2], T. Li [3], S. Zhang [4], S. Cherevko [5], C. Scheu [4], D. Raabe [2], G. Dehm [6], K. Mayrhofer [1, 5]*

[1]Department of Interface Chemistry and Surface Engineering (GO)
[2] Department of Microstructure Physics and Alloy Design (MA)
[3] now at: Ruhr-Universität Bochum
[4] Independent Max Planck Research Group on Nanoanalytics and Interfaces (NG)
[5] now at: Helmholtz Institute Erlangen-Nürnberg for Renewable Energies
[6] Department of Structure and Nano-/ Micromechanics of Materials (SN)

Electrocatalysis is key to clean energy conversion and storage technologies. During electrocatalytic reactions the surface composition of electrodes undergoes drastic changes that lead to efficiency decrease and structural degradation [1]. Up to now, particularly for the important oxygen evolution reaction (OER) on oxidic surfaces, the mechanisms underpinning the transformations and their influence on the reactivity and durability of catalysts remained largely unknown [2], mainly due to limitations in sufficiently analytically sensitive surface probing techniques. The resulting knowledge gap regarding the question how the topmost atomic layers behave and compositionally change, has hindered the development of high-performance, long-lasting electrocatalysts.

A close collaboration between the departments GO, MA, SN and the NG group was established, with the aim to develop an approach to characterize the temporal evolution of the topmost atomic layers of catalysts in operation. Iridium oxide formed on pure iridium films by anodic electrochemical oxidation OER was chosen as a model system. Advanced activity-stability analyses were performed by scanning flow cell connected to an inductively coupled plasma mass spectrometer (SFC-ICP-MS). In parallel, we performed high-end near-atomic-scale characterization by atom probe tomography (APT) and (scanning) transmission electron microscopy ((S)TEM), electron energy loss spectroscopy (EELS) and X-ray photoelectron spectroscopy (XPS). In addition, to resolve

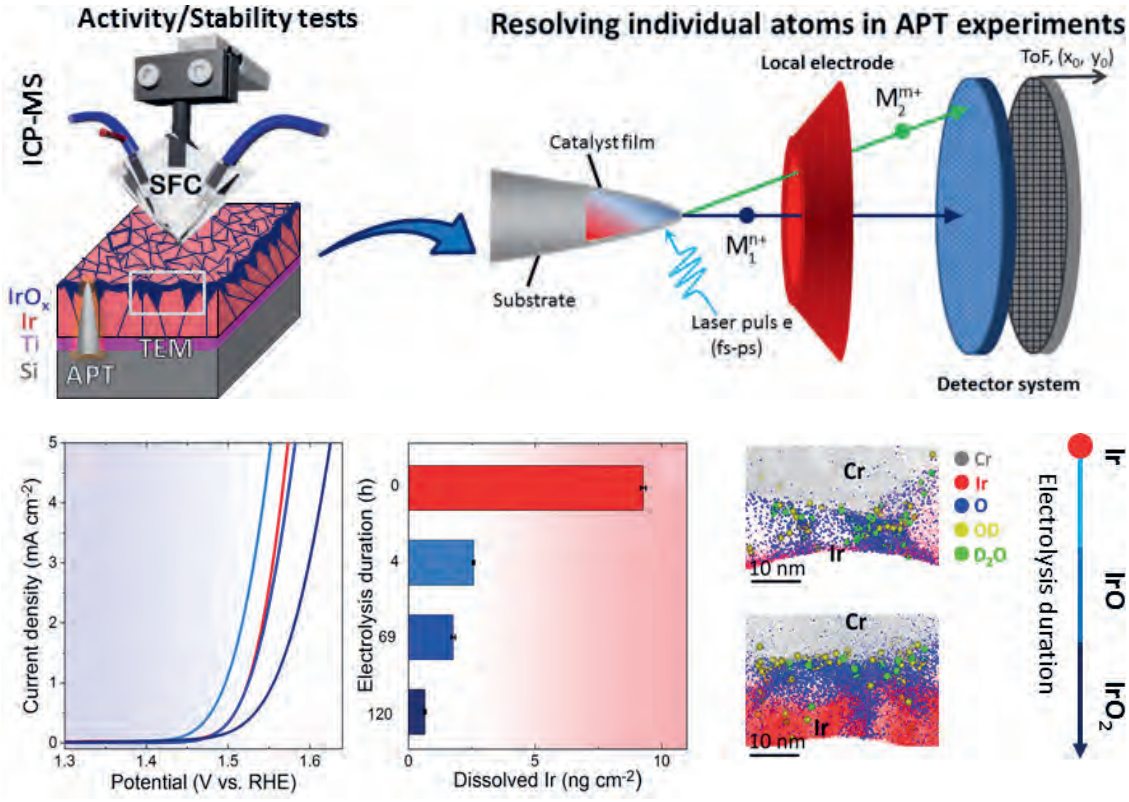


**Fig. 1:** *Combining SFC-ICP-MS with STEM and APT advanced understanding of electrocatalytic behaviour of Iridium OER catalysts.*

hydroxy-groups by APT in the electrochemically-grown oxides, proton-free deuterated electrolytes were used to avoid overlap with residual hydrogen from the ultra-high vacuum chamber.

This joint effort and the advanced characterization approach (Fig. 1) enabled to discover the formation of non-stoichiometric Ir-O species mixed with hydroxy-groups and water molecules during the short term electrolysis, providing a high electrocatalytic activity. The metastable Ir-O species gradually transform into $IrO_2$, which enabled to explain the observed decrease in activity and increase in stability [3]. The insights on the three-dimensional compositional distribution provided unique evidence of the chemical species residing at or near the outermost surface of Ir oxides and their transformation at near-atomic scale, which is critical for understanding the interplay between composition, reactivity and stability in electrocatalysis. In the future, this unique approach will be extended to other catalytic reactions and systems beyond OER and Ir-oxides. Combining advanced electrochemistry with APT and Identical Location Microscopy [4] will aid in unravelling the dynamic evolution of different nanoparticle catalysts commonly used in state of the art energy conversion and storage devices.

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# Electrochemical Semiconductor/Water Interfaces

*L. Yang [1], F. Niu [1], A. Erbe [1], S. Wippermann [1], M. Todorova [2], J. Neugebauer [2]*

[1] *Department of Interface Chemistry and Surface Engineering (GO)*
[2] *Department of Computational Materials Design (CM)*

Solid/liquid interfaces are of ubiquitous importance, e.g., in electrochemistry, electrocatalysis and corrosion. Often, metal electrodes are covered by semiconducting oxide films, and oxide/water interfaces also form as a consequence of corrosion processes. Emerging photoelectrochemical technologies, such as light-induced water splitting, employ semiconducting photoelectrodes. Therefore, many electrochemical interfaces of interest are in fact semiconductor/liquid interfaces. We utilize single-crystalline, atomically flat interfaces between semiconductors and liquid water as well-defined model systems to develop and validate methods, and to understand fundamental principles and processes.

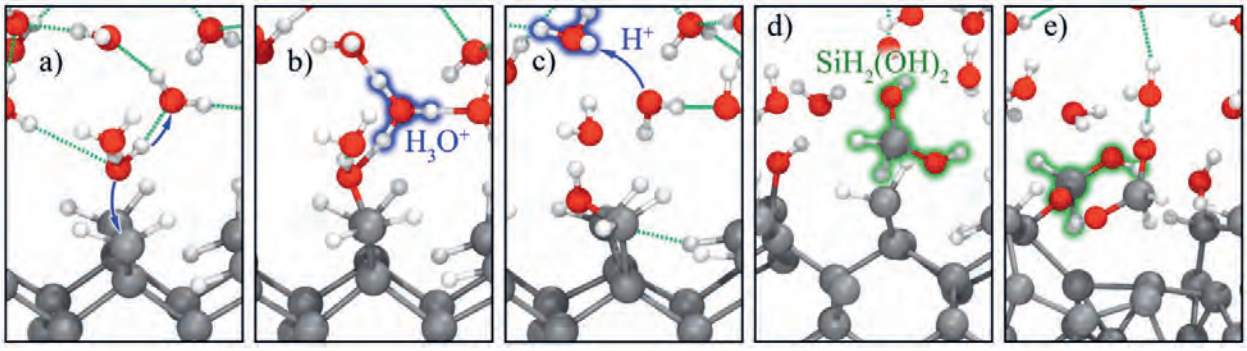


**Fig. 1:** *Snapshots of an ab initio MD simulation with applied electric field, showing initial oxidation steps of the solvated Si(100):H surface under anodic conditions, see text.*

Hydrogenated silicon and germanium surfaces in contact with liquid water are of particular interest in this context. They are transparent with respect to infrared light. Thus, optical fingerprints of electrochemical reactions and intermediates can be obtained in operando using attenuated total reflection infrared (ATRIR) spectroscopy. In water, silicon is known to irreversibly form porous oxide layers. The exact oxidation mechanism, however, is not yet understood. In addition, oxidation can be suppressed completely or allowed to proceed at controlled rates depending on the potential applied to the silicon electrode. Silicon is therefore of interest as a model system for corrosion. On the other hand, we find that germanium features a reversible potential-induced phase transition of the surface termination. It is therefore of interest as a model system to develop methods for predicting surface Pourbaix diagrams from first principles.

We use the modern theory of polarization, which introduces an electric field term directly into the density-functional theory (DFT) Hamiltonian, to describe electric fields in *ab initio* molecular dynamics (MD) simulations. Thereby, we can simulate the full electrochemical cell without a vacuum region. On the time scales accessible to our *ab initio* simulations, MD calculations demonstrate the solvated Si(100):H surface to be stable in the absence of applied electric fields and no interfacial reactions are observed. Once, however, the field is switched on, we observe characteristic field-induced surface reactions within a few ps, cf. Fig. 1: on the positively charged anodic surface, a $H_2O$ molecule dissociates (a). The $H^+$ is transferred to a neighbouring $H_2O$ molecule, whereas the $OH^-$ group binds to a surface Si atom, breaking a Si-Si backbond in the process (b). The proton is transported in accordance with the Grotthus mechanism towards the cathodic surface (c), where, at later stages when a sufficient number of protons has arrived, hydrogen evolution is observed. Eventually, a second water molecule dissociates and breaks the remaining Si-Si backbond of the surface $SiH_2OH$ group. The resulting $SiH_2(OH)_2$ molecule is then solvated (d). Often, an OH group within the solvated $SiH_2(OH)_2$ molecule deprotonates and subsequently binds to another surface Si atom, forming an Si-O-Si bridge (e). These are the first steps towards electrochemical oxidation of Si.

On the Ge(100):H surface, a qualitatively different process emerges. Following the approach outlined by Surendralal et al. [1], we introduced a potentiostat directly into the Quantum Espresso DFT package and perform MD simulations at constant electrode potential. At each *ab initio* MD time step, the electric field is adjusted so as to keep the potential difference at a target value of -1 V. A damping term is introduced to prevent any abrupt changes of the field, changing the electric field in a smooth and adiabatic way at all times. Fig. 2a shows the surface charge and the potential difference between the Ge surface and a computational counter electrode as a function of time.

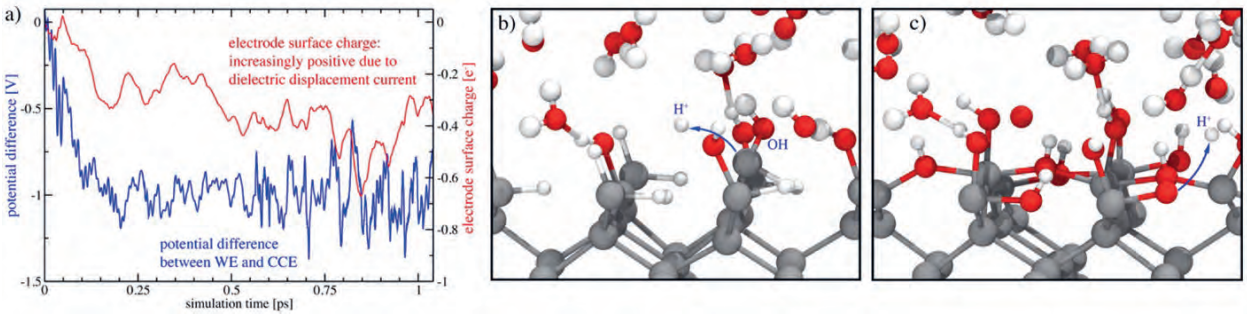


**Fig. 2**: *a) Surface charge and electrode potential as a function of time during ab initio MD simulations of solvated Ge(100):H surface. MD Snapshots of b) hydroxylation and c) oxidation events.*

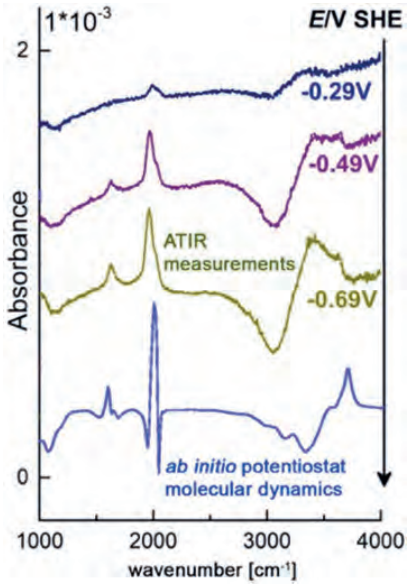


**Fig. 3:** *Infrared spectra of the Ge(100):H/$H_2O$ interface, measured by ATRIR spectroscopy and compared to predictions from ab initio potentiostat MD simulations.*

To keep the electrode potential constant, save for thermal fluctuations, the potentiostat must, however, continuously adjust the surface charge towards increasingly anodic conditions. We are thus observing a dielectric displacement current, caused by water reorientation and formation of the electrochemical double layer. The increasing fluctuations observed after 0.75 ps are due to an $OH^-$ ion approaching and attempting to hydroxylate the surface. A snapshot of the hydroxylation event is shown in Fig. 2b. On the completely hydroxylated surface the OH groups eventually move into the troughs between the rows of the surface Ge atoms and deprotonate, cf. Fig. 2c, and a thin surface oxide layer is formed.

Interestingly, in marked difference to our observations on Si(100):H, Ge hydroxylation and oxidation occur without breaking any Ge-Ge backbonds. The process thus resembles a surface phase transition. Indeed, ATRIR measurements confirm this transition to be potential-induced and reversible. Using our MD trajectories, we compute the difference between the vibrational spectra of the hydrogenated and hydroxylated Ge(100):H/$H_2O$ interfaces. The resulting spectra are compared to ATRIR measurements in Fig. 3 [2]. The spectra predicted from first principles coincide closely with the ATRIR measurements, confirming the transition in surface termination observed in our potentiostat MD simulations.

These two examples demonstrate that with our new methodological advances it is now possible to perform *ab initio* molecular dynamics calculations with applied electric field and at constant electrode potential. They also illustrate how our continuous methodological developments help to reveal the fundamental mechanisms of electrochemical and corrosion reactions at solid/liquid interfaces.

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# Passivity and Passivity Breakdown on Copper: Defect Formation during Oxygen Evolution and Effect of Chloride

*C. Toparli [1,3], A. Sarfraz [1], S. Hieke [2], A. Altin [1], C. Scheu [2], A.D. Wieck [4], M. Rohwerder [1], A. Erbe [1,5]*

[1] Department of Interface Chemistry and Surface Engineering (GO)
[2] Independent Max Planck Research Group on Nanoanalytics and Interfaces (NG)
[3] now at: Massachusetts Institute of Technology Cambridge, MA, USA
[4] Chair for Applied Solid State Physics, Ruhr-Universität Bochum
[5] Norwegian University of Science and Technology, Trondheim, Norway

Passivity breakdown is a major issue in corrosion. It is often assumed that passive films are simple, uniform and homogeneous oxide layers blocking the cation transfer from the metal surface to the electrolyte. However, recent advancement in surface analytical techniques show that almost all passive films have multilayer structure, including an inner layer, outer hydroxide part and also a barrier layer [1]. Passivity breakdown can occur due to several reasons during anodic polarisation up to the oxygen evolution reaction (OER). A key challenge remains the capture of the changes in the film *in situ* to obtain detailed insight into reactions. Aim of this work is to uncover passive film formation and its breakdown on Cu in relation to formation of point defects, electronic properties and chemical nature of oxides.

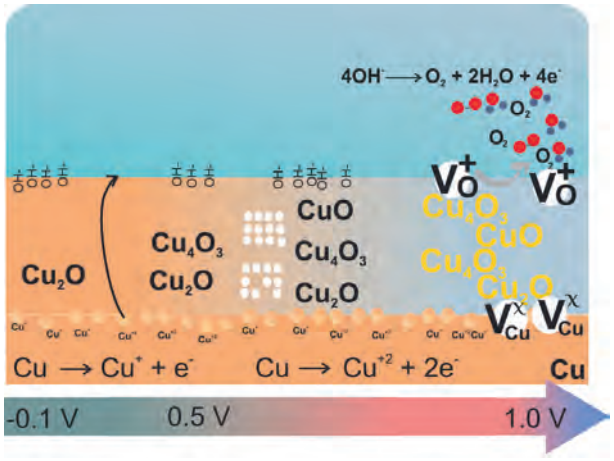


**Fig. 1:** *Scheme illustrating dominant oxide phases, and observed defect formation as function of electrode potential, on Cu in NaOH.*

In hydroxide, we systematically investigated the passive film formation, its breakdown accompanied by oxygen evolution, and the effect of $Cl^-$ on passivity breakdown by *in situ* spectroscopic ellipsometry (SE), *in situ* Raman spectroscopy and *in situ* photoluminescence spectroscopy (PL), completed by *ex situ* techniques. The thickness of the passive oxide layers was calculated from SE data by a model-independant first order perturbation approach [2], and confirmed *ex situ* as ~7 nm. Thicknesses of the passive films are weakly potential dependent [3], in disagreement with the point defect model [4]. The *in situ* Raman experiments results indicated that the mixed oxide $Cu_4O_3$ plays a prominent role in the passive film [3]. Both *in situ* PL spectra and *in situ* ellipsometry spectra showed that the passive film of Cu is a defective phase. Passivity breakdown through OER was accompanied by the formation of singly charged oxygen vacancies with *in situ* PL. At the onset of strong defect-related PL, the thickness of the oxide layer decreased, which shows that breakdown of the oxide layer is triggered by defect formation [5]. *Ex situ* Hall effect measurements in collaboration with the Ruhr-Universität Bochum show that both passive oxide and transpassive oxide have n-type conductivity, in contrast to literature data [1]. Overall, a rather complex mechanism of dissolution results as illustrated in Fig. 1.

The effect of $Cl^-$ on the properties of oxide film growing on Cu was studied using phosphate buffer saline (PBS, pH 7) [6]. Besides industrial relevance, Cu acts antibacterial. The corrosion mechanism of Cu in complex biological buffers is unknown. In PBS, corrosion products based on copper oxides, hydroxides, chlorides, phosphates, or mixed phases may develop. An early proposal for the corrosion mechanism of Cu in neutral $Cl^-$-containing media assumed that the initial corrosion product is CuCl, which transforms into $Cu_2O$. In later works, copper oxide formation in $Cl^-$-containing media was suggested to be a precipitation reaction rather than an electrochemical process. We observed that in PBS, the thickness of the growing film is dependent on the applied electrode potential. CuCl is only observed as a transient species before oxide formation. *Ex situ* surface analysis could not confirm the presence of CuCl (see Fig. 2). Cross sectional images show voids between the oxide layer and metal (Fig. 2). Inconsistencies became clear between *in situ* spectroscopy results and *ex situ* surface analysis. Based on observations and calculated predominance potential pH diagrams, the following model was proposed [6]. During anodic polarization, first $Cu_2O$ forms. This film is rich in point defects, as suggested by its absorption spectrum, some of these are likely oxygen vacancies. These can be compensated by uptake of $Cl^-$, resulting in the first step in a chloride-rich, $Cu_2O$-based layer. As soon as the elec-

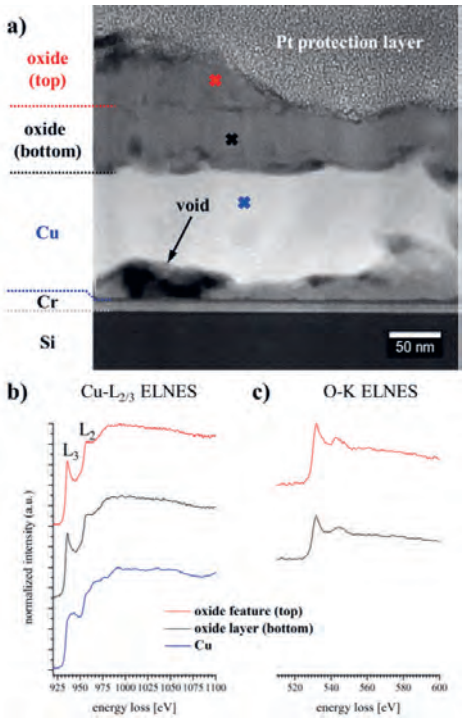


**Fig. 2:** *(a) Cross sectional scanning transmission electron micrograph shows the location where the presented energy electron loss spectra given in (b) and (c) were taken [6]. (b) Cu $L_{2/3}$ and (c) O K near-edge fine structures of the upper oxide feature (red), the lower oxide layer (black) and the Cu thin film (blue).*

trode potential increase triggers oxidation from $Cu^{I}$ to $Cu^{II}$, the formation of soluble $CuCl_4^{2-}$ sets in, which may have precursors inside the film, or adsorbed to the surface. The dissolution of copper proceeds via chloride incorporation in oxygen vacancies in the defective $Cu_2O$ [6]. As dissolution in the presence of biological material often proceeds at near neutral pH in an environment containing significant amounts of $Cl^-$, the results obtained in this work are relevant for the understanding of the surface electrochemistry of copper as antibacterial agent.

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# Grain Boundary Phase States

*A. Kwiatkowski da Silva [1], C. Liebscher [2], R. Hadian [3], B. Gault [1], D. Ponge [1], G. Dehm [2], J. Neugebauer [3], D. Raabe [1]*

[1] Department of Microstructure Physics and Alloy Design (MA)
[2] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[3] Department of Computational Materials Design (CM)

The local chemistry and structure of a grain boundary (GB) determines its energy, mobility, diffusivity, cohesive strength and sliding resistance, which directly affect the bulk materials' behaviour and properties such as impact toughness, creep resistance, fatigue, corrosion, and strength. GBs behave as quasi-two-dimensional phases, undergoing structural and chemical changes abruptly at critical values of thermodynamic parameters such as temperature, pressure and composition [1]. Recently, the term "complexion" was introduced to distinguish these equilibrium interfacial states from bulk phases [2]. GB phase states can be categorized by the type of transition that locally impacts GB properties through the formation of steps, facets or solute induced transitions of the GB core structure.

We have explored the impact of GB steps on GB mobility and discovered the atomistic mechanisms through molecular dynamics simulations. We found correlations between the type of steps that appear on the relaxed structure of a boundary and their migration energy barriers [3] as shown in Fig. 1. From this result we were able to conclude that the majority of general grain boundaries relax into steps with low symmetry, termed *kinked* boundaries which were shown to have the lowest migration barrier in comparison to flat and stepped boundaries. It was then observed that the facets in these *kinked* boundaries tend to coarsen in pure metals. This implies that general GBs dissociate into coarsely faceted segments, if faceting is not impeded or directed otherwise by alloying elements [4].

The generation and minimization of grain boundary structures is a precursor for migration simulations and we have designed an open access python package [5] that generates GB structures for atomistic simulations and additionally includes a minimization routine. Further *Jupyter* notebook scripts in the package give a step by step description on how to use the code to locate and produce GBs for *ab initio* or molecular dynamics simulations. It also serves as a platform to produce CSL properties for a given GB plane, such as CSL density.

Some of the extra functionalities of the code are as follows:

- Generation of different stepped structures
- Generation of large faceted structures
- Producing the displacement shift vectors (DSC) on a given GB plane. These vectors are conceptually considered to act as Burgers vectors of GB dislocations.

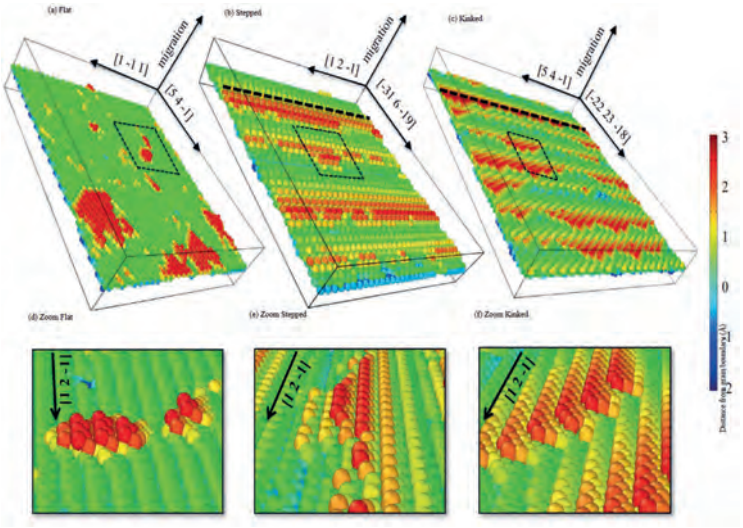


**Fig. 1:** *Migration mechanisms of flat (a), stepped (b) and kinked (c) grain boundaries. The colour code denotes height. Bulk atoms have been removed for clarity and only GB atoms are shown.*

The impact of phase transitions on the diffusivity or mobility of GBs has been intensively studied on idealized symmetric boundaries. In recent work, we could show that solute segregation is strongly anomalous in nanofaceted boundaries. In particular, the segregation of carbon (C) and iron (Fe) in multicrystalline silicon (Si) GBs is observed to occur at the facet junctions in contrast to the often assumed planar segregation at the facets themselves [6]. By using a combination of atomic resolution scanning transmission electron microscopy (STEM), atom probe tomography (APT) and molecular statics simulations, we were able to reveal that the atomic strain in the facet junctions dictates the segregation behaviour. Furthermore, we have systematically investigated the solute induced nanofaceting in asymmetric tilt grain boundaries. We could show that an initially flat, asymmetric copper (Cu) tilt GB develops silver (Ag) rich, nanometre sized facets upon controlled segregation as illustrated in Fig. 2 [7]. In combination with hybrid molecular dynamics and Monte Carlo simulations we established that this nanoscale GB phase transition is a result of a cascade of phase transitions and the

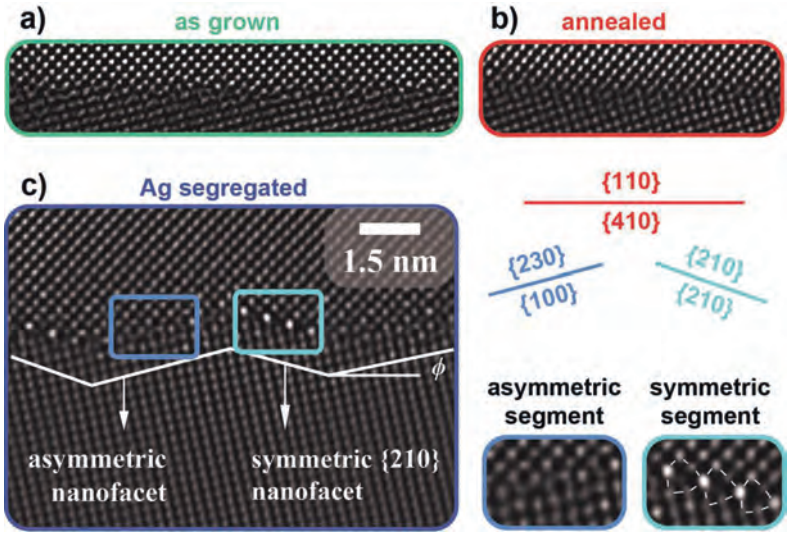


**Fig. 2:** *(a) Atomic structure of the asymmetric [001] Cu tilt grain boundary in the as grown state. (b) After annealing at 800ºC for 120 h. (c) Nanofaceted boundary after controlled Ag segregation annealed at 800ºC for 120 h.*

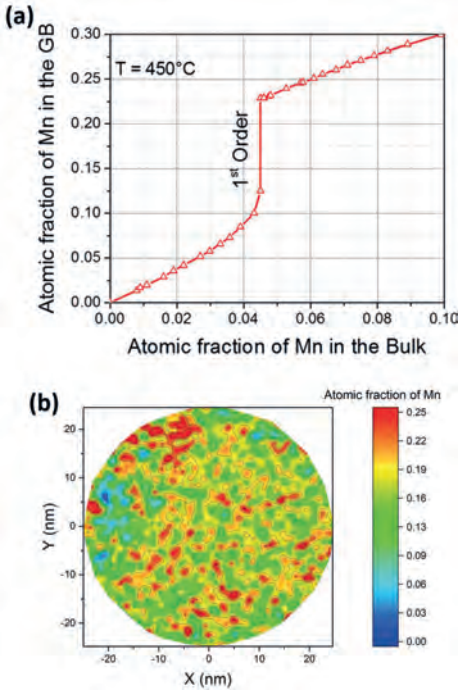


**Fig. 3:** *(a) Segregation isotherm at 450°C assuming metastable local equilibrium between the bulk and the grain boundary in a Fe-Mn BCC alloy. (b) 2D in-plane compositional analysis inside the grain boundary plane obtained by APT for a grain boundary from Fe-9 atomic % Mn solid solution, 50% cold-rolled, and annealed at 450 °C for 6 h.*

symmetric kite structure, shown in Fig. 2 c, is formed, due to its ability in taking up the highest amount of Ag atoms.

For solid-solid phase transformations, GB segregation is widely regarded as a pathway for phase transitions, since segregation to defects locally alters the thermodynamic driving force for phase nucleation by changing the chemical composition of the interfacial region. We developed an approach in order to quantitatively and qualitatively describe the Mn segregation in the BCC structure in Fe-Mn alloys which we systematically studied by Atom Probe Tomography (APT). This approach couples thermodynamic data from Calphad with a mean-field description of the grain boundary character what allows a more precise description of the segregation behaviour observed by APT than the more typical Langmuir-McLean segregation model [8]. The most important consequence of this model is that the presence of a spinodal region for the Fe-Mn BCC free-energy will lead to a first order transition of the grain boundary interface before the nucleation of austenite. This first order transition is typically represented in equilibrium segregation calculations as a discontinuous jump in the composition of the GB in function of the bulk composition (Fig. 3a). From a kinetics perspective, it implies the formation of metastable spinodal fluctuations (Fig. 3b) that tend to grow further with time at the segregated region, as observed by APT [4]. On the one hand, this increase in Mn content at the GB leads to an increase of the overall enthalpy of the boundary at lower temperatures and thus to embrittlement. On the other hand, these low-dimensional spinodal fluctuations on the GB act as precursor states to the nucleation of austenite when they become strong enough in composition amplitude and wavelength. Once austenite is formed, the amount of Mn segregated to the grain boundaries is drastically reduced and the toughness of the grain boundary is increased [9].

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# Dislocation Interactions with Twin Boundaries

*C. Kirchlechner [1], N.V. Malyar [1], M.K. Kini [1], W.S. Choi [2], S. Sandlöbes [2], R. Hadian [3], B. Grabowski [3]*

[1] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[2] Department of Microstructure Physics and Alloy Design (MA)
[3] Department of Computational Materials Design (CM)

Coherent Σ3 twin boundaries are certainly one of the most prominent interfaces in structural materials. Firstly, because they can be introduced by numerous processes like crystal growth, annealing, or even cold working. Secondly, because they simultaneously allow for an extraordinary high strength while maintaining an outstanding ductility, two properties which are classically mutually excluding themselves but are combined in bulk nano-twinned materials [1]. The combination of high strength and ductility is the "holy grail" in structural materials and renders damage tolerance. The fundamental origin of the damage tolerance is, however, still not understood and currently studied across several departments of the MPIE.

We are focusing on the behaviour of single dislocations at twin boundaries and their mutual interactions. Dislocations can transmit through a twin boundary in two ways: (i) the "ideal" or also "soft" mode, where the Burgers vector of the dislocation is a shared lattice vector in both twin-grains. And, (ii), the "hard" mode, where the Burgers vector of the dislocation is not a low indexed lattice vector in the second grain, which complicates slip transmission considerably. During the last years we have developed and applied a complementary toolbox [2] of *in situ* scanning electron microscopy (SEM), *in situ* Laue microdiffraction (μLaue), transmission electron microscopy (TEM) as well as atomistic simulations to unravel and quantify the mechanisms of slip transmission through grain and twin boundaries.

The *in situ* SEM experiments are well suited for monitoring collective slip transmission processes in terms of slip trace analysis (see Fig. 1). This technique is well established and enables to study large sample numbers, often exceeding 100 samples per study. Recently, we were able to measure the activation volume and strain rate sensitivity of ideal slip transmission of dislocations through a coherent Σ3(111) twin boundary in copper [3]. The results point towards a cross-slip like dislocation transmission mode with a strain rate sensitivity of the twinned bicrystals similar to the single crystal.

Complementary to our SEM work, the μLaue technique can quantify the collective dislocation storage in terms of geometrically necessary dislocations in the grain interior and at the twin boundary. Furthermore, the local deviatoric strain tensor and crystallographic orientation can be measured. Using the ability of μLaue to measure the local orientation and number of dislocations in a pile-up, we were able to identify the stress required for ideal dislocation slip transmission through a coherent Σ3(111) copper twin boundary for the first time [4]. Surprisingly, this slip transmission stress (17 MPa) agrees well with the stress required for dislocation cross-slip in copper at the same temperature. Our results indicate that in at least three out of 12 slip systems copper twin boundaries do not act as strong barriers for dislocation slip. This might be extremely important during the local stress relaxation at crack tips in bulk nano-twinned materials. The extraordinary strength of these systems might

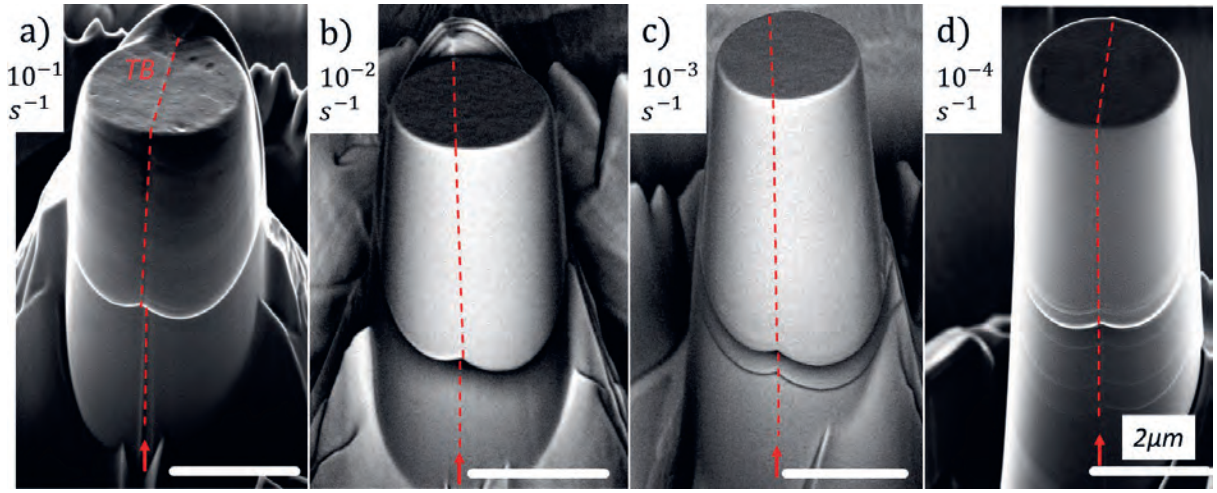


**Fig. 1:** *Micropillars deformed inside the SEM at different strain rates. The slip plane sharply kinks off at the location of the twin boundary. No significant differences in the activation of major slip steps can be identified.*

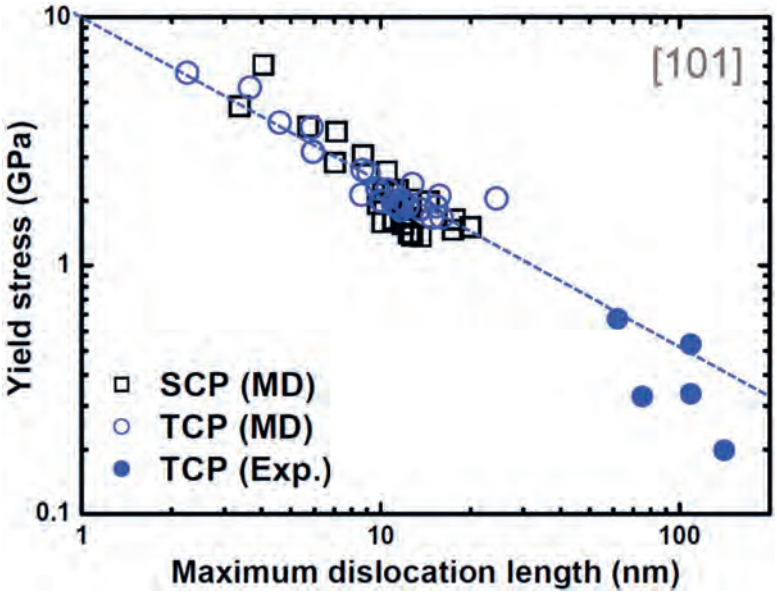


**Fig. 2:** *Correlation between the maximum dislocation length and the yield stress obtained from MD simulations for 42 nm sized nanopillars (open symbols) in comparison with experimental data from Imrich et al. [9]. SCP refers to single crystalline pillars and TCP to twin crystalline pillars. The extrapolation (blue dotted line) is based on a power fitting function and uses as input only the MD data for twin crystal pillars (blue empty points). The agreement with experiment is excellent.*

however be caused by compatibility requirements, which is currently investigated on nano-twinned silver thin films with twin thicknesses ranging from 10 nm to 1 µm.

*In situ* and *post mortem* TEM analysis are an ideal tool to understand the interactions of single dislocations with twin boundaries, as well as the impact of local chemistry on dislocation mobility. We have applied TEM not only on Σ3(111) boundaries in copper, but have also quantified the importance of twinning, double-twinning and slip transmission on the mechanical properties of Fe-Mn-C twinning-induced plasticity steel (TWIPs) [5,6].

The three experimental tools are finally complemented by MD simulations which shed light on possible mechanisms active during slip transfer [7, 8]. Our current work thereby focuses on the importance of the initial dislocation structure on the slip transmission properties [8]. For this purpose we have deformed pristine pillars requiring stresses close to the theoretical shear stress of copper for plastic deformation. Furthermore, we used high vacancy concentrations and subsequent thermal annealing to produce a natural dislocation network in our MD pillars (see Fig. 2). These pillars deformed at significantly lower stresses than the pristine ones. Also, the micropillars with a grown-in dislocation network exhibit slightly higher yield stresses than their single crystalline counter parts with similar dislocation structures. Snapshots taken during slip transmission point towards a double-hump like dislocation transfer mechanism which supports the experimental observations from SEM and µLaue on strain rate sensitivity and transmission stress.

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# Local Chemistry at Planar Defects in Off-stoichiometric Binary Alloys

*C. Liebscher [1], F. Stein [1], M. Slapakova [1], A. Zendegani [2], T. Hickel [2], J. Neugebauer [2], D. Palanisamy [3], D. Raabe [3], B. Gault [3]*

[1] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[2] Department of Computational Materials Design (CM)
[3] Department of Microstructure Physics and Alloy Design (MA)

Properties of materials are to a wide extent determined by the presence of defects. They may be either artificially introduced into the material or can be intrinsic defects. The stability and concentration of these defects is closely related to their atomic structure, which can already be complex for planar defects in pure elements or chemically ordered phases, such as Laves or Heusler alloys. In the case of multi-component alloys with off-stoichiometric compositions, the chemical degree of freedom adds another level of complexity. The excess atoms can form point defects (antisite atoms or vacancies) and can be accommodated by extended defects. Already a segregation of individual atoms yields an additional stabilization of these defects. Particularly fascinating becomes the interplay of local chemistry and planar defects, however, if defect structures and/or compositions are created that would not be present otherwise.

In the present article, we highlight two examples of binary intermetallic alloys that show such phenomena: First, we have observed novel atomic structures connected to planar stacking faults in phase-pure samples of the hexagonal Laves phase $NbFe_2$. They substantially change their concentration and therewith the mechanical performance of a phase, which is important for precipitation hardening in high-temperature steels [1-3]. Second, we have detected an unusual enrichment of Mn at twin boundaries in the binary $Al_{45}Mn_{55}$ Heusler alloy (τ-phase). These extended defects contribute to magnetic domain wall nucleation or act as pinning sites and are thus important for the magnetic response of a material, which is a potential low-cost replacement of medium performance ferrite-based magnets.

The significant increase in the defect density of the Laves phase $NbFe_2$ was observed with scanning transmission electron microscopy (STEM) in samples with 35 at.% Nb, while stoichiometric samples (33 at.% Nb) showed only isolated dislocations. Besides antisite occupation, various types of planar faults appear. We observed numerous extended planar defects parallel to the basal plane of the hexagonal structure, introducing Nb-enriched layers of various thicknesses, as well as a high number of confined basal and pyramidal planar faults. All types of observed basal and pyramidal faults contain structural motifs, which are characteristic for the crystal structure of the μ phase $Nb_6Fe_7$ (46 at.% Nb) in the same binary system. Interestingly, however, the

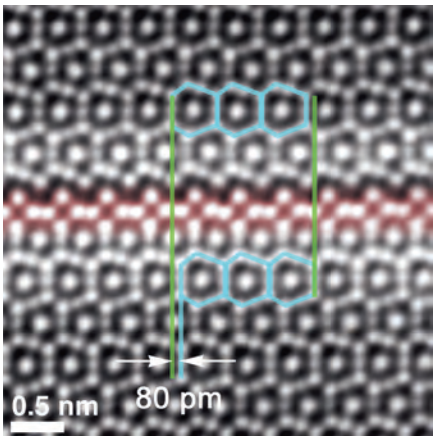


**Fig. 1a:** *Atomic resolution low angle annular dark-field (LAADF) STEM image of a basal fault in a Nb-rich $NbFe_2$ Laves phase with μ phase type building blocks. The shift of the upper and lower part and the single three-layer stack of the slab are highlighted.*

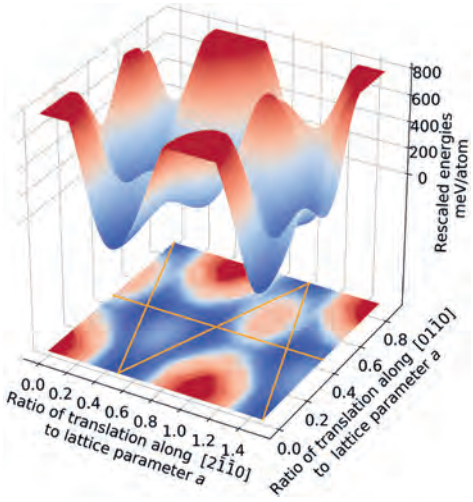


**Fig. 1b:** *The basal generalized stacking fault energy surface (γ surface) of the two half crystals in the STEM image. All structures along the orange lines reproduce in one projection the STEM image.*

stacking of the μ phase is not fulfilled in the atomic layers next to the defects, despite the increased Nb content. One of the variations in the stacking sequence is the omission of an Fe-layer, so-called Kagome layer, as shown in Fig. 1a.

We used *ab initio* calculations to determine the formation energies of these planar defects. A prerequisite was to find the exact crystallographic structure underlying the experimental STEM images, since the restriction to a single projection is still consistent

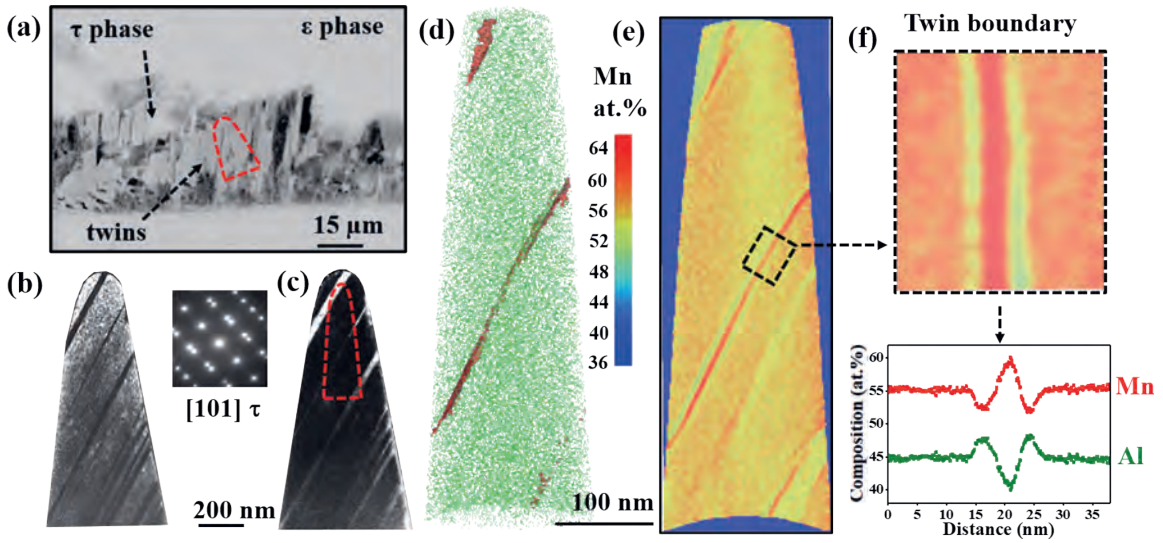


**Fig. 2:** *(a) Back-scattered electron SEM image of the $Al_{45}Mn_{55}$ ε phase sample annealed at 450 °C for 15 minutes showing massive growth of τ phase on ε phase grain boundaries. The red triangle is the location from where the atom probe tips have been extracted. (b) Bright field (BF) image taken near to [101] τ phase zone axis. (c) Dark field (DF) image taken from the twinning spot. (d) Atom probe reconstruction showing distribution of Al atoms (green colour) and iso-compositional interfaces with 60 at.% Mn (red colour) showing Mn enrichment confined to twins. (e) 2D composition plot with colour scale for Mn at.% across the APT tip reconstruction projected to the plane perpendicular to the viewing direction. (f) 2D and 1D composition plots showing Mn enrichment along the twin boundary.*

with multiple translational variants perpendicular to the image plane. Therefore, the generalized stacking fault energy (SFE) surface was determined by *ab initio* calculations (Fig. 1b). The energy of the most stable crystallographic Nb-enriched defect structures was then compared with a phase separation of the off-stoichiometric composition into a perfect Laves and a perfect μ phase. While the defects turned out to be not stable in equilibrium conditions, some of them become energetically favourable as compared to a phase separation that involves a laterally strained μ phase. This explains why a nanoprecipitation of μ phase is less likely than the observed extended defects.

The second example, $Al_{45}Mn_{55}$, is a metastable intermetallic phase with a $L1_0$ ordered structure. This compound, denoted as 'τ', evolves by suppressing the formation of equilibrium β-Mn (cubic) and $\gamma_2$ ($Al_8Mn_5$, rhombohedral) phases from the high temperature hexagonal-close packed ε phase and has a strong uniaxial magneto crystalline anisotropy. The microstructural development in the alloy takes place through massive mode and a large number density of defects such as twins, stacking faults and antiphase boundaries appear during the thermal history of the material [4]. Our combined electron microscopy and atom probe tomography approach revealed the structure and composition of some defects [5], as shown in Fig. 2. The extraordinary observation in this case, is the enrichment of twin boundaries by approx. ~8 at.% Mn with a confined depletion outside the boundaries. This evidences an occurrence of a short-range solute diffusion during the ε→τ-phase transformation. A more detailed study involving *ab initio* calculations is underway, and we aim to better understand the driving forces of this segregation behaviour and its effect to the defects on the magnetic properties for the $Al_{45}Mn_{55}$ alloy. This approach is also expanded to low rare earth containing high performance magnets such as Sm-Fe-Ti based, in collaboration with Professor Oliver Gutfleisch's Functional Materials group in TU Darmstadt. The obtained results and their interpretation will be used for improving the magnetic properties of these alloys by means of further tuning alloying and processing.

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# Tribology of Steels

*S. Brinckmann [1], M. Herbig [2]*

[1] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[2] Department of Microstructure Physics and Alloy Design (MA)

Friction of sliding components and surface wear occur in the majority of transportation and manufacturing systems. The associated friction induced energy losses are high, in combustion engines they are around 30-40%. Steels are often used for these applications as they offer low friction surfaces with ultra-mild wear volumes (<1×10$^{-7}$ mm$^3$ per periodic cycle). Steel contacts can be either unlubricated (e.g. in the food industry) or lubricated to further reduce friction and wear.

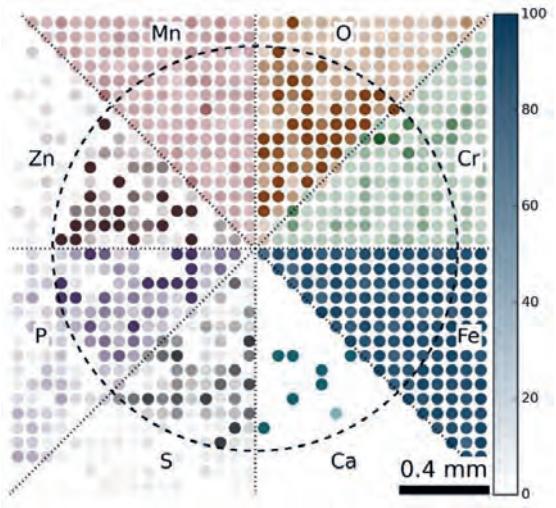


**Fig. 1:** *Distribution of elements in the macroscale cyclic contact as determined by quantitative electron probe microanalysis EPMA. The maxima are 100at.% for Fe; 5at.% for Cr, O; 1at.% for Mn; 0.5at.% for Zn;0.2at.% for P, S; 0.02at.% for Ca. The experiment was carried out using 100Cr6 steel on steel contact with ZDDP in a mineral oil.*

Lubricants use a number of additives that improve the wear resistance and reduce friction. Zinc-dialkyldithiophosphates (ZDDP) are currently the most frequently used anti-wear additives, which result in roughly 100 nm thin and amorphous surface layers that consist of material patches that have a few micrometer extension. However, improved environmental standards require a decrease in the use of phosphates and sulphates. To mirror the beneficial behaviour of ZDDPs onto next generation additives, the generation mechanisms of ZDDP-induced tribolayers have to be identified. To this end, we - in collaboration with colleagues at the Institute for Machine Elements and Systems Engineering, RWTH Aachen University - investigated the tribofilm generation by focusing on the mechanical activation of surface layer growth (Fig. 1).

We executed cyclic contact experiments (90 k cycles; 1.89 MPa contact pressure; frequency 2.5 Hz at macroscale and 0.33 Hz at microscale) at the macroscale (sphere radius = 27 mm) and microscale (sphere radius = 145 µm) and quantified the surface chemistry. The observed films are chemically and topographically similar to layers that evolve during conventional tribology [1]. In these layers, Zn, P and S are enriched compared to the contact outside and more oxygen is present. Moreover, the size of the film is similar to the Hertzian contact domain. This knowledge will be used to create a tribolayer growth model.

In addition to chemical surface layers, also the subsurface microstructure evolves during tribological loading. We studied the deformation of an austenitic [2,3] and pearlitic steel during microasperity friction. In pearlite, we observed that the cementite lamellae deform by bending (Fig. 2), undergo severe thickness changes and shear while only few lamellae fracture; despite of the brittle nature of cementite. The understanding of the ductile behaviour of cementite during microtribology requires a fundamental understanding of the local deformation. To this end, we executed microcantilever bending and micropillar compression experiments of pure cementite samples. Those experiments revealed that dislocation-mediated plasticity occurs as discete slip steps are present on the cantilever and pillar surface. The maximum plastic strain is on the order of 7% in pillar compression. However, the microscale experiments failed to exhibit severe bending as observed during microtribology. To further the insight of the severe bending, FEM simulations were executed to quantify the adiabatic heating due to plastic deformation. Those simulations revealed temperatures in excess of 600°C during microtribology.

The above described activities on pearlite target basic tribological principles and prepare the ground for understanding a complex phenomenon occurring during service in bearings: the formation of white etching cracks (WECs). These initiate below the bearing surface and eventually extend to the raceway what leads to catastrophic failure. Although this failure mode is known for more than 100 years and causes enormous economic costs worldwide so far neither the mechanism is understood nor are reliable countermeasures available. The research activities at the MPIE have revealed that failure by WEC is caused by a so far unknown crack propa-

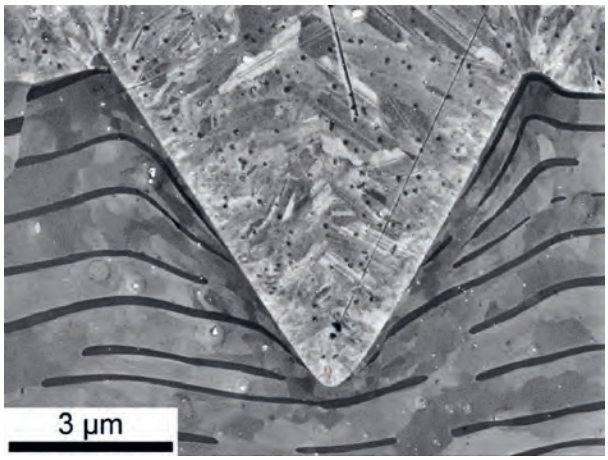


**Fig. 2:** *Cross-section of pearlite after microtribological experiment: cementite lamellae being embedded in ferrite can be deformed plastically although cementite on its own has only little ductility. The sample was enclosed by Ni for protection during cross-section preparation.*

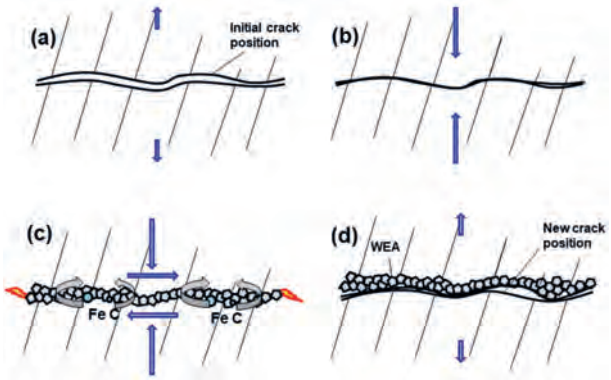


**Fig. 3:** *White etching crack (WEC) and white etching area (WEA) formation mechanism. During compressive loading cycles fracture surface rubbing occurs, leading to material transport between the fracture surfaces what causes a macroscopic change of the crack position.*

gation mechanism [4]. Cracks have been known to continuously extend until failure occurs and this holds also for WECs. However, WECs show additionally to that a unique particularity: they "roam" through the material, viz. they continuously change their position, leaving behind a severely plastically deformed area. This so called white etching area (WEA) consist of nanocrystalline ferrite surrounded by carbon (C) grain boundary segregation [5] as known also from the case of cold drawn pearlitic wires.

As WECs initiate within the bulk, their fracture surfaces are not oxidized. When these get in contact during a compressive loading cycle strong adhesive forces form and material can be transferred from one side of the fracture surface to the other. Many repetitive loading cycles lead to a macroscopic change in the crack position (Fig. 3). The element C plays a key role in the process [6] as it - on the one hand - stabilizes the WEA microstructure by lowering the grain boundary energy, whichreduces the driving force for dynamic recrystallization [5]. On the other hand, C forms a film on the fracture surfaces which prevents the complete closure of the crack and supposedly acts as a solid lubricant that facilitates fracture surface rubbing.

The formation of WECs involves the decomposition of carbides which act as a reservoir for C. Further research is targeted towards understanding precipitate stability and decomposition. The remarkable immunity of high nitrogen (N) bearing steels to WEC failure is elucidated by systematic comparison to the commonly employed high C bearing steels. Further, the influence of electric current in combination with deformation on the decomposition of cementite is currently being investigated. In future, tribological tests drawing cementite over ferrite will give insights into the processes occurring during WEC fracture surface rubbing. As the dislocation velocity influences solute drag, the influence of the deformation rate on cementite decomposition will be investigated using a custom-built rolling contact fatigue device. Further, the influence on hydrogen (H) on cementite decomposition will be investigated with a modified nanoindenter that allows *in situ* H charging.

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# Hydrogen Effect on the Mechanical Properties of Metallic Materials

*S. Brinckmann [1], J. Duarte [1], M. Rohwerder [2], H. Luo [2], Z. Li [3], D. Ponge [3], T. Hickel [4]*

[1] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[2] Department of Interface Chemistry and Surface Engineering (GO)
[3] Department of Microstructure Physics and Alloy Design (MA)
[4] Department of Computational Materials Design (CM)

**Experiments on hydrogen trapping sites:** The increasing use of high strength steels, Ni base superalloys and aluminium alloys led to a renewed interest in understanding H uptake and trapping in metallic materials. The strength of trapping and diffusivity of H depends on the microstructure. This investigation requires suitable methods for H detection. The Scanning Kelvin Probe Force Microscopy (SKPFM) is a high lateral resolution, unprecedented sensitivity technique for H detection that was applied for a number of different materials, e.g. Pd, Fe, duplex steel and Ni-Nb alloys [1-4]. The trapping sites inside a Fe-5 wt.-% Ni model alloy were characterized using a combination of Thermal Desorption Spectroscopy (TDS) and SKPFM (see Fig. 1*)*. The TDS detects no traps in the recrystallized material, but indicates at least two traps in the cold rolled material. They were identified as dislocations and vacancies with desorption energies of 29 and 38 kJ/mol (0.3eV and 0.39eV) [5]. The SKPFM and Kelvin Probe (KP) measurements give indirect confirmation that the vacancy density is higher close to inclusions, most probably at the oxide inclusion-matrix interface, and that even the recrystallized material has such H traps. In Fig. 1b), KP allows obtaining quantifiable potentials and shows that the average background signal is much higher for the cold rolled sample compared to the recrystallized one, indicating a 100 times higher H release rate. This means that the H release around inclusions detected by SKPFM is much lower in the recrystallized sample than in the cold rolled one. This example shows the advantage of using a combination of TDS and SKPFM for a more detailed trap characterization of materials.

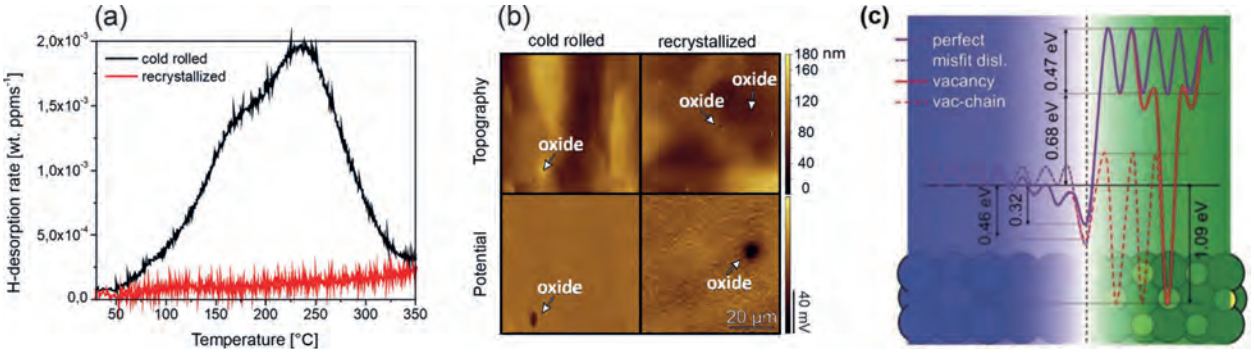


**Fig. 1:** *(a) TDS and (b) SKPFM map for a Fe-5 wt.% Ni alloy [5]. (c) Energy profiles of H at a (001)Fe/(001)TiC interface, which is perfect (purple solid), contains a misfit dislocation (purple dashed), a vacancy in the carbide (red solid), or a chain of vacancies starting at the interface (red dashed), see also [6].*

**Simulations on hydrogen trapping sites:** *Ab initio* based simulations allow us a systematic study of the H trapping next to precipitates and inclusions, taking the impact of vacancies as well as the possibility of H-enhanced decohesion into account. Investigations have, for example, been performed for cementite, k carbide, Cr carbides, and TiC, in the CM department and in collaboration with external groups. In the prototype case of TiC precipitates misfit dislocations and incoherencies have been simulated by well-defined crystal translations and modified orientation relationships, respectively [6]. The good agreement with trapping energies measured in TDS validates the reliability of this approach. We observe that the trapping of H to a perfectly coherent interface is moderate (0.32 eV) and is slightly enhanced (0.46 eV) for misfit dislocations (Fig. 1c). There are different scenarios for the trapping by C vacancies near the interface. Directly at the interface, a C vacancy yields a similar trapping energy as for misfit dislocations, while a vacancy insight the carbide shows a very deep trap with barriers of more than 1.7 eV. The most efficient trapping mechanism are chains and accumulations of C vacancies near the TiC interface to the matrix, a scenario that could explain the large traps at oxide-matrix interfaces, as measured by SKPFM and TDS.

**Influence of hydrogen on incipient plasticity in iron alloys:** The failure mechanisms that initiate at the atomic scale due to H absorption and interaction with trap binding sites, i.e. interfaces, precipitates or dislocations, can be studied independently by nanoindentation due to the small volume probed. In addition, *in situ* charging the sample with H avoids the formation of concentration gradients related to desorption. Two custom electrochemical cells were

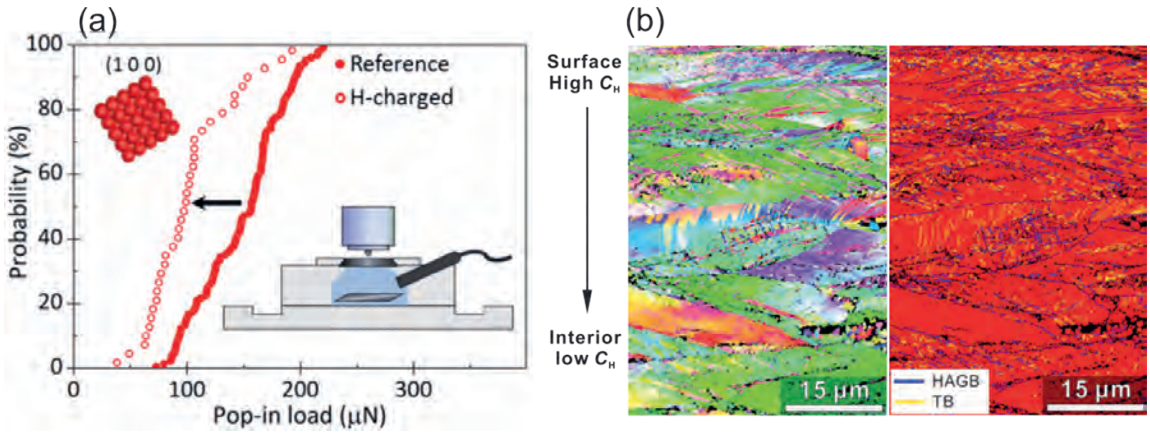


**Fig. 2:** *(a) Cumulative plot of the pop-in load for the (1 0 0) grain orientation showing a decrease related to H charging. Inset: back-side set-up for electrochemical charging. (b) Nanotwinned microstructure in a high entropy alloy with a high H concentration at the surface (top side) and low H concentration in the interior (bottom side). Inverse pole figure map of the grain orientation determined by electron backscatter diffraction (EBSD).*

built for *in situ* H charging during nanoindentation: "front-side" charging with the sample and indenter tip immersed into the electrolyte, and "back-side" charging where the analyzed region is never in contact with the solution. As case study, we investigate homogeneous nucleation of dislocations in bcc FeCr alloys depending on the H content. While directly charging with H in the back-side setup (inset in Fig. 2a), KP measurements over a Fe-20 wt.%Cr alloy showed a fast H diffusion rate towards the upper surface ($1.5x10^{-6}$ $cm^2/s$) as well as a pronounced release flow. During nanoindentation, a reduction in the pop-in load indicating the yield stress decrease with the increase of H content. The formation of multiple pop-ins provides evidence for the decrease in the resolved shear stress and enhanced dislocations nucleation. This behaviour is consistent with a multiscale simulation of homogeneous dislocation nucleation combining atomistic information (e.g., dislocation-core structure, H-H interaction) and a self-consistent iterative method for the local H concentration in a dislocation stress field [7]. According to that approach, the reduced critical shear stress can be explained as an effective decrease of the dislocation line energy due to the interaction with diffusible H.

**Hydrogen in CoCrFeMnNi High Entropy Alloy (HEA):** Besides the conventional alloys discussed above, we also probed the H effects on the novel high-entropy alloys which contain multiple principal elements in equiatomic or near-equiatomic concentrations. We demonstrated that H can be utilized for the case of an equiatomic CoCrFeMnNi HEA to tune beneficial strengthening and toughening mechanisms rather than undergoing catastrophic failure due to H embrittlement at room temperature [8]. Specifically, our work showed that a proper concentration of H actually jointly increases both strength and ductility of the CoCrFeMnNi HEA. This stress and ductility increase is owing to the fact that H can cause a significant increase in the nano-twin density, thereby increasing the alloy's work-hardening capability, and thus increasing both strength and ductility [8]. We further investigated the H effect on the CoCrFeMnNi HEA at cryogenic temperatures. It was found that the exceptional damage tolerance of this HEA at cryogenic temperatures can be maintained even when exposed in H containing environment [9]. This resistance is enabled by a self-accommodation mechanism: the higher the local H content, the higher is the twin formation rate. Accordingly, the H's through thickness diffusion gradient translates into a nano-twin gradient that counteracts material weakening by enhanced local strengthening (Fig. 2b). The beneficial effect of the gradient nano-twin structure overcompensates the H embrittlement, and hence leading to the absence of H-induced surface cracks upon tensile deformation at cryogenic temperatures [9]. Thus, these investigations provide new insights for designing H tolerant materials.

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# Nucleation and Growth of Stable Hydrides

*Y. Chang [1], I. Mouton [1], W. Lu [2], A. Breen [1], S. Zhang [3], S. Wang [4], D. Vogel [5], A. Ackermann [4], D. Dye [4], T.B. Britton [4], C. Scheu [3], T. Hickel [6], C. Liebscher [2], M. Rohwerder [5], G. Dehm [2], D. Raabe [1], B. Gault [1]*

[1] Department of Microstructure Physics and Alloy Design (MA)
[2] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[3] Independent Max Planck Group on Nanoanalytics and Interfaces (NG)
[4] Department of Materials Science & Engineering, Imperial College London
[5] Department of Interface Chemistry and Surface Engineering (GO)
[6] Department of Computational Materials Design (CM)

Hydrogen embrittlement (HE) is a significant challenge in high strength alloys were the ingress of H can cause a sudden and often catastrophic loss in ductility and premature failure. Ti and Zr based alloys are both known to be particularly prone to HE. Direct quantification of H in alloys with near-atomic resolution is critical to gain a better understanding of HE and has only recently become a possibility through the use of advanced atom probe tomography (APT) techniques. Isotope marking with deuterium (D) allows to discriminate D from within the specimen from the spurious residual H from the vacuum chamber of the microscope. Both Ti and Zr, and their respective alloys have a high affinity for hydrogen and are typical hydride formers.

We charged a Zircaloy-4 with D to form stable deuterides and successfully characterised the nanostructure of the deuteride growth front using APT. We observed by a combination of transmission electron microscopy and atom probe tomography the presence of an intermediate, metastable deuteride present at the interface with the metal, as well as rejection of Sn from the deuteride, with a significant enrichment of Sn at the growth front of up to 2 at.%. This behaviour suggests that Sn may help to retard further deuteride growth and have a significant influence on the growth rate. Such information could have significant implications for controlling hydride evolution in Zr based alloys and reducing the severity of DHC [1].

In parallel, significant efforts have been devoted to investigating hydride formation in titanium. Ti-hydrides are brittle phases which cause premature failure of Ti-alloys. Ti adopts either a hexagonal close-packed structure, (α) which has negligible solubility for H, and a body-centred cubic structure, (β) which can absorb significant amounts of H. The main model for embrittlement involves the growth of hydride films at interfaces that provide rapid transport of H, enhance segregation and thus accelerate hydride nucleation and growth, where crack initiates and propagates. We revealed by joint transmission electron microscopy and atom probe tomography that hydrides are prone to form at α/β interfaces and/or α lath boundaries in both pure-Ti and an array of alloys. The example of Ti-4 wt.%Mo is summarised in Fig. 2 (a-f). In contrast, Al-containing commercial alloys, such as Ti-6Al-4V and Ti-6Al-2Sn-4Zr-6Mo alloys, could dissolve slightly more H and do not show hydrides. The strength of the α matrix seems to play

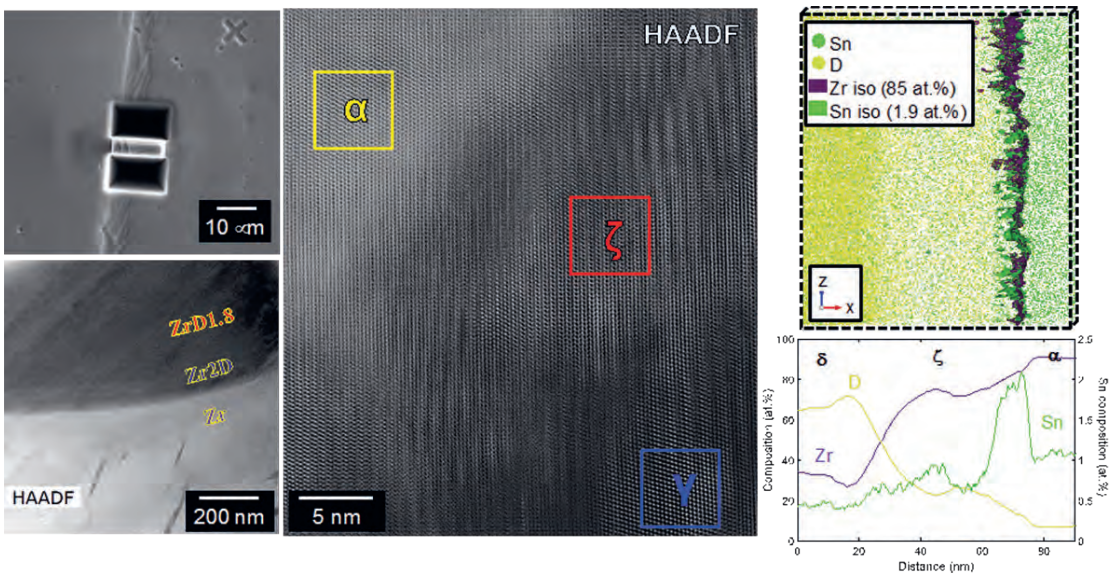


**Fig. 1:** *Focused-ion beam preparation of the specimen from a specific deuteride; conventional and high-resolution transmission electron microscopy of the deuteride-metal interface; Close-up on an atom probe tomography reconstruction and composition profile of the complex deuteride-metal interface.*

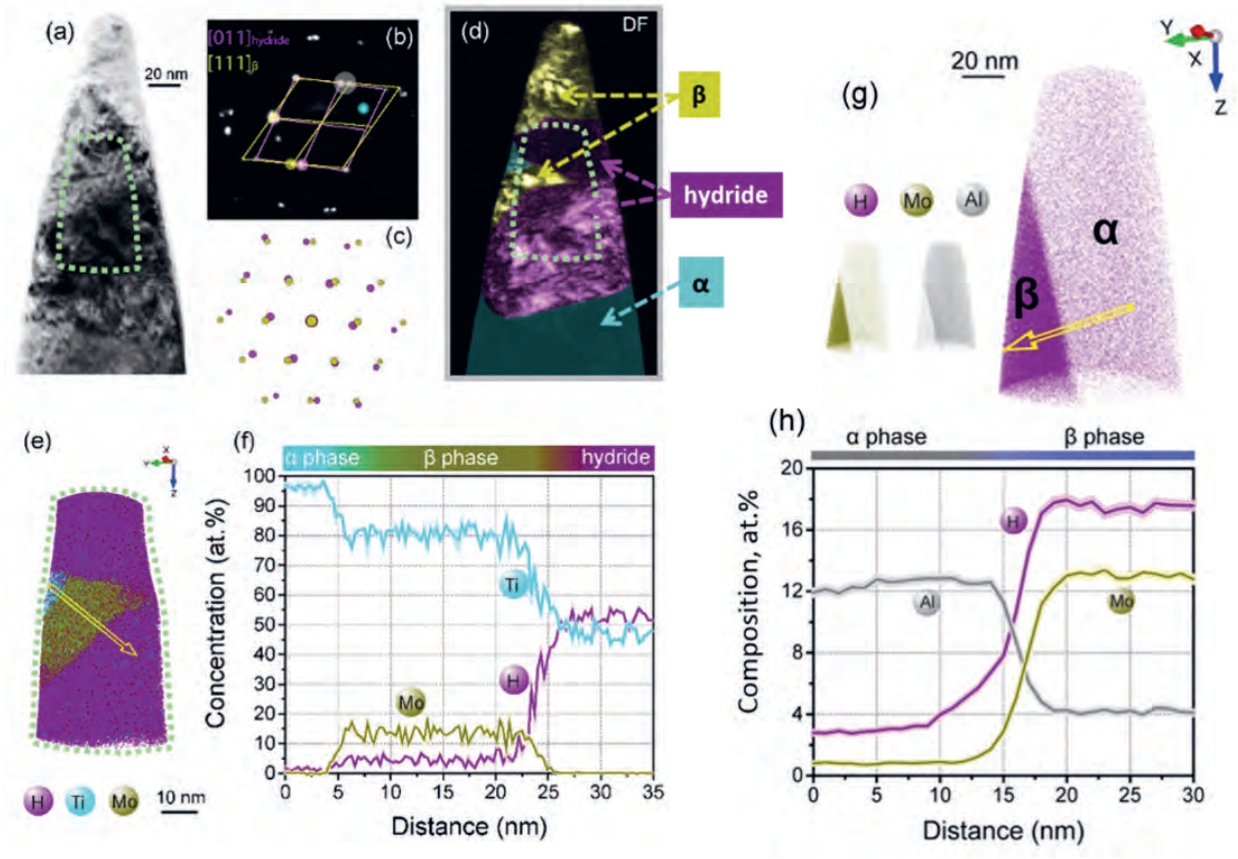


**Fig. 2:** *(a-f) Correlative TEM and APT analysis showing hydride formation at α/β interfaces in a Ti-4 wt.% Mo binary alloy; (g-h) H distribution and composition profile across the α/β interface in Ti-6Al-2Sn-4Zr-6Mo.*

a prominent role in hindering hydride formation, as the hydride growth must be accommodated by both elastic and plastic deformation. Therefore, the alloyed α phase probably requires greater supersaturation of H to create an adequate driving force for the formation of hydride. Our studies confirmed that Al alloying could increase H solubility in α and suppress hydride precipitation in Ti-alloys. The implication of our findings is that hydrogen embrittlement in commercial Ti alloys (with Al addition) near room temperature is probably not a consequence of hydride formation but the concentration of H in the β phase that can promote local decohesion or enable enhanced localized plasticity facilitating accelerated nucleation of cracks [2]. More work in this area, with a bridge to the CM department is underway through the appointment of a postdoctoral scientist joint between the groups of T. Hickel and B. Gault's ERC-Consolidator Grant (see p. 70 ), and the development of further infrastructure for gas-charging in collaboration with M. Rohwerder's group.

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# Combining Advanced Electron Microscopy Techniques with Atom Probe Tomography and Density-Functional Theory to Understand Materials' Behaviours

*C. Liebscher [2], T. Schwarz [1], M.J. Yao [1], P. Dey [3], I. Mouton [1], G. Stechmann [1], T. Hickel [3], D. Ponge [1], L.T. Stephenson [1], S. Zaefferer [1], G. Dehm [2], J. Neugebauer [3], C. Scheu [4], D. Raabe [1], M. Herbig [1], B. Gault [1]*

[1] Department of Microstructure Physics and Alloy Design (MA)
[2] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[3] Department of Computational Materials Design (CM)
[4] Independent Max Planck Group on Nanoanalytics and Interfaces (NG)

Over the past decades, it has become clear that understanding the interplay between structure, composition and properties requires the combination of advanced characterization techniques with compatible yet complementary strength. Electron microscopy and atom probe tomography form a good match as the former lacks the precise ppm-level compositional information whereas the latter does not allow for full structural analysis. In combination with *ab initio* simulation, which resolve their underlying chemo-mechanical coupling, a powerful toolbox for materials characterization becomes available.

A first example can be found in the combination of atom probe tomography with transmission Kikuchi diffraction. This technique exploits the diffraction of the electrons that have gone through the specimen to retrieve the local structure and grain orientation within the specimen. This is illustrated in Fig. 1, where a grain boundary is clearly imaged and characterized crystallographically in terms of its misorientation as well as chemically in terms of its local composition measured by atom probe. The study reveals strong segregation of Na and K impurities to the grain boundary in a $Cu(In,Ga)Se_2$ thin film used for solar cell application [1]. These solutes affect the degree of passivation of the grain and hence the transport properties of the film and the performance of the solar cell.

Moving up in scale, high-resolution scanning transmission electron microscopy (STEM) was performed on an atom probe specimen to reveal the atomic-scale structure of the material. A high-Mn weight-reduced Al-containing austenitic steel, strengthened by precipitation of coherent ordered κ-carbides upon heat treatment at 600°C was characterized [2]. Electron microscopy reveals the structure of the precipitates and their coherent interface with the matrix, as well as the local strain in the matrix with near-atomic resolution through advanced data processing. This information can be correlated with the compositional roughness of the interface observed in the atom probe data. The level of chemo-structural details from both techniques allowed to directly bridge to density functional theory calculations in order to understand how elastic strain fields impact the local concentrations of alloying elements at the atomic scale [3].

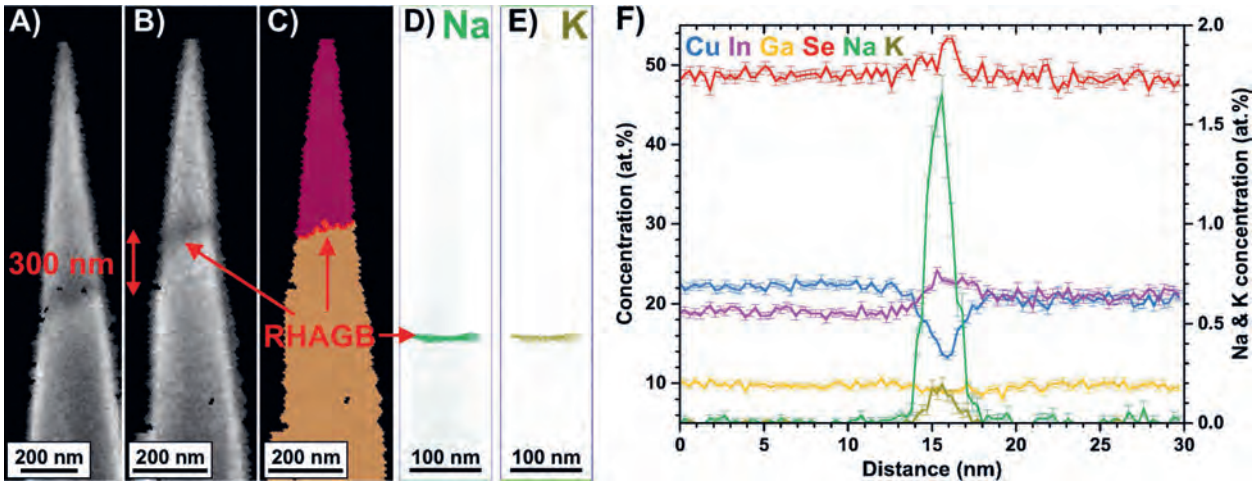


**Fig. 1:** *(A,B) Image quality maps from a transmission Kikuchi diffraction measurement taken directly on an atom probe tomography specimen. The dark contrast corresponds to a random high angle grain boundary (C) with a disorientation angle of 37.8°around the [201] axis. (D,E) Reconstructed atom probe data showing the Na and K distributions. (F) composition profile across the grain boundary reveals clear segregation [1].*

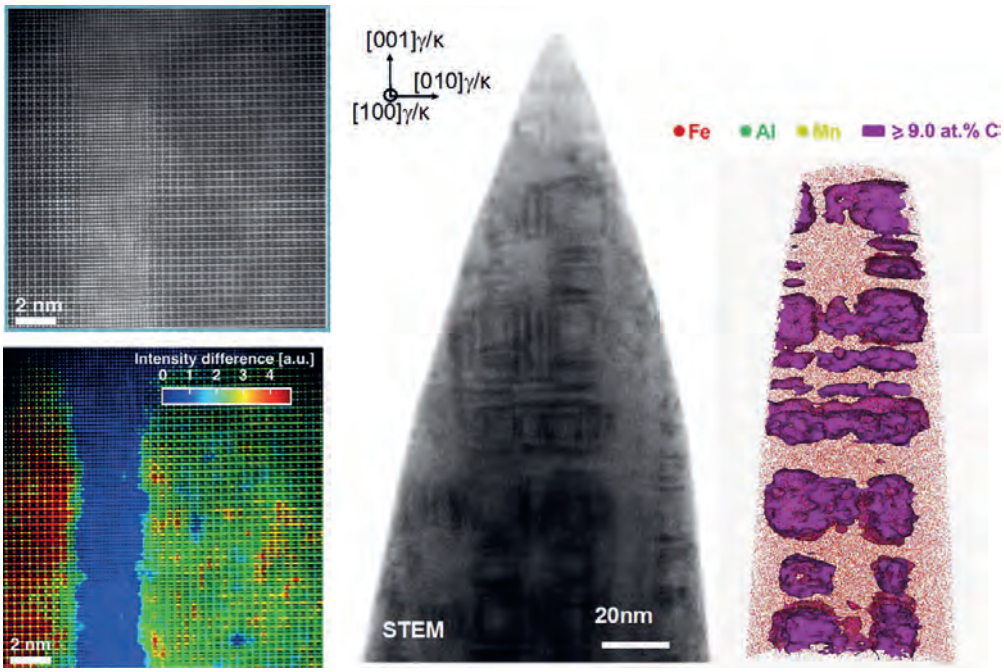


**Fig. 2:** *a) The close-up images are a high-angle-annular dark field (HAADF) image showing individual atomic columns that differ between the ordered precipitates (κ) and the matrix, as well as the corresponding atomic resolution strain $\varepsilon_{xx}$ map. b) Annular bight field (ABF) STEM image of a needle-shaped specimen showing cuboidal κ-carbides in an austenitic matrix. The corresponding reconstructed atom probe data is shown to scale and highlights the C distribution. c) The ab initio calculations explain how strain and the solubility of C in the matrix are connected [3].*

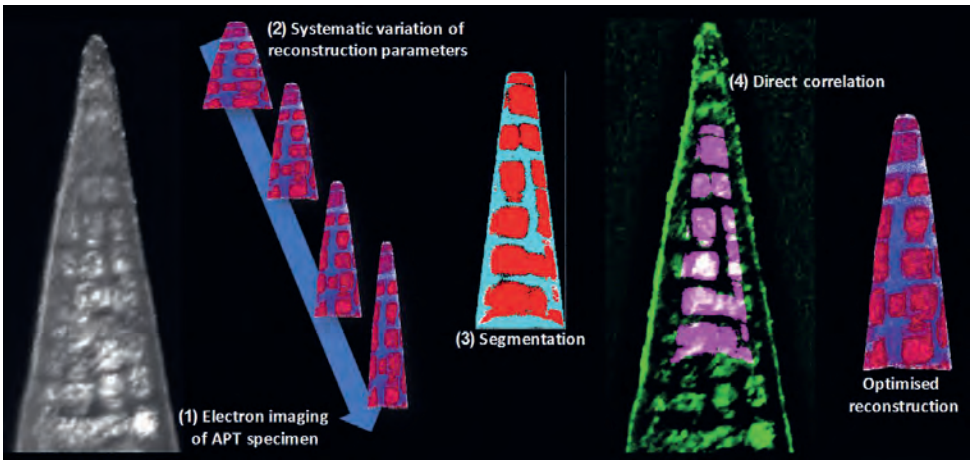


**Fig. 3:** *Step by step workflow for improving the fidelity of atom probe tomography reconstructions via digital image correlation with a transmission electron micrograph of the specimen acquired prior to the analysis [3].*

Finally, although significant effort was dedicated to developing protocols for correlative electron microscopy, atom probe tomography [4] as well as density functional theory (see p. 191), little has been done to truly combine the two streams of data and inform one technique with the results from the other. Here, we developed an approach that involved cross-correlation of a simulated electron image corresponding to the atom probe data with the electron micrograph of the specimen acquired prior to analysis. By systematically exploring the parameter space for reconstructing atom probe data and the possible rotations of the dataset with respect to the specimen, the results of the correlation is an optimised reconstruction of the atom probe data [5], as outlined in Fig.3.

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# Towards High Stiffness and Damage Tolerance: $Mo_2BC$ as a Model Material

*S. Gleich [1], R. Soler [2], J.-O. Achenbach [3], C. Kirchlechner [2], G. Dehm [2], C. Scheu [1], J.M. Schneider [3,4]*

[1] Independent Max Planck Research Group on Nanoanalytics and Interfaces (NG)
[2] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[3] Max Planck Fellow Group on Self-Reporting Materials
[4] RWTH Aachen University

High stiffness commonly comes at the expenses of a poor damage tolerance, as high strength and high fracture toughness have been traditionally found to be self-excluding. However, some materials have the promise to combine these properties. $Mo_2BC$ was predicted by *ab initio* calculations to exhibit both, an exceptional stiffness with a high Young's modulus of up to 470 GPa and a bulk modulus to shear modulus ratio indicating the possibility for moderate ductility [1]. Thus, from the calculated electronic structure point of view $Mo_2BC$ has the potential to combine the traditionally conflicting properties of high stiffness and damage tolerance. To explore whether this unusual combination can be confirmed by experiments, magnetron sputtering at different substrate temperatures was used to synthesize $Mo_2BC$ films for further studies by mechanical testing and microstructure characterization. First nanoindentation tests confirmed the predicted high Young's modulus and revealed plasticity by a visible material pile-up at the edge of the indent [1]. Additionally, $Mo_2BC$ coatings on ductile substrates exposed to tensile stresses were found to be significantly less prone to cracking than bench-mark TiAlN coatings [2]. Since the first screening experiments were successfully indicating damage tolerance, high stiffness and hardness, we decided to analyze the structure - property relationships in more detail.

**Nanostructure, hardness and Young's modulus:** The evolution of the nanostructure of $Mo_2BC$ coatings was studied as a function of the growth temperature and linked to the corresponding mechanical properties [3,4]. X-ray diffraction studies and advanced transmission electron microscopy investigations revealed a strong substrate temperature influence on the crystallinity of the bipolar pulsed direct current magnetron sputtered $Mo_2BC$ films. The coatings deposited at substrate temperatures between 380 °C to 630 °C range from partially amorphous for the coatings deposited at 380 °C to fully crystalline for the ones deposited at 630 °C (Fig. 1) [3]. This change in microstructure is also reflected in the mechanical response. The hardness and Young's modulus increased with increasing deposition temperature from 21 GPa to 28 GPa and 259 GPa to 462 GPa, respectively. We attributed this increase to the change in the nano- and microstructure and the corresponding changes in the average bond strength and stiffness [3]. Advanced scanning transmission electron microscopy studies in conjunction with atom probe tomography revealed a large number of defects within all deposited films. For example, Ar-rich Mo-B-C disordered clusters with a diameter of about 1.5 nm were observed in the films which are related to the magnetron sputtering process [3]. Besides these disordered clusters, the fully crystalline films deposited at 630 °C possess structural features at various length scales [3,4]. There are bundles of co-

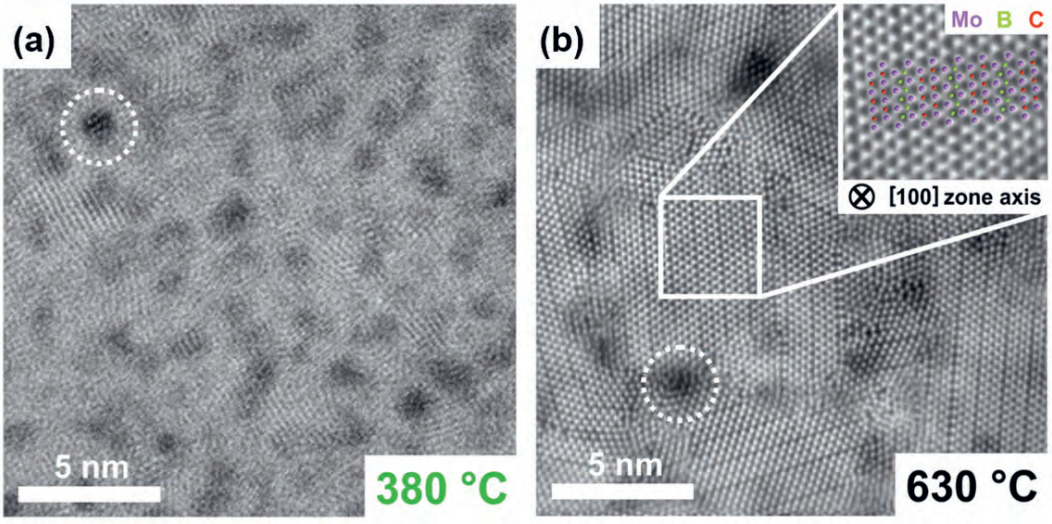


**Fig. 1:** *Plan-view scanning transmission electron microscopy images of the $Mo_2BC$ films deposited (a) at 380 °C and (b) 630 °C. Exemplary, Ar-rich Mo-B-C disordered clusters are marked by dotted circles. The enlarged region of the grain interior in (b) shows the stacking sequence in [100] orientation. The figures are taken from [3].*

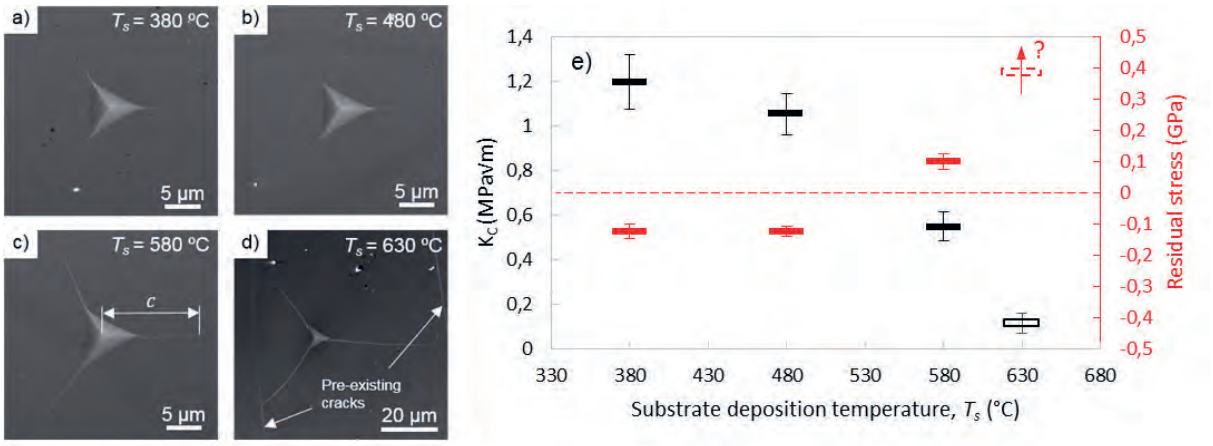


**Fig. 2:** *Nanoindentation induced cracks in $Mo_2BC$ coatings deposited on Si substrates at a) 380 °C, b) 480 °C, c) 580 °C and d) 630 °C. The film stresses and apparent fracture toughness of the $Mo_2BC$ films attached to the substrate are clearly related [6].*

lumnar grains (~10 nm in diameter) with dimensions of up to several micrometers in growth direction [4]. The atoms at the grain boundaries are less ordered compared to the grain interior, where stacking faults are present [4]. The thermal stability of the films was investigated by *ex situ* and *in situ* X-ray diffraction and transmission electron microscopy [5]. The partially amorphous film deposited at 380 °C transformed to fully crystalline during annealing resulting in grain sizes up to 1 µm at elevated temperatures. Up to 840 °C the interface to the Si substrate remained intact without delamination [5].

**Fracture toughness studies of $Mo_2BC$:** In order to obtain information on the fracture toughness, two different approaches were selected [6]. Indentation induced crack initiation was chosen to obtain the fracture toughness of the films attached to the substrate while notched cantilevers were used to obtain the fracture toughness of the films itself. The films grown at substrate temperatures of 380 and 480°C exhibit compressive stresses after cooling to room temperature, whereas the film grown at 580 °C shows tensile stresses after cooling [6]. The tensile stresses of the 630 °C deposited film are even larger, causing cracks when cooling down to room temperature, thus only a lower bound of the tensile film stress can be measured by wafer curvature with 0.4 GPa. Interestingly, indentation induced fracture leads to a lower apparent fracture toughness for the films grown at 630 °C compared to the lower deposition temperatures (Fig. 2). In contrast, notched cantilevers reveal the opposite trend, the higher the deposition temperature and crystallinity, the tougher the $Mo_2BC$ coating with a maximum average fracture toughness of 4.7±0.52MPa√m for the fully crystalline film deposited at 630 °C. The linear elastic slope during loading of the notched beams does not indicate plasticity. This is also supported by fractography revealing brittle fracture. However, fractography indicates intergranular fracture along the columnar grain boundaries of the grains with their nanometer sized column diameters [6]. Future experiments on large grained $Mo_2BC$ are required to resolve the fracture toughness of the bulk and to analyze dislocation plasticity.

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# Synthesis and High-Throughput Methods for High-Entropy Alloys

*Z. Li [1], H. Springer [1], D. Raabe [1], F. Körmann [2], C. Kirchlechner [3], C. Liebscher [3], W. Lu [3], G. Dehm [3], A. Ludwig [4]*

[1] Department of Microstructure Physics and Alloy Design (MA)
[2] Department of Computational Materials Design (CM)
[3] Department of Structure and Nano-/ Micromechanics of Materials (SN)
[4] Institute for Materials, Ruhr-Universität Bochum

High-entropy alloys (HEAs) are multi-component metallic materials consisting of four or more elements in high or even equimolar fractions [1-3]. The number of compositions explored is increasing rapidly due to the growing research efforts in this field driven by some promising mechanical HEA properties such as high fracture toughness at cryogenic temperatures. The main challenge that HEA research is facing is how to efficiently explore their huge compositional and microstructural spaces for novel materials with promising property profiles. Therefore, we have been working on different approaches for the combinatorial and high-throughput synthesis and processing of HEAs [3].

The first approach we employed is rapid alloy prototyping (RAP) which is a semi-continuous high-throughput bulk casting, rolling, heat treatment and sample preparation method developed at the MPIE, and has been successfully applied to screening weight-reduced TWIP-type steels, high strength martensitic steels and HEAs [3,4]. The RAP approach enables casting of five different alloys with tuned compositions of an alloy system in one operation. This is achieved by using a set of five copper moulds which can be moved stepwise inside the furnace. Following casting, the alloy blocks with a thickness of 10 mm and varying compositions are subsequently hot-rolled in air. This step is required for removing dendrites and casting porosity. After the final hot-rolling pass, the HEA plates are homogenized at high temperatures (e.g., 1200 °C) for several hours (e.g., 2 h) under Ar atmosphere, followed by water quenching. Since the homogenized HEA plates generally exhibit a large grain size, cold-rolling and annealing are required for refining the microstructure towards better mechanical properties. Thickness reduction by cold-rolling is generally higher than 50% to obtain a sufficiently high driving force for primary recrystallization. After these microstructure-tuning processing steps, samples for microstructure investigation and performance testing are machined from the alloy segments by spark erosion. Various characterization methods are then used for probing composition-microstructure-property relationships (Fig. 1).

The second high-throughput method for multi-component HEAs is utilizing diffusion multiples which can serve for alloy synthesis through systematic intermixing among blocks of pre-alloyed composition [3]. This allows three or more metal blocks to be placed in diffusional contact. Generally, such diffusion-multiple setups are subjected to a high temperature to induce thermal inter-diffusion to form continuously compositionally graded solid solutions and/or intermetallic compounds. In a diffusion-multiple assembly, the contacted surfaces of different metal blocks are required to be polished and cleaned without contamination. The aggregates are then treated in a hot isostatic pressing (HIP) process at high temperature (e.g., 1200 °C) for several hours to achieve intimate interfacial contacts of all constituent blocks. Subsequently, the diffusion multiple is heat-treated at a high tem-

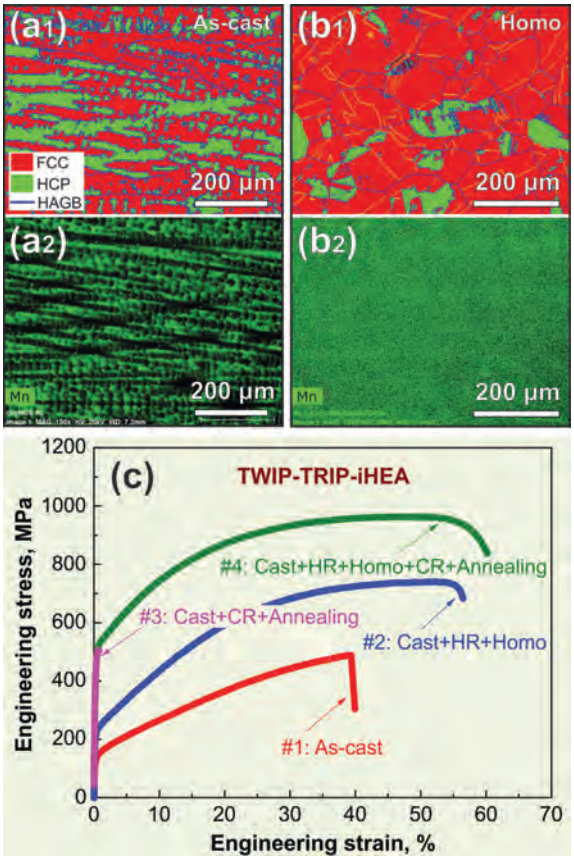


**Fig. 1:** *Microstructure, compositional homogeneity state (a,b) and tensile properties (c) of an interstitial high-entropy alloy ($Fe_{49.5}Mn_{30}Co_{10}Cr_{10}C_{0.5}$, at. %) in different processing conditions obtained after specific steps of rapid alloy prototyping [3]. FCC, HCP and HAGB refer to face-centred cubic phase, hexagonal close-packed phase and high-angle grain boundaries, respectively. "HR", "Homo" and "CR" refer to hot-rolling, homogenization and cold-rolling, respectively.*

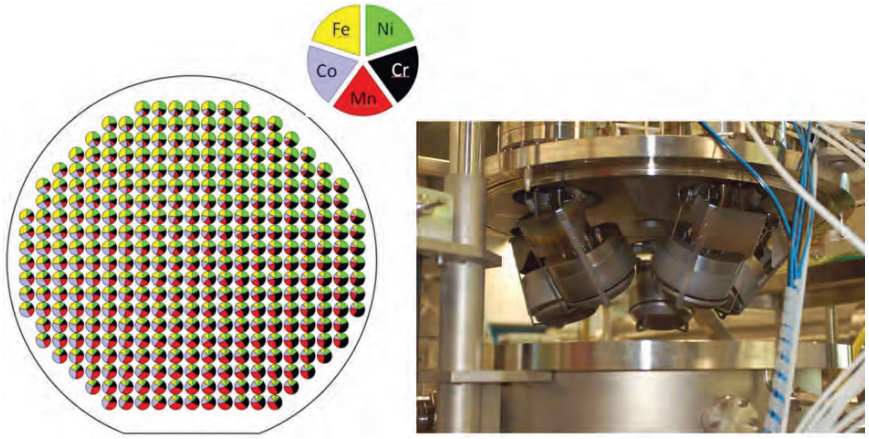


**Fig. 2:** *Field with varying quinary HEA compositions contained in a thin-film library of Cr-Mn-Fe-Co-Ni co-sputtered from individual single-element targets, indicating the relative concentrations at each of 342 EDS measurement points (EDS: energy dispersive X-ray spectroscopy). The legend identifies the elements and respective cathode positions in an opened co-sputter chamber [3].*

perature (e.g., 1200 °C) for a long period (generally above 24 h). The total time of heat-treatment at high-temperature is determined for achieving diffusion profiles with sufficiently large extension, so that the solid-solution phases and/or intermetallic compounds formed in the diffusion-multiple are large enough to be subsequently characterized without interference from neighbouring phases [3].

The third approach for the high-throughput synthesis of HEAs is combinatorial laser additive manufacturing (LAM) enabling synthesis of compositionally graded materials which allows many variants to be probed efficiently for instance by using established micromechanical testing methods [3]. The compositionally gradient part can be designed to include large compositional steps, and it can also proceed with a smoothly graded transition from one composition to another. Also, metal-matrix-composites, e.g., nano-particle reinforced HEA-based materials, with a compositionally graded matrix can be fabricated by LAM. This can be realized when one of the powders being transferred into the laser has a significantly higher melting temperature than the others, thereby avoiding that particles pre-alloy with powders of lower melting point [3].

The fourth high-throughput technique used for probing the large HEA space is pursued together with A. Ludwig at the Ruhr-Universität Bochum. His group synthesizes multinary thin-film materials libraries, i.e. well-defined and large thin-film composition gradients across a substrate wafer fabricated in a single experiment. Co-deposition from cathodes that are tilted with respect to the substrate plane results in wedge-shaped nanoscale thin films that are thickest from the geometrically closest edge of the substrate to thinnest at the farthest edge. Multiple cathodes evenly distributed around the centre of a substrate (3 cathodes: 120° separation, 4 cathodes: 90° separation, 5 cathodes: 72° separation) each produce such a wedge, with the resulting composition at any point on the substrate being the sum of the material arriving from each cathode (Fig. 2). Co-sputtered films are atom-scale mixtures of the materials that are often subsequently annealed to form thermodynamically stable phases and reduce defects.

To promote the efficient high-throughput development of HEAs, theoretical guidance is critically important, capable of suggesting suited mechanical or magnetic trends for the design of alloy compositions [5]. For instance, to design strong, tough and ductile HEAs, we found that phase (meta)stability of HEAs is an important feature which can be well tuned in terms of composition adjustment to introduce activation of athermal deformation mechanisms (TWIP/TRIP), thereby improving the range of accessible strength-ductility combinations [2,5]. Accordingly, parameter-free *ab initio* simulations and thermodynamic calculations are used to provide guidance for adjusting stacking fault energies and/or free energy differences between phases to assist the high-throughput HEA development [5].

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# A Rare-Earth Free Magnesium Alloy with Improved Intrinsic Ductility

*S. Sandlöbes [1,4], M. Friák [2,3], S. Korte-Kerzel [1], Z. Pei [3,5], J. Neugebauer [3], D. Raabe [4]*

[1] now at: Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Germany
[2] now at: Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Czech Republic
[3] Department of Computational Materials Design (CM)
[4] Department of Microstructure Physics and Alloy Design (MA)
[5] now at: Oak Ridge National Laboratory, Tennessee, USA

Magnesium and its alloys have a hexagonal crystal structure. Their wider application is hindered by their poor ductility. The lack of room temperature formability is caused by deformation being confined to $\{0001\}\langle 11\bar{2}0\rangle$ basal <a> dislocation slip which does not allow accommodation of strain along the crystal c-axis (Fig. 1).

Strain along the crystal c-axis can only be accommodated by the activation of non-basal slip in hexagonal crystals, i.e. it is crucial for compatible polycrystalline deformation of Mg [1]. Alloying with yttrium and rare earth (RE) elements has been shown to improve the room temperature ductility [1-3]. Recent studies revealed that such ductility increase in Mg-Y and Mg-RE alloys is caused by <c+a> dislocation slip providing out-of-basal-plane shear [1-3].

The activation of out-of-basal-plane shear through Y or RE elements in Mg is correlated with a decreased $I_1$ intrinsic stacking fault energy ($I_1$ SFE). The $I_1$ SFE decreases with increasing Y and RE concentration. This is used here as a parameter connected with the ductility increase in the Mg-Y and Mg-RE systems. We conducted *ab initio* assessments of the thermodynamic, energetic (elastic energy) and structural-volumetric interactions of yttrium and RE atoms in Mg in solid solution and their effects on the $I_1$ SFE to understand the origin of slip system selection. We developed a quantum mechanically guided treasure map for Mg alloying [4,5]. The idea is to start from a Mg-Y alloy that is ductile, yet, is commercially not attractive, and search for alloy compositions matching the reference system as closely as possible for selected element-specific properties. This proximity between two alloys is expressed by a similarity index $Y_c=1-\{\sum_\alpha w_\alpha(\alpha - \alpha_c)^2\}^{1/2}$ where the subscript c describes the chemical composition of the new alloy, α describes a selected set of element-specific properties and $w_\alpha$ are the weighting factors. This proximity factor $Y_c$ is referred to as yttrium-similarity index, YSI.

To determine a set of elemental properties and weighting factors we used density-functional theory to compute reference quantities for a set of solid-solution binary $Mg_{1-x}X_x$ alloys (x<<1) [4,5]. We identified three correlations: the atomic volume of pure solutes, their electronegativity and their bulk modulus. From the correlation coefficients we obtained the weight, $w_\alpha$. We screened 2850 ternary combinations (Fig. 2a) and identified 17 ternary alloys highlighted in Fig. 2b with YSI values ≥ 0.95. Fig. 2a shows a symmetric matrix of all 2850 solute pairs computed, where the respective solutes are given on the x- and y-axes. The intersection points of each solute pair of the y- and x-axis are marked by a coloured

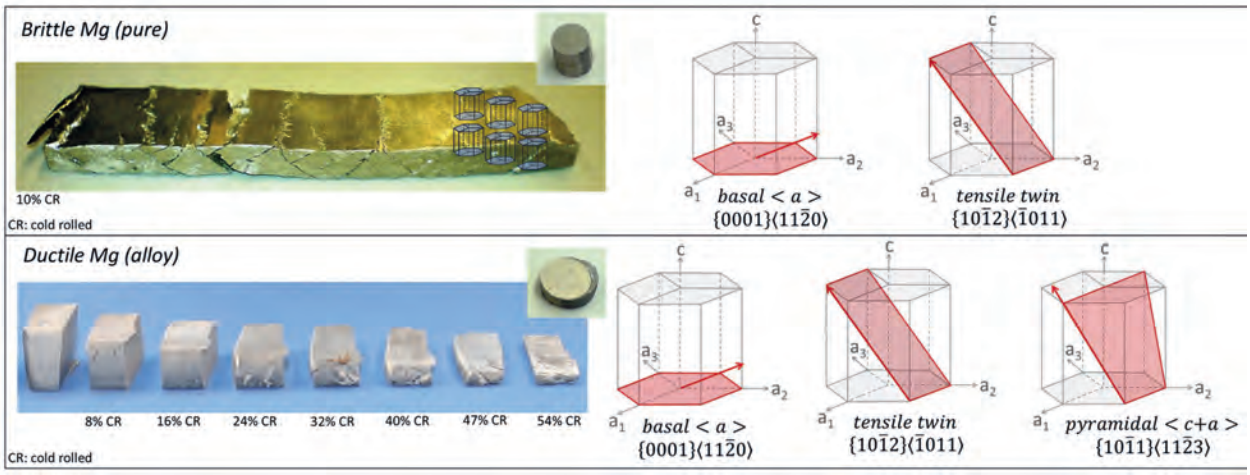


**Fig. 1:** *Pure polycrystalline magnesium fails brittle already at low strains (top row). The new Mg-1Al-0.1Ca alloy can be cold rolled to 54% thickness reduction (bottom row) [5].*

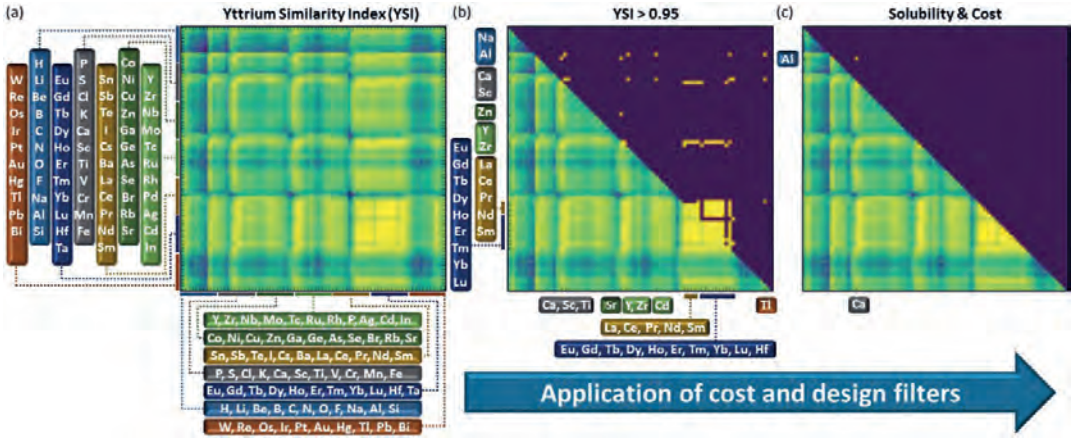


**Fig. 2:** *Yttrium-similarity index, YSI for the 2850 solute pairs computed in this study and visualized in the form of a symmetric matrix (a) with yellow indicating a high similarity and blue a low one. Solute pairs that have a high index (YSI>0.95) are shown in the upper triangular part in (b). Applying a cost and solubility filter only a single pair, Al-Ca, remains (c) [5].*

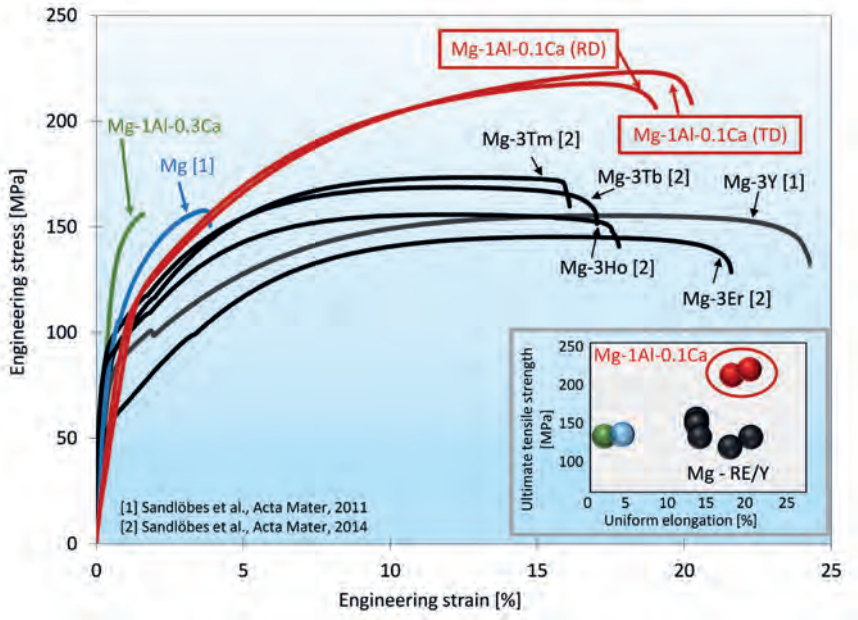


**Fig. 3:** *Engineering stress-strain curves of the new Mg-Al-Ca alloy shown in Fig. 1 in comparison with solid solution Mg-Y, Mg-RE, pure Mg and Mg-Al-0.3Ca [5]. The inset shows the ultimate tensile strength – uniform elongation diagram of the same alloys. RD: rolling direction; TD: transverse direction. Compositions in weight %.*

point indicating the similarity of that pair to Y. Yellow colour corresponds to a high similarity to Y (high YSI) and blue to a low YSI. In the upper triangle of Fig. 2b only those solute pairs with an YSI above 0.95 (i.e. 95% or higher similarity to Y) are shown. The solutes are listed at the x- and y-axis in Fig. 2b. From this list 11 alloys are RE/Y-free. We applied a second filter ruling out element pairs which are incompatible with recycling constraints, toxic, not sufficiently soluble in Mg or too expensive so that only one alloy system remains, viz. Mg-Al-Ca [4-6]. With this result we synthesized a new material, namely, Mg-1Al-0.1Ca (wt.%). Fig. 3 shows the tensile stress-strain behaviour of the new alloy in comparison with pure Mg and binary solid solution Mg-RE and Mg-Y alloys revealing superior mechanical properties.

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# Advanced Lightweight Steels

*D. Ponge [2], T. Hickel [1], M. Herbig [2], B. Gault [2], S. Zaefferer [2], P. Shanthraj [2], F. Roters [2], C. Scheu [3], J. Neugebauer [1], D. Raabe [2]*

[1] Department of Computational Materials Design (CM)
[2] Department of Microstructure Physics and Alloy Design (MA)
[3] Independent Max Planck Research Group on Nanoanalytics and Interfaces (NG)

High-Mn lightweight steels offer a very good combination of high strength, ductility and toughness together with a reduced mass density due to their high Al content. For clarifying the mechanisms responsible for the outstanding mechanical properties, we collaborated on this topic among several departments at the MPIE. The aim was to understand especially the origin of the high strain hardening rate in the as quenched state (devoid of κ-carbides) [1] and in the precipitation hardened state (containing L'$1_2$-type κ-carbides) and the mechanisms of precipitation hardening [2]. For this purpose, the microstructure evolution of a high-Mn lightweight steel (Fe-30.4Mn-8Al-1.2C, wt.%) was studied after interrupted tensile testing by electron channeling contrast imaging (ECCI), transmission electron microscopy (TEM), atom probe tomography (APT) and correlative TEM/APT. To quantify the precipitation strengthening, the anti-phase boundary (APB) energy of the $(Fe,Mn)_3AlC$ κ-carbides was determined by *ab initio* calculations. The seemingly inconsistent outcomes of theory and experiment led to new insights into the mechanisms of precipitation strengthening in these steels.

**Strain hardening:** Interestingly, the material deforms in both conditions (as quenched or precipitation hardened) by planar slip, indicating a low cross slip frequency. This results in a low rate of dynamic recovery and, therefore, a high apparent strain hardening rate. Here, we observe a gradual reduction of the spacing between the co-planar slip bands with increasing strain, which leads to constantly high strain hardening (Fig. 1). To further confirm this mechanism, the flow stress was calculated from the coplanar slip band spacing on the basis of the dislocation passing stresses. The good agreement between the calculated values and the tensile test data confirms that dynamic slip band refinement is the main strain hardening mechanism.

Precipitation hardening is increasing the yield stress, but the strain hardening behaviour is nearly the same like in the κ free condition (Fig. 1). Again planar slip and dynamic slip band refinement were identified as governing deformation mechanisms. The resulting strain hardening rate is high enough to compensate the negative strain hardening rate caused by shearing and fragmenting the *κ*-carbide precipitates. The latter is connected with dislocation penetration and the dragging out of carbon and other elements by these dislocations, which leads

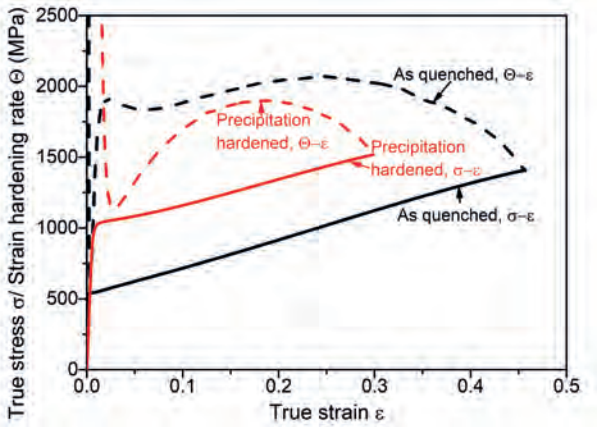


**Fig. 1:** *True stress-strain curve of the alloy in precipitation hardened state (red solid line) in comparison to that of the alloy in the as quenched state (black solid line). The strain hardening curves Θ–ε of both states are shown as dashed lines.*

to a reduction of the APB energy in the κ-carbides as detailed below. Especially at higher strains, the shearing and fragmentation of the *κ*-carbides leads to a reduction of the apparent strain hardening rate in comparison to the as quenched state.

**Precipitation hardening**: A heat treatment at 600°C for 24 h resulted in the formation of *κ*-carbide precipitates and an increase in the proof stress. In order to better interpret the resulting hardening, the particle size, shape and inter-spacing needs to be analysed. This is ambiguous with TEM alone, since it only provides a 2D projected image of the microstructure. Therefore, to achieve a better topological characterization of the precipitate morphology and arrangement, APT analysis was performed. Fig. 2 shows a representative κ/γ microstructure observed in the reconstructed 3D atom maps by APT.

Fig. 3 shows TEM micrographs of a deformed sample. The whole precipitation structure is shown to be sheared along a fine line, indicating the shearing of κ-carbide precipitates by dislocations on the same glide plane.

To quantify the precipitation strengthening effect, the APB energy of the L'$1_2$ –type $(Fe,Mn)_3AlC$ κ-carbides has been determined by *ab initio* calculations. The energies for the stoichiometric carbides turned out to be much too high to explain the observed shearing by dislocations. We realized that this is related to a reduced C content in the precipitates. Instead of a stoichiometric C content of 20 at.%, the actual C concentration of κ-carbide is in the order

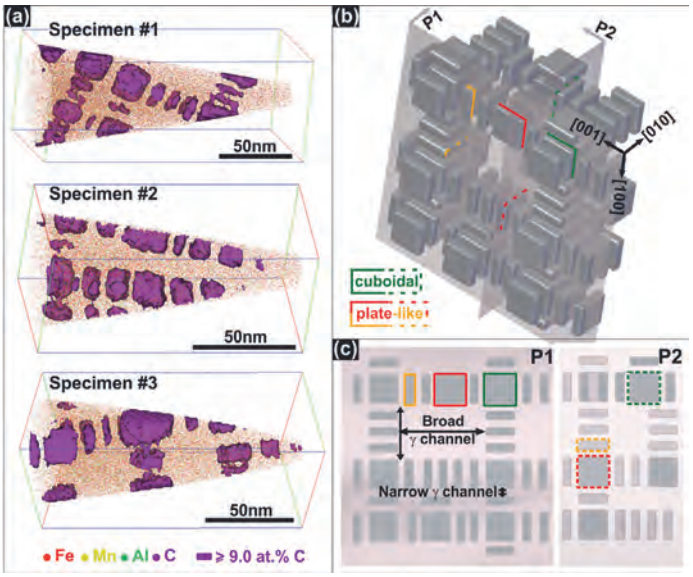


**Fig. 2:** *Morphology and arrangement of κ-carbide precipitates by APT (3D) and 2D sketches: (a) three representative reconstructed 3D APT maps of Fe (red), Mn (yellow), Al (green) and C (purple) atoms. The κ-carbide precipitates are visualized with 9 at.% C iso-concentration surfaces. (b) Schematic illustration of 3D morphology and arrangement of κ-carbide precipitates based on APT observations. (c) 2D projections of the κ/γ microstructure along <001> directions highlighted in (b), reflecting the TEM observations [2].*

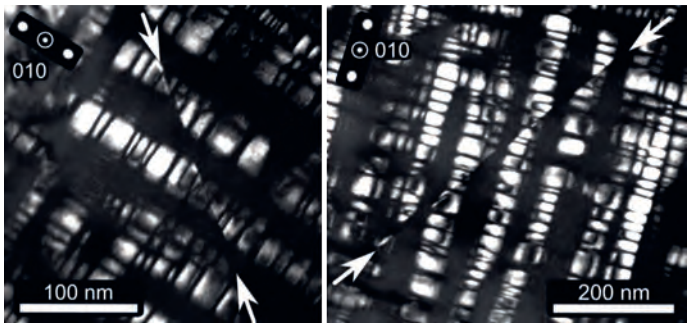


**Fig. 3:** *DF-TEM images showing sheared κ-carbides at a strain of 0.02 (with g=(010) superlattice reflection used for DF imaging and viewing direction close to the [110] zone axis) [2].*

of 13 at.% [3]. Therefore, two extreme cases were studied, namely, a full occupancy of the body-centred interstitial sites by C and a C-free $L1_2$ $Fe_3Al$ structure. The resulting $\gamma_{APB}$ value of κ-carbide in the current alloy is expected to lie in the range of ~350-700 mJ/m$^2$. The measured particle radius of around 10 nm indicates that for the given volume fraction of around 0.2, the strengthening is then in the range of 900-1800 MPa. However, experimentally, the κ-carbides introduced upon ageing were found to increase the yield strength only by ~500 MPa.

This discrepancy can be explained by the influence of dislocation pile-up stresses at the κ-carbide interfaces that assist particle shearing. The pile-up of dislocations in the grain interior has been observed in the as quenched state with short range ordering [1]. This is difficult to be captured by ECCI or TEM here in the precipitation hardened state due to the high number density of precipitates. Calculations [2] indicate that a pile-up size of 4-8 dislocations is required to reduce the macroscopic strengthening effect to ~500 MPa, which, based on previous experimental observations [1], is a reasonable assumption. An additional reason for the lower experimental yield strength increase by κ-carbide precipitation compared to the calculated value is the reduced concentration of alloying elements in the matrix due to κ-carbide formation. This leads to a reduced solid solution strengthening of the matrix and a reduced tendency for short range ordering [1]. Both mechanisms reduce the effective strengthening contributed by precipitation hardening.

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# Deploying Machine Learning to Extract Meaningful Materials Science Information from Advanced Microscopy

*S. Zhang [1], Y. Wei [2], A.J. Breen [2], M. Herbig [2], B. Gault [2], C. Scheu [1], C. Freysoldt [3], C. Liebscher [4]*

[1] Independent Max Planck Group on Nanoanalytics and Interfaces (NG)
[2] Department of Microstructure Physics and Alloy Design (MA)
[3] Department of Computational Materials Design (CM)
[4] Department of Structure and Nano-/ Micromechanics of Materials (SN)

Advanced microscopy and spectroscopy offer unique opportunities to study the structure, composition, and bonding state of individual atoms from within complex, engineering materials. Such information can be collected at a spatial resolution of as small as 0.1 nm with the help of aberration correction. With advancements in electron source brightness and detection efficiency, acquiring spatial maps in 2D and even 3D has become a routine practice, generating ever bigger datasets to handle.

Researchers at the MPIE now routinely make use of tools from the big data community [1,2]. As an example, nonnegative matrix factorization (NMF) algorithms are applied to electron energy loss spectroscopy (EELS) datasets. Fig.1 shows a sparse representation of an EELS spectrum imaging, using three spectral components and their spatial contribution maps to approximate spectra from 500 pixels. The differences in spectral features and their spatial origins are presented without the need to inspect 500 individual spectra. For example, the Ti-$L_3$ edge of component 3 has a peak position shifted to the left compared to the other components, corresponding to a reduced oxidation state of Ti. The spatial maps of component 3 reveals such reduced species come from the interface between the $TiO_2$ nanoparticle and the AlOOH matrix [3].

Dimension reduction of big data benefits researchers not only in presenting the data. Also, the subsequent data handling becomes less exhaustive and the quantification less biased [2].

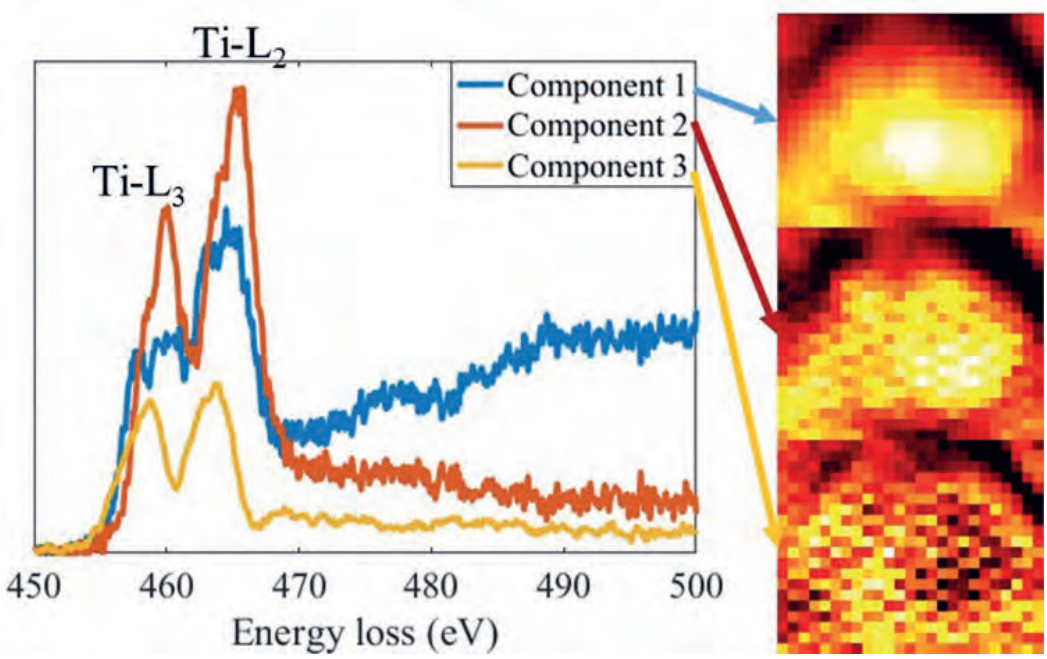


**Fig. 1:** *Three major spectral components of 500 electron energy loss spectra of Ti-$L_3$ and -$L_2$ edges, and their spatial contribution maps. The pixel size is 2 × 2 nm² [3].*

A second example came from the analysis of the field desorption patterns obtained from atom probe tomography (APT). APT maps the 3D position and chemical identity of up to a billion atoms in a material. The pattern formed on the single-particle detector often reveals traces of the crystallographic structure and orientation of the specimen. However, it remains largely under-utilised due to the lack of efficient and accurate extraction techniques. We have proposed a mixture of feature detection, machine learning and deep learning to enable automatic identification of crystallographic patterns observed on atom probe detector maps. Preliminary results exploiting theoretical geometric relationships have been very promising. A

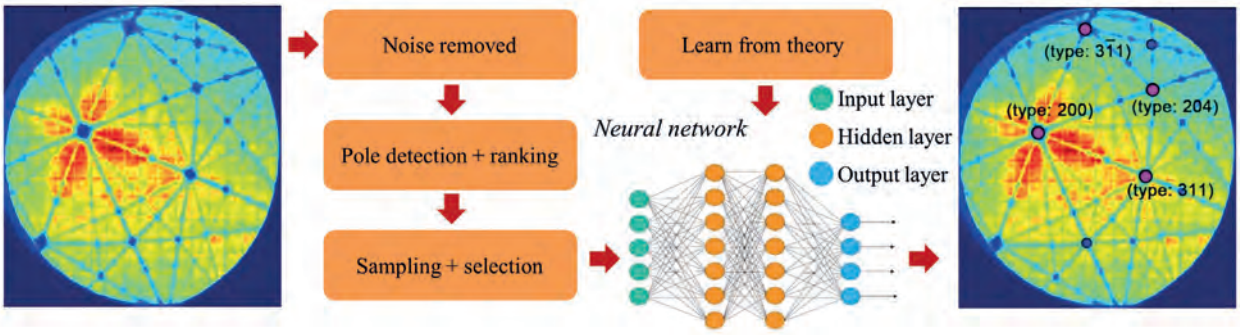


**Fig. 2:** *Complete workflow of automated identification of grain orientation via a deep neural network.*

flow-chart outlining this process is shown in Fig. 2. For detector hit-maps obtained from pure-Al specimens, our approach correctly characterised the orientation of single crystals with 98% confidence.

A database of experimental images for training was built, but for more complex materials systems and low-symmetry crystallographic structures there is not enough labelled data yet. This offers unique opportunities to bridge with the CM department. By full-scale, theory-driven forward calculations of such maps we can build large databases from which the machine learning algorithms will learn and refine the data analysis, as well as systematically explore the ultimate limits of APT crystallography in multi-phase multi-component samples.

Further forays into deploying big-data methodologies to advanced microscopies will be a future focus at the MPIE, as a collaborative project was recently awarded funding within the BigMax network (see p. 53) to pursue approaches to better evaluate large spectral dataset from scanning transmission electron microscopy (STEM) and extract atomic-scale compositional and structural information. In particular, we develop an automatic classification of high-resolution STEM image-series into distinct spatial regions according to the actual microstructure of the sample in order to detect, e.g., intra-grain variations or inter-grain differences even in very noisy data. Any advances in the analysis will be directly used to push the experimental measurement conditions to their limits.

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# *Ab initio*-Derived Semiconductor Surface and Interface Phase Diagrams

*L. Lymperakis [1], C. Freysoldt [1], S. Wippermann [2], J. Neugebauer [1]*

[1] *Department of Computational Materials Design (CM)*
[2] *Department of Interface Chemistry and Surface Engineering (GO)*

III-V semiconductors have shaped optoelectronic technology for decades, and progressively enter power electronics, solar cells, and quantum technology. The bulk materials and nanostructures for actual devices are produced by controlled growth, be it in gas phase epitaxy, wet chemistry, or colloidal synthesis. Surfaces and interfaces therefore play a dominant role in determining the materials' properties. Surface effects may alter the chemical composition and provide routes to surface engineer growth in order to obtain materials with targeted properties. An alternative path to achieve tailored materials is the controlled wet-chemical assembly of dissimilar components into nanostructured materials. Both approaches depend critically on the ability to understand and control the physics and chemistry at the surfaces and at the interfaces. Here, we investigate these and highlight recent insights obtained by *ab initio* modelling into growth processes of semiconductor alloys and nanostructures.

Today's power light emitting diodes (LEDs) employ $In_xGa_{1-x}N$ alloys as active zone for light generation. While the $In_xGa_{1-x}N$ system allows for continuously tuning the colour from UV (pure GaN) to infrared (pure InN) in principle, the lack of homogeneous alloys with more than 30% Indium content forces us to down-convert blue light from low-In concentration devices. Detailed investigations on the bulk thermodynamics of these alloys suggest a favourable ordered phase at the technologically relevant In content of 33%, but only at low temperatures [1]. However, recent experimental findings indicate that this order even occurs at temperatures as high as 950 K. In order to resolve this discrepancy we employed DFT calculations and investigated In incorporation in the GaN(0001) surfaces. For growth under N rich conditions the (0001) III-Nitride surfaces reconstruct in order to obey the electron counting rule. The latter results in a 2×2 N adatom reconstruction which leaves ¾ of the surface metal atoms four-fold coordinated in a $sp^3$ configuration and ¼ of them triply coordinated in a planar $sp^2$ configuration. Although, the stronger Ga-N bonds are expected to result in preferential incorporation of In at the low coordinated surface sites, our calculations reveal a novel reconstruction mechanism, elastically frustrated rehybridization (EFR), that contradicts this conventional picture: due to their large atomic radius, In atoms at the triply coordinated sites are hindered from re-hybridizing to the $sp^2$ configuration [2]. Instead, they preferentially incorporate to four-fold coordinated surface sites where rehybridization of the triply coordinated Ga is allowed.

The effect of the above mentioned EFR mechanism on the alloy compositional limits is significant. We have calculated the chemical potential of In at the surface as a function of the surface In content. As it is revealed in Fig. 1 the chemical potential remains essentially flat for low surface In contents where In is substituted only at sites obeying the EFR mechanism. However, increasing the In concentration from ¼ to

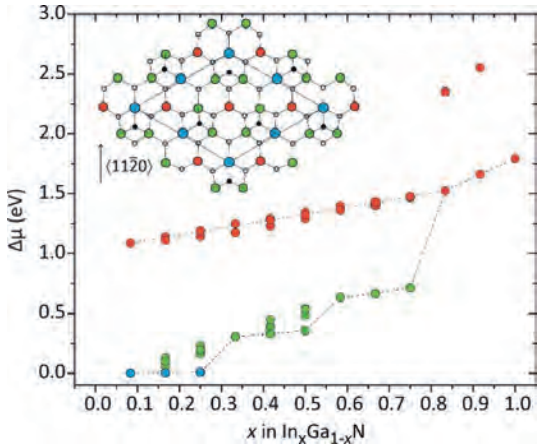


**Fig. 1:** *Chemical potential Δμ of In at the surface as a function of composition x. Green/blue and red dots correspond to the lowest- and higher-energy configuration/s for each x, respectively. The dashed lines are guidelines for the eye. (Inset) Top view of the lowest energy (2√3 x 2√3)R30° $In_{0.25}Ga_{0.75}N$ reconstruction. Small/black dots denote the N adatoms and small/open balls the N atoms. Blue balls indicate the In atoms and red and green balls the ×3 and ×4 coordinated inequivalent Ga atoms, respectively.*

⅓ increases the In chemical potential by ~ 0.3 eV, cf. Fig. 1. This corresponds to a ≈5-fold increase of the In-flux in molecular beam epitaxy growth (MBE). Such a huge increase in the In-flux would eventually switch the growth conditions to In-rich, resulting in the formation of In droplets and poor growth morphology. These trends in the computed chemical potential as function of the In content explain the observed experimental limitations in achieving higher In concentrations. Nevertheless, EFR may also provide efficient pathways to surface engineer growth and overcome the bulk solubility limits in other semiconductors alloys. Boron containing III-Nitride ternary alloys are a characteristic example: while the bulk solubility limit of B in GaN is restricted to less than 2%, B can be incorporated at the surface with contents as high as 25% forming an ordered 2×2 phase in the basal plane [3].

Surfaces and interfaces also govern the growth of semiconductor nanostructures. Nanocrystals (NCs)

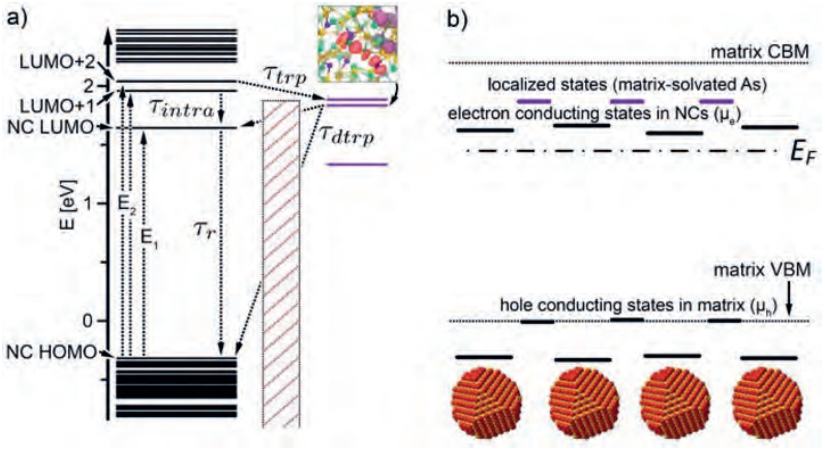


**Fig. 2:** *Model of ambipolar photoresponse of InAs NCs with $Sn_2S_6^{4-}$ ligands. Hot electrons promoted to the LUMO+1/+2 states can undergo intraband relaxation or get trapped by localized states that originate from matrix-solvated As, which are situated above the NC LUMO, but below the matrix conduction band edge. In the NC solid, the mobility edge for majority carriers (electrons) is associated with the NC LUMO states and the hole-conducting states are given by the matrix band edge. Copyright 2018 Nature Publishing Group.*

with controlled shape and composition can be used as "artificial atoms" to create semiconductors with superior properties, e.g., for emerging optoelectronic and photonic technologies [4]. As a prototypical example, InAs NCs are colloidally synthesized, capped with $Sn_2S_6^{4-}$ molecular metal chalcogenide complexes (MCCs), and subsequently assembled into quantum dot solids: Following solution casting and subsequent annealing, the NCs arrange in superlattice structures. After solution casting, gentle heat treatment decomposes the MCCs and results in a $SnS_2$ matrix encapsulating the InAs NCs. The resulting InAs/$SnS_2$ quantum dot solid exhibits promising transport properties, measured, e.g., by field-effect transconductance. The understanding of NC nucleation, growth, superlattice formation and assembly processes is still in its infancy, though. Often, this leads to unexpected results when process parameters are varied.

We systematically investigated the interaction of $Sn_2S_6^{4-}$ MCCs with InAs surfaces. Contrary to common assumptions drawn from studies using organic ligands, we found that the MCCs are not adsorbed as intact structural units, but rather they decompose upon contact with the NC surface, and form a passivation layer surrounding the NCs. The adsorption of intact $Sn_2S_6^{4-}$ MCCs on the passivated NP surfaces becomes then possible. However, $Sn_2S_6^{4-}$ is unstable towards dissociation into tetrahedral $SnS_4$ units, and the most stable structural units identified consist of passivated NCs embedded in amorphous $SnS_x$ matrices. As an additional effect, sulphur displaces As and is incorporated into the NC subsurface layer. These theoretical predictions were later confirmed by angle-resolved X-ray photoelectron and Raman spectroscopy.

In order to model the temperature-induced decomposition of $Sn_2S_6^{4-}$ ligands adsorbed on the NC surfaces and the formation of amorphous matrices, we performed *ab initio* MD simulations where structural motifs, validated by experiments, were explicitly included as starting points of annealing cycles. We systematically explored variations in the density and stoichiometry of the amorphous matrix, generating a series of structural models of NC solids corresponding to different colloidal synthesis conditions. A number of defect states were identified that are expected to play a key role in determining the electronic and transport properties of the NC solids. We could trace the origin of the measured negative photoconductivity to the presence of As dopants: as a consequence of subsurface sulphur incorporation, As atoms diffuse into the matrix. They preferentially occupy Sn lattice sites and create localized donor states above the NC mobility edge, but below the matrix conduction band edge, cf. Fig. 2. These donor states act as traps and are responsible for the measured negative photoconductivity. By adjusting the colloidal synthesis conditions, we show how to suppress the formation of these trap states [5].

These two examples illustrate how addressing fundamental questions in semiconductor surface growth by computer simulations not only helps to rationalize experimental observations, but also to guide the design of alternative processing routes to overcome present-day compositional and defect-related limitations.

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# Solute Segregation at Grain Boundaries in Al Based on New Concepts in Machine Learning and Experiment

*L. Huber [1], H. Zhao [2], R. Hadian [1], B. Gault [2], D. Ponge [2], B. Grabowski [1], J. Neugebauer [1], D. Raabe [2]*

[1] Department of Computational Materials Design (CM)
[2] Department of Microstructure Physics and Alloy Design (MA)

Even very low concentrations of alloying elements can have a significant impact on the nominal material properties in a metallic alloy. One of the main mechanisms for this is the segregation of solute atoms to grain boundaries (GBs), where they can impact microstructural evolution to a degree beyond what their nominal alloying concentration would suggest. With modern experimental techniques, we are now able to measure solute concentration at particular boundaries with high accuracy [1], and can even resolve the segregation of solute atoms to particular GB sites [2]. Modelling, however, has lagged behind these developments and there is a strong need for new techniques and deeper understanding to bridge the gap between experimental measurements and atomistic simulations.

In general the solute concentration at the GB depends on the solute density of states (DOS) (i.e. segregation energies), and occupation probability for those states, which is a function of the site energy, the temperature, and the alloy composition. Here, we have developed a computational framework using classical embedded atom method potentials to evaluate the segregation energy of six different solutes to 38 unique GBs in Al – a total of more than 1.4 million segregation energies. Fig. 1(a) shows the DOS for Mg segregation aggregated across all 38 boundaries, while figs. 1(b) and (c) show examples of individual DOS for two special GBs for each solute. Alongside the DOS in fig. 1(a) we plot the corresponding Fermi-Dirac occupation curve, which takes into account that each site can be occupied by only a single atom.

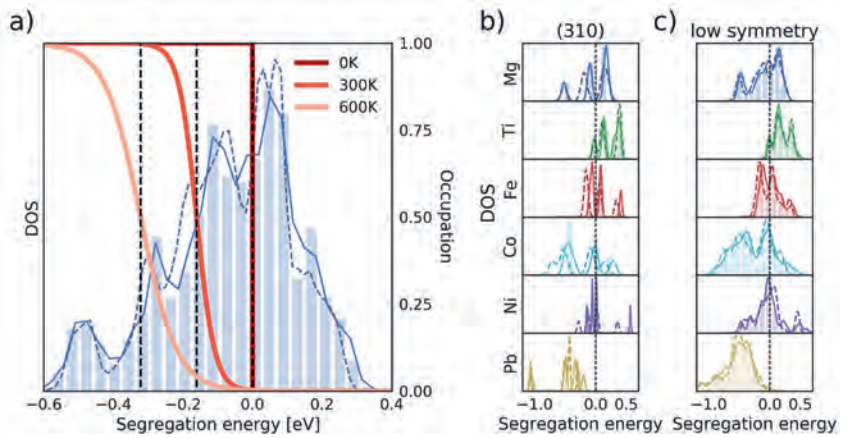


**Fig. 1:** *(a) The aggregated DOS across all 38 GBs for Mg segregation, as a histogram (blue bars) and smoothed distribution (solid blue line). The occupation probability at three different temperatures for a bulk concentration of 0.2 at.% (red lines) is also shown. (b and c) DOS for each of the solutes at (b) the highly-symmetric (310) GB and (c) a low-symmetry boundary. Smoothed machine-learned predictions for the DOS are shown using dashed lines in all subfigures.*

Using this rich data set, we demonstrate two new paths forward for modelling solute-GB segregation [3]. First, we have applied machine learning techniques to make accurate predictions of the segregation DOS based purely on the solute-free GB structure. This reduces the number of atomistic calculations needed to obtain the DOS for a new GB from the number of GB sites at that boundary down to one. Second, we observe that except for a few very symmetric GBs, a Gaussian distribution is often a good estimate for the DOS. With this insight, we go beyond the widely used Langmuir-McLean (LM) model by treating the DOS using its second moment, where we now have three fitting parameters instead of two – i.e. the distribution normalization, mean segregation energy, and distribution variance, instead of the LM model's saturation limit and "effective" segregation energy.

In fig. 2 we demonstrate that both the machine learning approach and Gaussian best-fit give good predictions over a broad temperature range. In contrast, the LM model – which approximates the entire segregation DOS with a single-energy Dirac-delta function – systematically fails to describe solute-GB concentration as a function of temperature. This machine learning technique opens the door to multi-scale modelling methods where larger length scales are informed by atomistic segregation data, while the Gaussian DOS approximation offers a direct link between experimental concentration measurements and atomistic simulations due to the physical interpretability of its fit parameters.

In parallel, we have used atom probe tomography (APT) to study segregation at Σ13(001) GBs in an Al-6.22%Zn-2.46%Mg-2.13%Cu alloy (wt.%), which

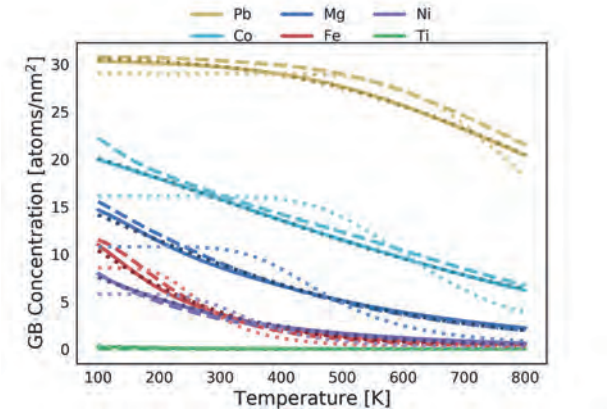


**Fig. 2:** *Solute-GB concentration isotherms at the GB for all six solutes with a nominal concentration of 0.2 at.%. Results are shown for calculated segregation energies (solid lines), machine-learned energies (dashed lines), Langmuir-McLean best-fit (light dotted lines), and Gaussian best-fit (dark dotted lines).*

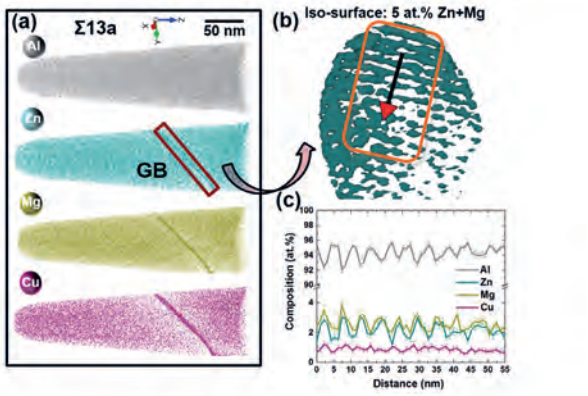


**Fig. 3:** *Atom probe tomography results obtained on a Σ13 GB in the as-quenched state: (a) Atom maps of all elements; (b) Distribution of solutes within the grain boundary (region indicated by the red rectangle in (a)); (c) Corresponding one-dimensional composition profile along the arrow in (b).*

belongs to the high strength Al-7XXX series. To begin, we solution heat treated the material at 475°C for 1 hour before water quenching [4]. We then prepared APT samples using a FEI Helios plasma focused ion beam (PFIB) with a Xe source and acquired near-atomic-scale compositional information using a Cameca LEAP5000XR local electrode atom probe instrument. With a conventional Ga source for FIB, the quality of atom probe data is compromised by the strong segregation of Ga to Al GBs, which also leads to embrittlement. The use of the Xe-source has allowed us to obtain the first ever set of reliable APT data for grain boundary composition in Al-alloys.

Analysis of one of the resulting APT measurements for the as-quenched Al-Zn-Mg-Cu alloy is shown in fig. 3. The location of the GB is highlighted with a red box in fig. 3(a), while isosurfaces of 5 at.% Zn+Mg are shown in fig. 3(b) for the cross sectional slice from this region. Fig. 3(a) demonstrates that all solute species, i.e. Zn, Mg, and Cu, have already segregated to the GB by the end of the quench. We see in fig. 3(b) that this segregation follows periodic patterns throughout the entire GB. These segregation patterns are formed due to the preferential segregation of Zn and Mg to particular sites, similar to observations from our simulations. The corresponding composition profile along the pattern axis is shown in Fig. 3(c). A periodic distribution is revealed, with 5 nm distance between the peaks. The segregation patterns and compositional analysis indicate that this phenomenon can be related to the periodic alternating structure within the grain boundary [2] or faceted grain boundary as Liebscher et al. studied in multicrystalline Si [5]. Facetted boundaries can be studied using our computational methodology in a piece-wise fashion, and we plan to extend our research in this direction.

Going forward, a deeper integration of these cutting edge experimental and simulation techniques will be used to advance our understanding of solute segregation at GBs. As indicated by our simulation work, the GB normal plane can have a strong influence on the amount of segregation. In light of this observation, we will perform further experiments which fully characterize all five GB parameters. This will allow us to directly compare both the degree of segregation and its spatial patterning as predicted by theory and observed in experiment.

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# Magnetic Disorder in Materials: *Ab initio* Methods and Applications

*I. Stockem, O. Hegde, O. Waseda, C. Freysoldt, T. Hickel*

Department of Computational Materials Design (CM)

A majority of the material systems investigated at the MPIE, including for instance advanced high-strength steels, Ni-based superalloys, high-entropy Cantor alloys or magnetocaloric alloys, show magnetism at the atomic scale. Ferromagnetic or other ordered magnetic configurations, that form the ground state of the material, are nowadays routinely computed in density functional theory (DFT). In technological applications most of the above mentioned materials are, however, operating well above their ordering temperature. Consequently, the magnetic entropy yields highly disordered (i.e. unstable) magnetic configurations and high-frequency fluctuations, which are not captured in conventional DFT calculations.

In the CM department, employing our own DFT code S/PHI/nx gives us the chance to implement and apply techniques tailored for these challenges. In the group of C. Freysoldt a novel way of constraining the local magnetic density to atomic moments of arbitrary magnitude and direction was developed [1]. It uses the concept of Lagrange multipliers, similarly to the way a normalization of the wave function is ensured during the electronic structure minimization cycle. Extensive performance tests revealed that this approach yields substantially faster and more stable convergence than the consideration of penalty terms with auxiliary magnetic fields implemented in other codes. In this way, magnetic disorder in materials from steels up to Fe-based superconductors became accessible.

The fluctuations in the magnetic disorder have been addressed with two different strategies: The spin-space averaging (SSA) technique has been developed by F. Körmann [2] to simulate phonons in the paramagnetic regime. It is based on the assumption that the changes in the magnetic configurations occur on a much shorter time scale than the atomic vibrations. An average over all magnetic configurations contained in a supercell, in which up- and down spins are distributed according to the concept of special quasirandom structures (SQS), simulates the magnetic fluctuation, but preserves the structural symmetries. The SSA approach quantitatively reproduces the experimentally observed softening of phonons when heating the material across the magnetic transition temperature.

Based on this success, the group of T. Hickel applied the SSA technique for the relaxation of atoms next to structural defects in paramagnetic materials. It is fully clear that a single disordered magnetic structure would yield artificial forces that are inconsistent with the structural symmetry. To make the averaging of forces during the relaxation efficient, several synchronous DFT calculations, an on-the-fly averaging of forces and an external structure optimization have been employed. The combination of different codes and the implementation of the complex simulations protocol were substantially simplified by using pyiron, the novel integrated development environment of the CM department (see p. 48).

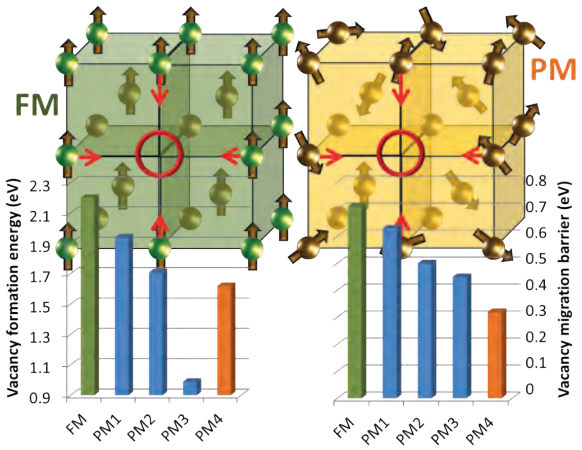


**Fig. 1:** *Vacancy formation (left) and migration (right) energies in the ferromagnetic (FM) and paramagnetic (PM) state. In the PM state no relaxation (PM1), a ferromagnetic relaxation (PM2), a relaxation of individual paramagnetic snapshots (PM3) and a relaxation according to averaged paramagnetic forces (PM4) are compared.*

The application of this technique to vacancies in bcc Fe yields remarkable relaxation effects. It turns out that the formation as well as the migration energy are substantially reduced by magnetic disorder (compare FM and PM2 in Fig. 1). More importantly, however, the correct relaxation of the atomic positions yields an additional reduction of these energies by the same order of magnitude (compare PM1 and PM4 in Fig. 1). Therefore, using relaxations in ordered magnetic states for the determination of paramagnetic vacancy formation energies (PM2 in Fig. 1) fails to be accurate.

The second strategy to consider magnetic fluctuations is the application of atomistic spin dynamics (ASD) at finite temperatures. This approach becomes particularly attractive if combined with *ab initio* molecular dynamics (AIMD). For this purpose, I. Stockem [3] has developed in a close collaboration with Linköping University (B. Alling) an alternating scheme (Fig. 2), in which every ASD step receives an updated set of atomic positions and therewith

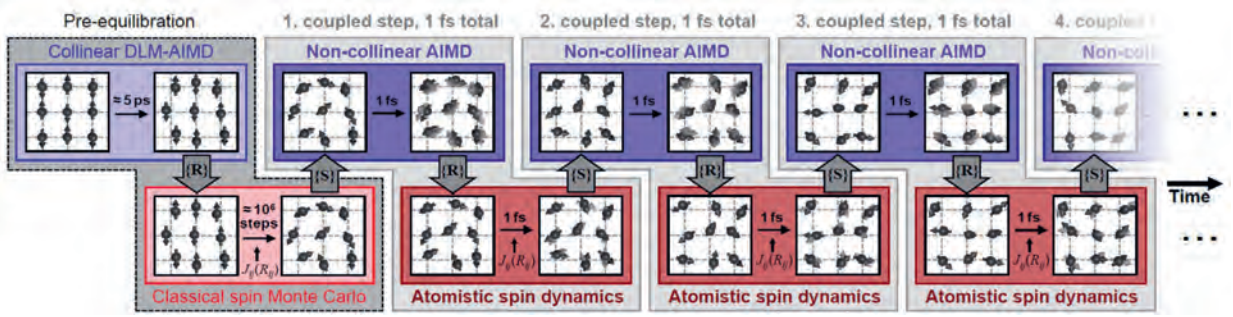


**Fig. 2:** *Alternating scheme, combining ab initio molecular dynamics (AIMD) for disordered local moments (DLM) with atomistic spin dynamics.*

magnetic interaction parameters, and every AIMD step receives an updated set of magnetic moments, which are constrained during the *ab initio* calculation of forces. In this way mutual coupling effects become accessible.

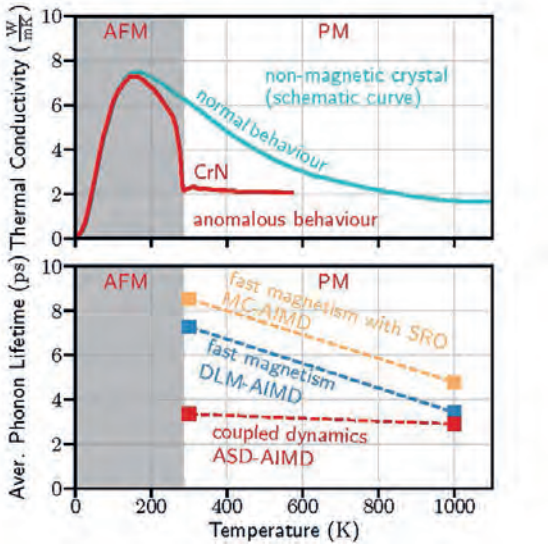


**Fig. 3:** *Experimentally observed anomaly of the hermal conductivities of CrN (top) compared to the averaged phonon lifetime as obtained with different simulation techniques (bottom).*

Indeed, the application of this scheme to CrN has lead to interesting insights: Although there is no long-range magnetic order in the paramagnetic state, the spin orientations of neighbouring Cr atoms depend clearly on the distances of these atoms: As two neighbouring Cr atoms approach during the vibration, their spins tend to point into opposite directions. If they are further away from each other, the corresponding spins prefer an orientation into the same direction. Furthermore, the mutual coupling of the spin orientations and the distance between the neighbouring Cr atoms prevents the spin system from a fast decay compared to the spin dynamics of an uncoupled vibrating lattice.

We studied the influence of this dynamic coupling on phonon lifetimes in CrN. The relevance of short range order (SRO) effects are highlighted by a comparison with alternative methods (Fig. 3): If the directions of the magnetic moments are randomly changed at each step (DLM-AIMD), the magnetic subsystem shows no SRO, neither in space nor time. If the atomic configurations are determined by Monte-Carlo simulations, the spins exhibit a temperature-dependent SRO in space, but not in time. We realize that only our coupled ASD-AIMD approach, which includes SRO in space and time, yields a vanishing temperature dependence of the resulting phonon lifetimes. This explains an anomalous temperature dependence of the thermal conductivity of CrN in its paramagnetic state, which was observed experimentally, but not understood before (Fig. 3).

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# Applying an *ab initio* Potentiostat to Elucidate the Fundamental Mechanism behind Mg Corrosion

*S. Surendralal [1], M. Todorova [1], S. Wippermann [2], J. Neugebauer [1]*

[1] Department of Computational Materials Design (CM)
[2] Department of Interface Chemistry and Surface Engineering (GO)

Solid/liquid interfaces are at the heart of many applications of practical importance. Examples are batteries, electro catalysis, fuel cells or corrosion. To understand and eventually overcome the technological challenges faced in these applications requires accurate modelling techniques. Electronic structure calculations are free of fitting parameters and provide insights at the atomistic level. They are thus the method of choice, provided that we are able to overcome the issues impeding the modelling of constant electrode potential conditions, essential for the realistic description of solid/liquid interfaces. We recently developed a method that successfully addresses these issues (see p. 47) and provides an *ab initio* potentiostat [1], thus enabling calculations under applied bias in complete analogy to electrochemical experiments.

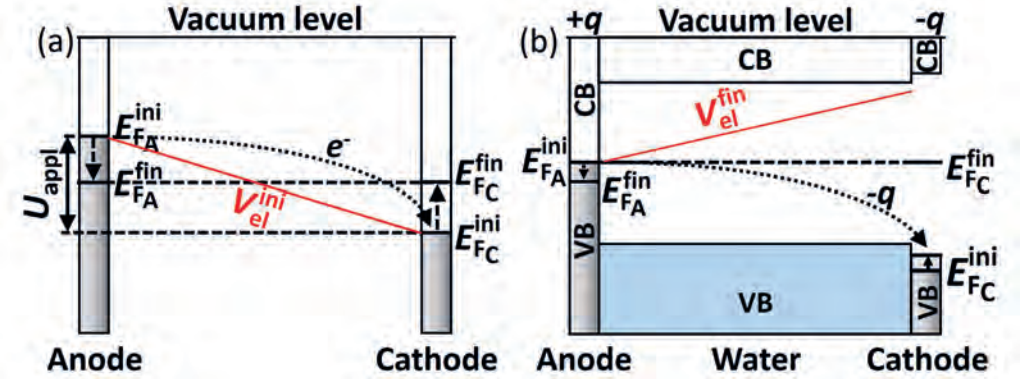


**Fig. 1:** *Schematic representation of the concept used to realize an electrolytic cell. (a) Alignment between two metal electrodes before (superscript "ini") and after (superscript "fin") charge transfer. The charge transfer leads to equal Fermi energies $E_F$, preventing the realization of an electric field. The red line shows the electrostatic potential before the charge transfer. (b) A doped semiconductor electrode allows us to control the position of the Fermi level. The type (here, p type) and concentration of dopants controls the polarity and magnitude of the field. The red line shows the electrostatic potential realized by the charge transfer. The slope of the potential is proportional to the induced electric field.*

We had to overcome two key challenges. To ensure a constant electrode potential *U* electrons are transferred from the anode (positively charged electrode) to the cathode (negatively charged electrode). The ensuing electric field drives negatively charged ions, such as $OH^-$, to the positively charged anode and positively charged ions, such as $H^+$ (protons), to the negatively charged cathode. This means that electrodes are thermodynamically open to both electrons and protons, and thus fundamentally grand canonical. This is difficult to realize in a standard density functional theory (DFT) code where the particles and electrons in the cell remain constant. However, a full electrolytic (or electrochemical) cell contains both the positively and the negatively charged electrode and is canonical for both electrons and protons. By realizing a canonical setup in a DFT calculation we retain a constant number of electrons and protons throughout the calculation and circumvent the described difficulty. This setup enables us to describe a realistic electrochemical system, if we are able realize an electric field between the two electrodes. This is challenging in a standard DFT code with periodic boundary conditions, because the necessity of having a different Fermi level on each electrode, a requirement to realizing a potentiostat and thus an electric field between the two electrodes, contradicts the mandatory condition for a constant Fermi level throughout a cell (see Fig.1a). To overcome this fundamental limitation while still using a standard DFT code we introduced a novel type of computational electrode by replacing one of the metal electrodes by a doped semiconductor (Fig.1b). In cases where the semiconductor is not doped and the Fermi level of the metal electrode falls within the band gap of the semiconductor electrode the two electrodes are decoupled and there is no charge transfer between them. If we dope the semiconductor electrode *p*-type the ensuing charge transfer from the metal electrode will charge the semiconductor negative and make it the cathode, as seen in Fig.1b. Conversely, doping the semiconductor electrode *n*-type will result in charge transfer to the metal electrode, charging the semiconductor electrode positive and making it

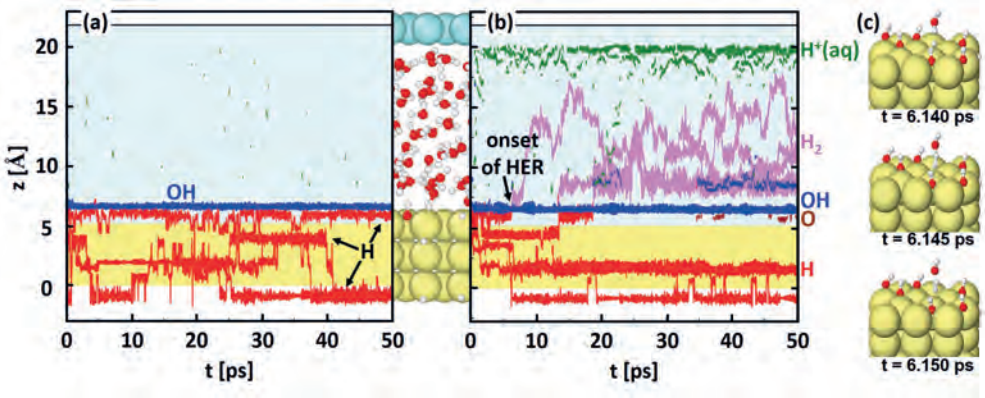


**Fig. 2:** *Ab initio computed trajectories of the atomic and molecular species formed when Mg is exposed to water for (a) open circuit conditions and (b) applying a linear increasing voltage. Trajectories are shown in a projection along the normal to the Mg surface. Blue, red, violet, green, and brown lines mark OH, H, $H_2$, $H^+$(aq.), and O, respectively. The onset of the $H_2$ evolution reaction is indicated in (b) by a black arrow. To focus on the relevant reaction products Mg-water trajectories are shown as yellow (blue) colored background. The atomic geometry of the electrolytic cell is visualized in the figure between (a) and (b). Atoms are shown as colored spheres: Mg (yellow), Ne (turquoise), oxygen (red), hydrogen (gray). (c) Snapshots of the HER extracted from the MD trajectory of the system under applied bias potential.*

the anode. The charge transfer induces a potential bias *U* and an electric field. Controlling the doping charge *q* enables us to control the bias and the field.

We identified Ne as the most suitable semiconductor electrode, as it possesses the following characteristics: (i) its band gap, although significantly reduced in DFT calculations, remains sufficiently large and is suitably aligned, (ii) Ne is van der Waals bonded and has a negligible deformation potential, (iii) it is chemically inert, so that chemisorption or alloy formation at the electrode are suppressed, (iv) even a single layer of Ne prevents permeation of water molecules and its residues. To dope the Ne electrode we use pseudo-atoms with fractional proton numbers. This gives us flexibility regarding the charge on the electrode by not restricting us to integer numbers, as explicit dopants would have. The full control we retain over the electrode charge is a central element to constructing a static or dynamic potentiostat.

Utilizing pyiron (see p. 48) allowed us to implement a charge control feedback-loop outside the DFT code. This way we can employ the new approach with any DFT code and without having to make changes to the underlying code. We were thus able to employ a standard DFT code (VASP) to study one of the key puzzles in corrosion science – the anomalous hydrogen evolution at an anodically polarized Mg electrode. According to fundamental corrosion concepts, $H_2$ evolution should occur only at the negatively charged cathode via a reaction consuming electrons, i.e. $2H^+ + 2e^- \rightarrow H_2$. The counterintuitive behaviour observed at anodically polarized Mg in contact with water has been known for 150 years, but the atomistic mechanism of the reaction is yet unknown. At open circuit conditions, i.e. without an applied electric field, we observe spontaneous dissociation of water molecules at the Mg surface (cf. Fig. 2a) and a subsequent adsorption of OH on the surface up to a maximum coverage of 1/3 ML (monolayer), but no $H_2$ formation. Following anodic polarization of Mg (cf. Fig. 2b) the OH coverage increases to 1 ML and we observe $H_2$ evolution. Since our *ab initio* setup allows us to inspect the reaction at the atomic level, we extract relevant snapshots from the molecular dynamics trajectory (see Fig. 2c) to study the reactions. As can be seen, a water molecule binds to an H atom adsorbed on the Mg surface, dissociates and leaves a $H_2$ molecule and an $OH^-$ ion. While this reaction looks like a "conventional" Heyrovsky reaction in an alkaline medium, $H_{ad} + H_2O + e^- \rightarrow H_2 + OH^-$, its occurrence at the anode, where electrons are deficient, contradicts present concepts in electrochemistry. A careful inspection of the electronic structure reveals that, even under the condition of a positively charged Mg surface, the adsorbed H is not charge neutral, but negatively charged $H^-$. Thus, H itself, rather than the anode provide the required excess electron, and the ensuing reaction becomes $H^-_{ad} + H_2O \rightarrow H_2 + OH^-$. In the absence of a potential (open circuit conditions), the reaction does not occur [see Fig. 2(a)], because the attractive electrostatic interaction between the $OH^-$ ion and the anode, which is critical to make this reaction exothermic, is absent. Being able to unravel this long standing corrosion science question shows the power of the new potentiostat approach and its potential to address a wide range of questions related to electrochemistry and corrosion.

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## PART IV.

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*Kahl Zilnyk,* M.Sc. (Brazil), Escola de Engenharia de Lorena, University of São Paulo (EEL-USP)/BR, Humboldt Research Fellowship for Postdoctoral Researchers; Dec 2015 to Feb 2016

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*Dr. Dominique Chatain* (France), Aix-Marseille Université, CINaM (CNRS)/FR; Jul 2017

*Ran Chen,* B.Sc. (China), Shanghai Jiao Tong University (SJTU)/CN, China Scholarship Council (CSC); Feb 2015 to Jan 2017

*Dr. Serhiy Cherevko* (Ukraine), Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN) /DE, Postdoctoral Research Fellow; Dec 2011 to Aug 2018

*Dr. Wonseok Choi* (Korea), Korean Institute of Science & Technology (KAIST)/KR; Jul to Aug 2018

*Ning Dang*, M.Sc. (China), Baihang University/CN; Nov 2017 to Jan 2018

*Farnaz Abdollahzadeh Davani,* M.Sc. (Iran), University of Sistan and Baluchestan/IR; Feb 2017 to Feb 2019

*Dr. Palanisamy Dhanalakshmi* (India), Indian Institute of Science, Bangalore/IN; Apr 2017 to Apr 2018

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*Isnaldi Rodrigues de Souza Filho,* M.Sc. (Brazil), Escola de Engenharia de Lorena, University of São Paulo (EEL-USP)/BR; Oct 2017 to Sep 2018

*Jorge Luis Martins Guerra Filho,* M.Sc. (Brazil), Universidade Federal do Rio de Janeiro (UFRJ)/BR; May 2017 to Apr 2020

*Axel Forslund* (Sweden), Royal Institute of Technology/SE; May to Jun 2018

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*Dr. Martin Friák* (Czech), Institute of Physics of Materials of the Academy of Sciences of the Czech Republic (IPM Brno)/CZ; Dec 2016; Feb 2017; Oct 2017; Jun 2018

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*Dr. Junying Hu* (China), State Key Laboratory of Oil and Gas/CN, Chinese Scholarship Council; Sep 2016 to Sep 2017

*Dr. Pradeep Konda Gokuldoss* (India), RWTH Aachen University/DE; May 2014 to Apr 2018

*Dr. Mark Greiner* (Canada), MPI für Chemische Energiekonversion, Mülheim a.d.R./DE; Jul to Aug 2018

*Dr. James Griffiths* (UK), Cambridge/UK; Apr 2016

*Yueling Guo,* M.Sc. (China), Beihang University/CN, Chinese Scholarship Council (CSC); Oct 2017 to Sep 2019

*Dr. Ivan Gutierrez-Urrutia* (Spain), Research Center for Strategic Materials, National Institute for Materials Science/JP; Jul 2017

*Dr. Masood Hafez* (Iran), VDM Metals GmbH/DE; Feb 2015 to Dec 2016

*Michael Haines*, B.Sc. (USA), University of Tennessee/US; Jan to Jul 2018

*Dr. Nima Hamidi* (Iran), Institut für Theoretische Physik, AG Computersimulationen und Theorie komplexer Fluide, TU Berlin/DE; Feb 2015 to Jan 2016

*Ian Harding,* M.Sc. (USA), Brown University/US; May to Jun 2018

*Dr. Jinshan He* (China), Beijing University/CN; Jul to Aug 2018

*Anders Holten* (Denmark), University of Copenhagen/DK, Visiting Researcher; Nov 2015 to Apr 2016

*Prof. Toshiaki Horiuchi* (Japan), Hokkaido University of Science/JP; Feb to Mar 2016; Aug 2016; Oct 2017; Aug 2018

*Dr. Junying Hu* (China), State Key Laboratory of Oil and Gas/CN, Chinese Scholarship Council; Sep 2016 to Sep 2017

*Dr. Qingyun Hu* (China), Ruhr University Bochum/DE, RESOLV Fellow; Mar 2014 to Aug 2018

*Mingda Huang,* M.Sc. (China), Xi'an Jiaotong University/CN, Chinese Scholarship Council (CSC); Oct 2017 to Sep 2019

*Dr. Yuji Ikeda* (Japan), Kyoto University/JP, Mai 2017 to Apr 2018

*Hyeji Im,* M.Sc. (Korea), Korean Institute of Science & Technology (KAIST), Seoul/KR; Jul 2017 to Feb 2018

*Dr. Shoji Ishibashi* (Japan), National Institute of Advanced Industrial Science and Technology/JP; Feb 2018; Mai to Oct 2018

*Prof. Balila Nagamani Jaya* (India), Indian Institute of Technology Bombay/IN; May to Jun 2017, Jul 2018

*Dr. Darja Jenko* (Slovenia), Institute of Metals and Technology (IMT)/SI; Jul 2017 to Jul 2018

*Hosun Jun,* B.Sc. (Korea), Korean Institute of Science & Technology (KAIST), Seoul/KR; Jun 2018 to Jan 2019

*Dr. Reza Darvishi Kamachali* (Iran), Tehran University, Tehran/IR; Heisenberg Fellowship; Feb 2018 to Jan 2021

*Sho Katsura,* M.Sc. (Japan), Kobe Steel/JP; Oct 2017 to Sep 2018

*Mehrin Peyman Khanipour,* M.Sc. (Iran), Forschungszentrum Jülich/DE; Aug 2016 to Jul 2017

*Dr. Jong-Hee Kim* (Korea), POSCO (Pohang Iron and Steel Company)/KR; Dec 2017 to Dec 2018

*Julius Knöppel,* M.Sc. (Germany), Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN) /DE; Dec 2017 to Dec 2018

*Peter Konijnenberg*, Dipl.-Ing. (The Netherlands), Bruker Nano GmbH, Berlin/DE; Jan 2014 to Dec 2018

*Assist. Prof. Dr. Maciej Krzwiecki* (Poland), Silesian University of Technology/PL; several short-term research visits; 2012 to 2018

*Ankit Kumar,* M.Sc. (India), Indian Institute of Technology Roorkee/IN, TU Delft /NL; Nov 2015 to Jul 2017

*Dr. Alisson Kwiatkowski da Silva* (Brazil), Universidade Estadual de Ponta Grossa, UEPG (State University of Ponta Grossa)/BR, Brazilian Government (Science Without Borders); Apr 2015 to Sep 2018

*Dr. Minjie Lai* (China), Northwestern Polytechnical University, Xi'an/CN, China Scholarship Council (CSC); Aug 2012 to Aug 2016

*Dr. Christopher Laursen* (USA), University of Wyoming/US; Jan to Apr 2018

*Juan Li*, M.Sc. (China), University of Science and Technology Beijing/CN; since Oct 2015

*Zhuangming Li,* M.Sc. (China), University of Science and Technology Beijing (USTB)/CN; Jul to Oct 2018

*Chuanlai Liu,* M.Sc. (China), Shanghai Jiao Tong University/CN, China Scholarship Council (CSC); Oct 2015 to Sep 2017; Feb 2018

*Andreas Lücke* (Germany), Universität Paderborn/DE, for research exchange; Jan to May 2016

*Wei Luo*, M.Sc. (China), Central South University/CN, China Scholarship Council (CSC); Nov 2014 to Oct 2017

*Caleb Massey,* M.Sc. (USA), University of Tennessee/US; Oct to Nov 2017

*Nidhin George Mathews* (India), Indian Institute of Technology Bombay/IN; Jul 2018

*Sami Meddeb,* B.Sc. (Tunesia), PHELMA, Grenoble (INP)/FR; May to Jul 2018

*Prof. Sai Ramudu Mekka* (India), Indian Institute of Technology Roorkee/IN, MPG-DST Partner Group; Mar 2017 to Feb 2020

*Maisam Merali* (UK), University of Cambridge/UK; Jul to Aug 2018

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*Dr. Kristiane Ann Kathrin Rusitzka* (Germany), Max-Planck-Institut für Eisenforschung/DE, Experiment!-Fellow (VW Foundation); Jun 2017 to Jun 2018

*Dr. Ryoji Sahara* (Japan), National Institute for Materials Science/JP, Jul 2015 to Jun 2016

*Dr. Maria Samdim* (Brazil), Universidade de São Paulo (EEL-USP)/BR; Apr 2016; Jun 2017; Mar 2018

*Daniel Sandbeck,* M.Sc. (Germany), Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN)/DE; Aug 2016 to Jul 2017

*Prof. Hugo Sandim* (Brazil), Universidade de São Paulo (EEL-USP)/BR; Apr 2016; Jun 2017; Mar 2018

*Dr. Vitalij Schmidt* (Germany), Münster University/DE; Mar 2016 to Mar 2017

*Anton Schneider* (France), CEA Saclay/FR; Jan 2018

*Dr. Torsten Schwarz* (Germany), RWTH Aachen University/DE; Sep 2015 to Apr 2016

*Kai Alexander Schwenzfeier,* M.Sc. (Germany), TU Wien/AT; Jul 2015 to Nov 2018

*Dr. Karo Sedighiani* (Iran), TU Delft/NL; Apr 2017 to Mar 2020

*Javiera Aguirre Sepúlveda*, M.Sc. (Chile), Pontificia Universidad Católica de Chile/CL; Jan to Jul 2018

*Andreja Šestan* (Slovenia), Jožef Stefan Institute (JSI)/SI; Aug 2017 to Aug 2018

*Dr. Pratheek Shanthraj* (India), North Carolina State University/US; Aachen Institute for Advanced Study in Computational Engineering Science (AICES); Jun 2014 to May 2016; Jun 2018 to May 2020

*Dr. Alexander Shapeev* (Russia), Skoltech, Stolkovo Innovation Center/RU, Apr 2018

*Ariel Sheskin,* B.Sc. (Israel), Technion/IL; Minerva Scholarship; Aug 2016 to Sep 2016

*Dr. Reinhard Sigel* (Germany), German University in Cairo (GUC)/ EG; Feb to Dec 2017

*Gabriel da Silva,* Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN)/DE; Dec 2017 to Dec 2018

*Dr. Sanjay Singh* (India), Max-Planck-Institut für Chemische Physik fester Stoffe/DE; Jul 2016

*Dr. Michaela Šlapáková* (Czech Republic), Charles University Prague/CZ; Sep 2015 to Aug 2016; Mar to Apr 2017

*Purvesh Soni,* M.Sc. (India), RWTH Aachen University/DE; Sep 2015 to Aug 2018

*Florian Speck,* M.Sc. (Germany), Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN)/DE; Jan to Jul 2017

*Prashanth Srinivasan* (India), TU Delft/NL, Apr 2018; Oct 2018; Dec 2018

*Dr. Irina Stockem* (Germany), Linköping University/SE, Aug 2016 to Feb 2017, Aug 2018 to Jul 2019

*Dr. Andreas Stoffers* (Germany), RWTH Aachen University/DE; Sept 2015 to Aug 2016; Jan to Jun 2017

*Prof. Bob Svendsen* (USA/Germany), RWTH Aachen University/DE; cooperation with RWTH Aachen University; since Mar 2012

*Dr. Agnieszka Szczepaniak* (Poland), Wroclaw University/PL; Jan to Jun 2018

*Haleh Taghinejadi* (UK), University of Cambridge/UK; Jul to Aug 2017

*Chris Talbot* (UK), University of Cambridge/UK; Jul to Aug 2018

*Xiaodong Tan,* M.Sc. (China), Northeastern University, Shenyang/CN, China Scholarship Council (CSC); Oct 2015 to Sep 2016

*Komomo Tani* (Japan), Advanced Technology Research Laboratories, Nippon Steel & Sumitomo Metal Corporation/JP; Jul 2016 to Jun 2018

*Dr. Shunsuke Taniguchi* (Japan), Advanced Technology Research Laboratories, Nippon Steel & Sumitomo Metal Corporation/JP; May 2016 to Apr 2017

*Stefanie Tecklenburg,* M.Sc. (Germany), Ruhr Universität Bochum/DE; Jan 2016 to Jan 2018

*Katie Tidd* (UK), University of Cambridge/UK; Jul to Aug 2017

*Konstantina Traka,* M.Sc. (Greece), National Technical University of Athens/GR, TU Delft/NL; Jul 2017 to Jun 2019

*Dr. Mizuki Tsuboi* (Japan), Kyoto University/JP; Jul 2017 to Aug 2018

*Daniel Varley* (UK), University of Cambridge/UK; Jul to Aug 2016

*Ruben Bueno Villoro* (Spain), Universitat Autonoma de Barcelona/ES; Jul to Aug 2017; Feb to Jun 2018

*Lixiao Wang,* M.Sc. (China), Tsinghua University/CN, China Scholarship Council (CSC); Mar 2016 to Aug 2016

*Dr. Xiaoxiang Wu* (China), Ruhr Universität Bochum/DE, Apr 2017 to Dec 2018

*Dr. Yun Wu* (China), Shanghai University/CN; Jan to Aug 2018

*Jinghua Xin* (China), Central South University/CN, Sep 2015 to Sep 2016

*Konatsu Yamada* (Japan), Hokkaido University of Science/JP; Aug 2018

*Suhyun Yoo* (Korea), Ruhr Universität Bochum/DE; Mar 2016 to Feb 2018

*Kooknoh Yoon,* M.Sc. (Korea), Seoul National University/KR, Scholarship of 'Research Exchange Program' between Korea and ERC (EU); Sep 2018 to Aug 2019

*Dr. Janez Zavašnik* (Slovenia), Jožef Stefan Institute (JSI)/SI; Aug 2017 to Aug 2018

*Dr. Han Zhang* (China), Tsinghua University, Beijing/CN; Jan to Jun 2016

*Dr. Jian Zhang* (China), Xi'an Jiaotong University/CN; Apr to Jul 2018

*Jiecen Zhang*, M.Sc. (China), Northeastern University, Shenyang/CN, China Scholarship Council (CSC); Oct 2015 to Sep 2016

*Huan Zhao,* M.Sc. (China), Chongqing University/CN, China Scholarship Council (CSC); Oct 2014 to Sep 2019

*Tian Rong Zhu* (UK), University of Cambridge/UK; Jul to Aug 2016

# Scientific Honours

## 2015 (not included in the Scientific Report 2013 - 2015)

*Prof. Dierk Raabe* was awarded the Certificate of Excellence in Reviewing from Acta Materialia & Elsevier in recognition of significant contributions made to the quality of the journal, 2015

*Prof. Paulo Rangel Rios* from Universidade Federal Fluminense (UFF), Rio de Janeiro (Brazil) has been awarded a Return Fellowship of the Humboldt Research Award, Dec 2015

*Dr. Franz Roters* became member of the Editorial Board of Philosophical Magazine and Philosophical Magazine Letters, Oct 2015

*Dr. Cem Tasan* former leader of the group Adaptive Structural Materials (until Dec 2015) won the Freigeist Fellowship of the Volkswagen Foundation, Jun 2015

*Dr. Markus Valtiner* was elected as member-at-large for the Biointerfaces Division of the American Vacuum Society, Oct 2015

*Dr. Markus Valtiner* received an ERC Starting Grant for the project “CSI.interface - A molecular interface science approach: Decoding single molecular reactions and interactions at dynamic solid/liquid interfaces”, Dec 2015

*Ali Zendegani* received the Larry Kaufman Scholarship 2015 to present his research on “First-principles study of thermodynamic properties of the Q phase in Al-Cu-Mg-Si” at the CALPHAD XLIV conference, Loano (Italy), May 2015

## 2016

*Christian Broß* has been honoured by the Chamber of Industry and Commerce (IHK) Düsseldorf being one of the Best Trainees 2016, Oct 2016

*Christian Broß* won the Max Planck Trainee Prize by the Max Planck Society, one of the best trainees of all Max Planck Institutes, Sep 2016

*Christian Broß* received the 1st Poster Award at the Conference Mikpräp 2015, Solingen (Germany) with his poster “Study of New Methods to Analyse Chromium-Nickel Steels”, Jun 2016

*Dr. Vijayshankar Dandapani* was selected to give an invited talk at the Gordon Research Conference 2016 on Aqueous Corrosion, New London (USA), Jul 2016

*Dr. Martin Diehl* received the Deutsche Gesellschaft für Materialkunde e.V. (DGM) – Nachwuchspreis, Sep 2016

*Dr. Andreas Erbe and Dr. Michael Auinger* received the Best Paper Award for the years 2014 - 2015 from EOS (Journal of the European Optical Society) for their paper “Effect of surface roughness on optical heating of metals”, Sep 2016

*Herbert Faul* was lent the honourary needle in silver with thanks and recognition for his 10 years honourary engagement in professional training by Niederrheinische Industrie- und Handelskammer, Duisburg-Wesel-Kleve (Germany), Aug 2016

*Dr. Martin Friák, Dr. Stefanie Sandlöbes, Z. Pei, Dr. Duangcheng Ma, Prof. Bob Svendsen, Prof. Dierk Raabe and Prof. Jörg Neugebauer* won one of three poster prizes with the poster “An ab initio high throughput approach to identify MG-alloys with exceptionally high yield strength” at the 80$^{th}$ Annual Meeting of the German Physical Society (DPG) in Regensburg (Germany). The shown results are based on a close interdisciplinary work between scientists of the two departments “Computational Material Design” and “Microstructure Physics and Alloy Design”, Mar 2016

*Dr. Baptiste Gault* was awarded the Volkswagen Foundation ‘Experiment!’ research project on “Enabling atomic-scale tomography of biological material”, Oct 2016

*Dr. Michael Herbig* received 1.468 Mio € funding by the BMBF for his junior research group "Materials Science of Mechanical Contacts", Sep 2016

*Stefan Hieke* received a Travel Award from the DGE (Deutsche Gesellschaft für Elektronenmikroskopie) to participate at the European Microscopy Conference EMC 2016 in Lyon (France) Sep 2016

*Dr. Nejc Hodnik* got a Marie-Curie Intra-European Fellowship „ElWBinsTEM - Development of electrochemical water based in-situ TEM and study of platinum based nanoparticles potential- and time-dependent changes", Apr 2014 to Mar 2016

*Dr. Motomichi Koyama*, *Dr. Asif Bashir and PD Dr. Michael Rohwerder* received the Japan Institute of Metals and Materials Metallography Award (Fine work prize), Mar 2016

*Nataliya Malyar* received one of two prestigious Best Poster Awards at the Gordon Research Conference 2016 in Lewiston, Maine (USA), Aug 2016

*Prof. Jörg Neugebauer* was awarded the 2015 Ernst Mach Medal of the Czech Academy of Sciences, May 2016

*Julian Rechmann* obtained a Best Poster Award at the 16th International Conference on Organized Molecular Films (ICOMF16), Helsinki (Finland), Jul 2016

*Dr. Hauke Springer, Dr. Cem Tasan and Prof. Dierk Raabe* received the Werner Koester Award for the paper "A novel roll bonding methodology for the cross-scale analysis of phase properties and interactions in multiphase structural materials" published in IJMR 106 (2015), 3-14, Sep 2016

*Dr. Frank Stein and Irina Wossack* received the Best Paper Award of the Alloy Phase Diagram International Commission for the year 2015, Jul 2016

*Daniel Varley* won the 2016 European Placement Prize of the University of Cambridge for his work on high-temperature polymer electrolyte membrane fuel cells, which he performed during his two-month summer internship in the independent research group of Prof. Christina Scheu, Nov 2016

*Dr. Aleksandar R. Zeradjanin* was selected to give an invited lecture at the 67th Annual Meeting of the International Society of Electrochemistry (ISE) and was invited to chair the session at the Symposium: "Novel Materials and Devices for Energy Conversion and Storage", Haag (The Netherlands), Aug 2016

## 2017

*Priyanshu Bajaj* received the Best Poster Award: ADDMAT conference, Tiruvanantapuram (India), Dez 2017

*Janine Birnbach* received the Apprentice Prize for one of the best final exams in the profession of laboratory technician, Chamber of Industry and Commerce (IHK) Düsseldorf (Germany), Oct 2017

*Heidi Bögershausen and Luca Bender* gained the 2nd poster prize at the „Fachtagung für Mikroskopie und Präparation (MikPräp) 2017", Solingen (Germany) with their poster about „Haushalts- und Lebensmittel als alternative Ätzmethoden", Apr 2017

*Dr. Martin Diehl, Christian Broß and Prof. Dierk Raabe* won the 3rd poster prize with the poster „Quasi in situ Untersuchung der statischen Rekristallisation in DC 04 Stahl" at the „Fachtagung für Mikroskopie und Präparation (MikPräp) 2017", Solingen (Germany), Apr 2017

*Till Freieck* won the Max Planck Trainee Prize by the Max Planck Society, one of the best trainees of all Max Planck Institutes, Aug 2017

*Dr. Blazej Grabowski* received the Acta Journals Outstanding Review Award for 2016, Apr 2017

*Dr. Michael Herbig* has been awarded the Certificate of Excellence in Reviewing from Scripta Materialia for 2016, Mar 2017

*Dr. Michael Herbig* was honoured with the AIME Champion H. Mathewson Award 2017 by the Minerals, Metals & Materials Society (TMS), Jan 2017

*Dr. Michael Herbig* received the Outstanding Reviewer Award by Acta/Scripta Materialia, 2017

*Shyam Katnagallu and Zirong Peng* have been awarded with the IFES Student Award of the International Field Emission Society, Aug 2017

*Dr. Christoph Kirchlechner* has received the Heinz Maier-Leibnitz Preis 2017 (DFG), Berlin (Germany), May 2017

*H. Knoll, S. Ocylok, A. Weisheit, H. Springer, E. Jägle and D. Raabe* have been selected for the "Best of Steel 2017" for the article "Combinatorial Alloy Design by Laser Additive Manufacturing", May 2017

*Dr. Fritz Körmann* received the VIDI-Preis of the Dutch Science Foundation (NWO) for „Advancing finite-temperature ab initio techniques to explore chemically complex multi-component alloys", Jul 2017

*Dipl.-Ing. Philipp Kürnsteiner* won the M&M (Microscopy & Microanalysis) Student Paper Award 2017 with his paper "In-process Precipitation During Laser Additive Manufacturing Investigated by Atom Probe Tomography". The Prize is annually awarded by the Microanalysis Society, Aug 2017

*Xiaolin Li* received an "Editor Choice Award 2016" from the Journal of Phase Equilibria and Diffusion, Feb 2017

*Chuanlai Liu* has been awarded with the Best Oral Presentation Award at the EUROMAT 2017 in Thessaloniki (Greece), Sep 2017

*Wei Luo* was awarded with the "Best Student Talk Award" at the Nanobrücken 2017 conference in Manchester (UK), Apr 2017

*Max-Planck-Institut für Eisenforschung GmbH* reaches the 3rd best position in the Humboldt-Ranking among all non-university research organizations in Germany with 30 won scholarships between 2012 and 2016, Sep 2017

*Claudia Merola* received the Best Poster Award at the 64th American Vacuum Society conference in Tampa, FL (USA), Nov 2017

*Enrico Pizzutilo* participated in the 67th Lindau Nobel Laureate Meeting, Lake Constance (Germany), Jun 2017

*Prof. Dierk Raabe* is Vice Chair of the Gordon Research Conference on Physical Metallurgy held at the University of New England in Biddeford, Maine (USA), Jul 2017

*Prof. Dierk Raabe* is Senator of Helmholtz Society since 2017

*Dr. Martin Rabe* got a Marie Sklodowska-Curie European Fellowship "Smart cc - Designing novel smart sensor interfaces based on a biologically abundant peptide motif: coiled-coils", Jun 2017 to May 2019

*Dr. Michael Rohwerder* received the Excellent Poster Award for the poster entitled: "Novel Zinc-Nanocomposite Coatings for Intelligent Corrosion Protection"at the 11th International Conference on Zinc and Zinc Alloy Coated Steel Sheet (Galvatech 2017) in Tokyo (Japan), Nov 2017

*Dr. Rafael Soler* was awarded with the Best Poster Award at the ECI Conference (Engineering Conference International) on Small Scale Mechanics, Dubrovnik (Croatia), Oct 2017

*Dr. Aleksandar R. Zeradjanin* received a Travel Award for Young Electrochemists, in recognition of the quality of scientific research and contribution to the 68th ISE (International Society of Electrochemistry) Annual Meeting, Providence (USA), Aug 2017

## 2018

*Lamya Abdellaoui* won the Best Oral Communication Award at the "1st International Meeting on Alternative and Green Energies" (IMAGE18) in Mohammedia (Morocco), May 2018

*Prof. Gerhard Dehm* received an ERC Advanced Grant for the project "GB-CORRELATE - Correlating the State and Properties of Grain Boundaries", Mar 2018

*Dr. Poulumi Dey* received one of two Best Poster Awards at the 3rd International Conference on Metals and Hydrogen „SteelyHydrogen2018" in Ghent (Belgium), May 2018

*Aniruddha Dutta* won the German Science Slam Championship 2018. In the final eight researchers competed against each other, Wiesbaden (Germany), Nov 2018

*Dr. Eric A. Jägle* visited the Tokyo Institute of Technology, Tokyo (Japan), Department of Materials Science and Engineering as specially Appointed Assistant Professor, Mar 2018 to Feb 2020

*Dr. Baptiste Gault* received an ERC Consolidator Grant for the project „SHINE - Seeing Hydrogen in Matter", Feb 2018

*Dr. Simon Geiger* was awarded the prize of the German Chemical Society (GDCh) for his dissertation titled "Stability investigations of iridium-based catalysts towards acidic water splitting", Aug 2018

*Daniel Göhl* received a DAAD Fellowship for a research short-term stay at Yuriy Román's Group, Massachusetts Institute of Technology (USA), Sep 2018 to Dec 2018

*Ankit Gupta* won one of two 2018 Travel Awards sponsored by the journal "Materials" for his paper on "First-principles investigation of thermodynamics and precipitation kinetics in Al-Sc alloys". Ankit Gupta presented his work at the "TMS 2018 Annual Meeting and Exhibition, Phoenix (USA), Mar 2018

*Dr. Tilmann Hickel* received the Acta Journals Outstanding Review Award for 2017, Apr 2018

*Dr. Stefan Hieke* was awarded with a EMS (European Microscopy Society) Scholarship 2018 to present his work at the 19th International Microscopy Congress (IMC19) in Sydney (Australia), Sep 2018

*Dr. Stefan Hieke* was one of 50 selected participants of the Young Scientist Assembly of the International Federation of Societies for Microscopy held before the 19th International Microscopy Congress (IMC19) in Sydney (Australia), Sep 2018

*Dr. Reza Darvishi Kamachali* was awarded the Heisenberg Fellowship by the German Research Foundation to pursue his research on materials microstructures, Jan 2018

*Dr. Christoph Kirchlechner* was awarded with the Certificate of Excellence in Reviewing by Acta Materialia and Scripta Materialia, Apr 2018

*Philipp Kürnsteiner* received the Acta Materialia Student Award 2017 for the best publication of the previous year for the paper "Massive nanoprecipitation in an Fe-19Ni-xAl maraging steel triggered by the intrinsic heat treatment during laser metal deposition", Aug 2018

*Dr. Marc Ledendecker* received a DAAD Fellowship for a research short-term stay at Alivisatos Group, University of California, Berkeley (USA), Jun to Sep 2018

*Dr. Christian Liebscher's* paper on "Strain-Induced Asymmetric Line Segregation at Faceted Si Grain Boundaries" was selected as cover story in Physical Review Letters 121(1), Jul 2018

*Maisam Merali* won the 2018 European Placement Prize of the University of Cambridge for his work on phase relations in the Co-Ti system, which he performed during his two-month summer internship in the group Intermetallic Materials of the SN department, Nov 2018

*Prof. Dierk Raabe* has been honoured with The Seidmann Family Lecture Series Award, Tel Aviv University (Israel), 2018

*Prof. Dierk Raabe and Dr. Michael Herbig and their co-authors* have been awarded with the AIME Champion H. Mathewson Award 2018 by The Minerals, Metals & Materials Society (TMS) for their Publication "Autonomous Filling of Grain-Boundary Cavaties during Creep Loading in Fe-Mo Alloys". (Zhang, S., Fang, H., Gramsma, M.E. et al. Metall and Mat Trans A (2016) 47: 4831. https://doi.org/10.1007/s11661-016-3642-0), Jan 2018

*Prof. Christina Scheu* was nominated to serve as panel member of the strategic evaluation of the research field Matter of the Helmholtz Association, 2018

*Prof. Christina Scheu* has been elected as a member of the evaluation board for the "EFRE.NRW 2014–2020 „NeueWerkstoffe.NRW" (European Regional Development Fund of the State of North Rhine-Westphalia), 2018

*Dr. Cidem Toparli* won an ISE Prize "Oronzio and Niccolò De Nora Foundation Young Author Prize" for her paper "In situ and operando observation of surface oxides during oxygen evolution reaction on copper" in Electrochim. Acta 236 (2017) 104, Aug 2018

# Participation in Research Programmes

## National:

### BMBF

„ECCO2 - Combinatorial electrocatalytic CO2 reduction“, BMBF „Technologies for Sustainability and Climate Protection“, Oct 2011 - Sep 2016

„KoWUB - Novel corrosion protection coatings compatible with hot forming“, BMBF, May 2012 – May 2015

„MANGANESE - Mechanistic investigations of model and applied electrodes for the oxygen evolution“, BMBF, May 2015 – Oct 2019

„NanoSolar - Semiconducting nanocomposites with tailored optical and electronic properties”, BMBF NanoMatFutur, Jan 2014 – Dec 2019

„Optimizing solar cell efficiency based on 3-dimensinal chemical analysis on the atomistic scale (Optimierung des Wirkungsgrades von Solarzellen basierend auf 3-dimensionalen chemischen Analysen auf atomarer Skala)“, BMBF NanoMatFutur, Feb 2013 – Aug 2015

„RADIKAL - Resource-saving material substitution by additive & intelligent FeAl material concepts adapted for light and functional building“, BMBF MatRessource, Feb 2013 – Mar 2016

„RAVE-K - Ressource friendly design for precious metal containing switch materials for low voltage applications“, BMBF MatRessource, Jun 2013 – May 2016

„UGSLIT - Ultra-high-strength, weight-reduced steels for resource-saving lightweight construction in transport applications“, BMBF, Aug 2016 – Mar 2018

„White Etching Crack - Knowledge-based design of wear resistant bearing steels by atomic-scale characterization as countermeasure against white-etching crack failure in wind power plants“, BMBF, Sep 2016 – Aug 2021

### BMWi

„Development of HTPEM fuel cells with improved degradation behaviour via detailed structure and chemical analysis“, BMWi, AiF Projekt GmbH, Jan 2015 – Nov 2017

„PtTM@HGS - Development of cost-efficient, high performance gas diffusion electrodes for polymer electrolyte membrane fuel cells (PEM-FC) with low Platinum loading and novel hollow graphitic spheres as support”, BMWi, Apr 2016 – Mar 2019

### DFG

***DFG Priority Programmes, Collaborative Research Centres & Transregio Projects***

„Broadband reflecting fibers with tailored structures inspired by desert ants”, DFG SPP 1839: Tailored Disorder - A science- and engineering-based approach to materials design for advanced photonic applications, Jul 2015 – Dec 2018

„Correlative study towards experimental validation of the high throughput methodology (S02)”, DFG SFB 1232: From colored states to evolutionary structural materials, Jul 2016 – Jun 2020

„Coupling phenomena in magnetocaloric materials: From thin layers to composites”, DFG SPP 1599: Caloric Effects in Ferroic Materials: New Concepts for Cooling, Sep 2012 – Dec 2018

„Electro-plasticity in Al-Cu eutectic alloys”, DFG SPP 1959: Manipulation of matter controlled by electric and magnetic fields: Towards novel synthesis and processing routes of inorganic materials, Jul 2016 – Dec 2019

„Evolution of strengthening phases under in-service stresses and temperatures: phase-field and experimental study”, DFG SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical States in Applied Materials, Jul 2017 – Dec 2019

„Investigation and enhancement on bonding by cold bulk metal forming processes", DFG SPP 1640: Joining by Plastic Deformation, Nov 2011 – Dec 2018

„Investigations of the local alloy composition by means of atom probe tomography (A04)", DFG CRC/Transregios, TRR 103: From Atoms to Turbine Blades - A Scientific Approach for Developing the Next Generation of Single Crystal Superalloys, Jan 2012 – Dec 2019

„Mechano-chemical coupling during precipitate formation in Al-based alloys", DFG SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical States in Applied Materials, Jul 2015 – Apr 2019

„Metallic nanowires on the atomic scale: Electronic and vibrational coupling in real world systems", DFG Forschungsgruppe 1700, Jul 2016 – Dec 2019

„Metal oxide nanostructures for electrochemical and photoelectrochemical water splitting", DFG SPP 1613: Fuels Produced Regeneratively Through Light-Driven Water Splitting: Clarification of the Elemental Processes Involved and Prospects for Implementation in Technological Concepts, Jan 2017 – Mar 2019

„Micromechanisms of the electro-plastic effect in magnesium alloys investigated by means of electron microscopy", DFG SPP 1959: Manipulation of matter controlled by electric and magnetic fields: Towards novel synthesis and processing routes of inorganic materials, Jul 2016 – Dec 2019

„Modeling bainitic transformations during press hardening", DFG SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical, Jan 2015 – Dec 2016

„PaCCman - Particle-strengthened Compositionally Complex Alloys - interlinking powder synthesis, additive manufacturing, microstructure evolution and deformation mechanisms", DFG SPP 2006: Compositionally Complex Alloys - High Entropy Alloys (CCA - HEA), Jul 2017 – Dec 2020

„Phase-field-based chemomechanical models for phase transitions and dislocation-microstructure interaction in metallic alloys with application to kappa-carbides", DFG SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical States in Applied Materials, Jun 2017 – Dec 2019

„Quantum mechanically guided design of ultra-strong and damage-tolerant glasses", DFG SPP 1594: Topological Engineering of Ultra-Strong Glasses, Dec 2015 – Oct 2019

„Steel - *Ab Initio*. Quantum Mechanics Guided Design of New Fe-based Materials", DFG SFB 761, 1st period: July 2007 – June 2011, 2nd period: Jul 2011 – Jun 2015, 3rd period: Jul 2015 – Jun 2019

Projects at MPIE in frame of SFB 761:

- A 02 *Ab initio* thermodynamics und kinetics in the Fe-Mn-Al-C system, Jul 2007 – Jun 2019
- A 07 Microstructure mechanics and fundamentals of concurrent twinning and martensite formation, Jul 2007 – Jun 2019
- A 09 *Ab initio* based mesoscale simulation of hydrogen embrittlement, Jul 2011 – Jun 2019
- C 01 Microstructure analytics, Jul 2015 – Jun 2019
- C 04 Fatigue, damage and stress corrosion cracking under cyclic loading, Jul 2007 – Jun 2019
- C 08 3D atomic analysis of the local chemical composition by atom probe tomography, Jul 2011 – Jun 2019
- C 10 Deformation behavior of multi-phase steels, Jul 2015 – Jun 2019
- T 4 Influence of microstructure on hydrogen embrittlement in Cr-alloyed high-Mn steels, Jul 2015 – Dec 2018

„Synthetic dental composite materials inspired by the hierarchical organization of shark tooth enameloid", DFG SPP 1420: Biomimetic Materials Research: Functionality by Hierarchical Structuring of Materials, Aug 2013 – Dec 2016

„Tailored precipitation (B2, $L2_1$) strengthened, compositionally complex FeAlCr (Mn, Co, Ni, Ti) alloys for high temperature applications", DFG SPP 2006: Compositionally Complex Alloys - High Entropy Alloys (CCA - HEA), Jan 2018 – Dec 2020

„Thermo-chemo-mechanical coupling during thermomechanical processing of microalloyed steels", DFG SPP 1713: Strong Coupling of Thermo-Chemical and Thermo-Mechanical States in Applied Materials, Jun 2014 – Dec 2017

„Towards self-healing metals by employing optimally-dispersed Ti-Ni shape memory nano-particles“, DFG SPP 1568: Design and Generic Principles of Self-Healing Materials, Apr 2014 – Dec 2017

„TRIP-iCCAs - Interstitial transformation-induced plasticity-assisted quinary compositionally complex alloys: Design, structure and mechanical behavior”, DFG SPP 2006: Compositionally Complex Alloys - High Entropy Alloys (CCA - HEA), Jul 2017 – Dec 2020

„Understanding the damage initiation at microstructural scale (B03)“, DFG CRC/Transregios, TRR 188: Damage Controlled Forming Processes, Feb 2017 – Dec 2020

„Understanding the role of trigger signal spreading, release rate of suitable active agents and their transport rate for optimal healing in extrinsic self-healing materials”, DFG SPP 1568: Design and Generic Principles of Self-Healing Materials, May 2014 – Jun 2018

***DFG Research Grants***

„Ab initio based calculation of the stability of selected TCP precipitates in steels: Temperature and interface effects“, DFG Research Grant, Feb 2017 – Jan 2020

„AHEAD - Analysis of the Stability of High Entropy Alloys by Dewetting of Thin Films“, DFG-ANR, Mar 2017 – Jul 2020

„Automated analysis and validation of interatomic potentials for application in Materials Science“, DFG Research Grant, Jan 2019 – Dec 2021

„Can high strength and moderate ductility be combined in wear resistant coatings? A fundamental plasticity study of $X_2BC$ nanolaminates (X=Hf, Mo)“, DFG Research Grant, Oct 2016 – Dec 2019

„Consistent physically-based modeling of dynamic recrystallization under hot working conditions“, DFG Research Grant, Apr 2016 – Apr 2019

„Correlation of growth, structure, optical and electronic properties of novel $Nb_3O_7(OH)$ and $Nb_2O_5$ nanostructures”, DFG Research Grant, Jul 2017 – Jun 2020

„CORRKEST - Correlative characterization of co-evaporated $Cu_2ZnSnSe_4$ thin-films“, DFG Research Grant, Apr 2016 – Dec 2019

„Diffusion in high entropy alloys: Development and application of an experiment-ab initio approach“, DFG Research Grant, Jan 2019 – Dec 2021

„Exploring Multinary Nanoparticles by Combinatorial Sputtering into Ionic Liquids and Advanced Transmission Electron Microscopy“, DFG Research Grant, Dec 2016 – Dec 2019

„Fracture initiation in FCC and BCC metals during tribology“, DFG Research Grant, Oct 2017 – Sep 2020

„From interatomic potentials to phase diagrams: Integrated tools for validation and fitting“, DFG Research Grant, Jan 2019 – Dec 2021

„Fundamentals of molecular adhesion for the prediction of macroscopic adhesion at electrified interfaces“, DFG Research Grant, Dec 2015 – Dec 2018

„Hydrogen-microstructure interactions in iron-based alloys at small scales: from amorphous, via nanocrystals, to polycrystals“, DFG Research Grant, Sep 2016 – Aug 2018

„Lamellar Fe-Al in situ composite materials: microstructure and mechanical properties”, DFG Research Grant, Jan 2013 – Aug 2016

„Magnetism in iron alloys: thermodynamics, kinetics and defects”, DFG-ANR, Feb 2017 – Jan 2020

„Materials World Network: Fundamentals of Peptide Materials - Experimental and Simulation Probes”, DFG-NSF, Sep 2013 – Nov 2016

„Precipitation kinetics during non-linear heat treatment in Laser Additive Manufacturing”, DFG Research Grant, Jun 2016 – Apr 2019

„Rare-earth based alloys for hard-magnetic applications: Temperature and pressure dependent phase stabilities“, DFG-ANR, Jan 2017 – Jun 2020

„Structure, phase formation and properties of metallic glasses manipulated by electric current”, DFG Research Grant, May 2017 – Dec 2020

„Study of grain-boundary-dislocation interactions by advanced in situ µLaue diffraction“, DFG Research Grant, Jan 2015 – Jan 2019

„The effective pH at the solid-liquid interface and the local ion distribution during complex electrochemical reactions“, DFG Research Grant, Mar 2014 – Mar 2017

„Understanding the role of dislocation distribution(s) on the slip transfer across twin-boundaries“, DFG Research Grant, Aug 2015 - Dec 2018

„xMicroFatigue - X-ray Laue Microscopy to Understand Fatigue Damage“, DFG-ANR, Feb 2017 – Feb 2020

**DFG Cluster of Excellence**

„Electrochemistry on „dry surfaces“: electrode potential and structural order in nanoscopic electrolyte layers“, DFG Cluster of Excellence 1069 RESOLV (Ruhr Explores Solvation), Aug 2013 – Dec 2018

„Probing the molecular structure of extended solvated surfaces and interfaces“, DFG Cluster of Excellence 1069 RESOLV (Ruhr Explores Solvation), Mar 2014 – Feb 2017

„Stability of electrode materials in an electrochemical environment”, DFG Cluster of Excellence 1069 RESOLV (Ruhr Explores Solvation), Mar 2016 – Feb 2019

„Zinc oxide – water interfaces: interaction-driven structural evolution“, DFG Cluster of Excellence 1069 RESOLV (Ruhr Explores Solvation), Feb 2015 – Jul 2016

**Max Planck Society**

„AProLAM - Advanced Alloy and Process Design for laser Additive Manufacturing of Metals“, MPG - FhG cooperation, Apr 2015 – Dec 2018

„Combinatorial design of novel rare-earth free, high-entropy based permanent magnets“, Indian Institute of Technology, Madras, Max Planck Partner Group with India, Jun 2018 – May 2021

„Initial wear - Early detection of material wear in high-precision machine tools“, MPG - FhG cooperation, Jan 2014 – Dec 2016

„International Max Planck Research School for Interface Controlled Materials for Energy Conversion IMPRS-SurMat (IMPRS - SurMat)“, Max Planck Society, Jan 2016 – Dec 2021

„Designing Damage Tolerant Functional Oxide Nanostructures: Damage Tolerance Studies on Barium Titanate at Small Length Scales“, Indian Institute of Technology Bombay, Max Planck Partner Group with India, Mar 2017 – Mar 2020

„MaxNet BigMax - Max Planck Research Network on big-data-driven material science“, Research Cooperaion, Max Planck Society, Mar 2017 – Mar 2022

„MaxNet Energy“, Research Cooperation, Max Planck Society, Jan 2014 – Dec 2018

„Stress and defects driven phase transformations“, Indian Institute of Technology, Roorkee, Max Planck Partner Group with India, Apr 2017 – Apr 2020

**Leibniz Association**

„CarMON - New Carbon-Metal Oxide Nanohybrids for Efficient Energy Storage and Water Desalination”, Leibniz Competition, May 2017 – Apr 2020

**Volkswagen Stiftung**

„A new class of smart materials: Switching strength for future´s safety”, Experiment!, Jan 2017 – Apr 2018

„Seeing atoms in biological materials”, Experiment!, Jan 2017 – Jun 2018

**KSB Stiftung**

„Investigation of structural transformations at grain boundaries in Ti and Ti alloys by high-resolution and in-situ transmission electron microscopy“, KSB Stiftung, Jan 2018 – Dec 2018

# International:

**Christian Doppler Society**

Christian Doppler Laboratory „Diffusion and segregation mechanisms during production of high strength steel sheet" (original title: "Diffusions- und Segregationsvorgänge bei der Produktion hochfesten Stahlbands") Jan 2008 – Dec 2015

**FWO - Fonds Wetenschapelijk Onderzoek**

„PredictCor - Knowledge and technology platform for prediction of durability and lifetime of organic coated metals under long-term environmental corrosion", FWO/NL, Jan 2018 – Dec 2021

**European Union**

***European Research Council***

„GB-CORRELATE - Correlating the State and Properties of Grain Boundaries", ERC Advanced Grant, Horizon 2020, Aug 2018 – Jul 2023

„SHINE - Seeing Hydrogen in Matter", ERC Consolidator Grant, Horizon 2020, Feb 2018 – Jan 2023

„SMARTMET - Adaptive nanostructures in next generation metallic materials: Converting mechanically unstable structures into smart engineering alloys", ERC Advanced Grant, FP 7, Feb 2012 – Jan 2017

„TIME-BRIDGE - Time-scale bridging potentials for realistic molecular dynamics simulations", ERC Starting Grant, Horizon 2020, Jul 2015 – Jun 2020

***Marie Skłodowska-Curie Actions (FP7 and Horizon 2020)***

„EIWBinsTEM - Development of electrochemical water based in-situ TEM and study of platinium based nanoparticles potential- and time-dependent changes", Marie Curie Intra European Fellowship, FP7, Apr 13 – Mar 2016

„Smartcc - Designing novel smart sensor interfaces based on a biologically abundant peptide motif", Marie Skłodowska-Curie European Fellowship, Horizon 2020, Jun 2017 – May 2019

„SOMATAI - Soft Matter at Aqueous Interfaces", Marie Curie Initial Training Network, FP7, Oct 2012 – Mar 2016

***Collaborative Projects (FP7 and Horizon 2020)***

„AccMet - Accelerated Metallurgy - the accelerated discovery of alloy formulations using combinatorial principles", Collaborative project, FP7, Jun 2011 – Jun 2016

„EPPL - Enhanced Power Pilot Line", ENIAC Joint Undertaking, FP7, May 2013 – Sep 2016

„HERCULES-2 - Fuel flexible, near-zero emissions, adaptive performance marine engine", Horizon 2020 Societal Challenges - Smart, Green And Integrated Transport, May 2015 – Oct 2018

„PowerBase - Enhanced substrates and GaN pilot lines enabling compact power applications", The ECSEL Joint Undertaking, FP7, May 2015 – Apr 2018

***RFCS (Research Fund for Coal and Steel)***

„JOINOX - Guidelines for use of welded stainless steel in corrosive environments", RFCS, Sep 2012 – Feb 2016

„LIGHTOUGH - Screening of tough lightweight Fe-Mn-Al-C steels using high throughput methodologies", RFCS, Jul 2015 – Dec 2018

„MicroCorr - Improving steel product durability through alloy coating microstructure", RFCS, Sep 2015 – Feb 2019

„MuSTMef - Multi Scale Simulation Techniques for Metal Forming", RFCS, Jul 2016 – Jun 2020

„OPTIBOS - New developments and optimisation of high strength boron treated steels through the application of advanced boron onitoring techniques", RFCS, Jul 2012 – Dec 2015

„TOOLMART - New Metallurgical Tools for optimum design of modern Ultra High Strength Low Carbon Martensitic Steels", RFCS, Jul 2013 – Dec 2016

**European Space Agency (ESA)**

„On Beryllium Alloy & Composite Development for Space and Non-Space Application", Jan 2014 – Dec 2016

**FFG (Austrian Research Promotion Agency)**

„Fundamentals and tools for integrated computational modeling and experimental characterization of materials in the atomic to micrometer scale range", Project A1.23 (COMET II) / Project P1.1 (COMET III), Aug 2018 – Dec 2022

# Collaboration with National and International Research Institutes

## National:

Brandenburgische Technische Universität Cottbus-Senftenberg: Lehrstuhl Konstruktion und Fertigung (KuF), Cottbus

Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin

Deutsche Akademie der Naturforscher Leopoldina, Halle

Deutsches Zentrum für Luft- und Raumfahrt (DLR), Bonn

Forschungszentrum Jülich GmbH, Jülich

Forschungszentrum Jülich GmbH: Ernst Ruska-Centrum für Mikroskopie und Spektroskopie mit Elektronen (ER-C), Jülich

Forschungszentrum Jülich GmbH: Institute of Complex Systems Soft Condensed Matter (ICS-3), Jülich

Forschungszentrum Jülich GmbH: Institut für Energie- und Klimaforschung, Werkstoffstruktur und -eigenschaften (IEK-2), Jülich

Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V., München

Fraunhofer Institut für Lasertechnik (ILT), Aachen

Fraunhofer Institut für Produktionstechnologie (IPT), Aachen

Fraunhofer Institut für Werkstoffmechanik (IWM), Freiburg

Fraunhofer-Institut für Werkstoff- und Strahltechnik (IWS), Dresden

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für allgemeine Werkstoffeigenschaften, Erlangen

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für Feststoff- und Grenzflächen-verfahrenstechnik, Erlangen

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für Korrosion und Oberflächentechnik, Erlangen

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für Kunststofftechnik, Erlangen

Friedrich-Alexander-Universität Erlangen-Nürnberg: Lehrstuhl für Werkstoffkunde und Technologie der Metalle, Erlangen

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Heinrich-Heine-Universität Düsseldorf: Institut für Experimentelle Physik der kondensierten Materie, Düsseldorf

Heinrich-Heine-Universität Düsseldorf: Institut für Medizinische Mikrobiologie und Krankenhaushygiene, Düsseldorf

Heinrich-Heine-Universität Düsseldorf: Institut für Theoretische Physik, Düsseldorf

Heinrich-Heine-Universität Düsseldorf: Lehrstuhl für anorganische Chemie, Düsseldorf

Heinrich-Heine-Universität Düsseldorf: Lehrstuhl für organische Chemie, Düsseldorf

Helmholtz-Institut Erlangen-Nürnberg (HI ERN) für Erneuerbare Energien, Erlangen

Helmholtz-Zentrum Berlin, Berlin

Helmholtz-Zentrum-Berlin für Materialien und Energie, Berlin

Helmholtz-Zentrum Geesthacht, Zentrum für Material- und Küstenforschung, Mg Innovation Center (MagIC), Geesthacht

Humboldt Universität zu Berlin: Institut für Mathematik, Berlin
IFW Dresden, Institute for Complex Materials, Dresden
Karlsruher Institut für Technologie (KIT): Institut für Angewandte Materialien – Werkstoffkunde (IAM), Karlsruhe
Karlsruher Institut für Technologie (KIT): Institut für Technikfolgenabschätzung und Systemanalyse, Karlsruhe
Karlsruher Institut für Technologie (KIT): Institut für thermische Strömungsmaschinen, Karlsruhe
Leibniz-Institut für Analytische Wissenschaften e.V. (ISAS), Dortmund
Leibniz-Institut für Festkörper- und Werkstoffforschung(IFW): Institut für komplexe Materialien, Dresden
Leibniz-Institut für Neue Materialien (INM), Saarbrücken
Leibniz-Institut für Plasmaforschung und Technologie (INP), Greifswald
Leibniz-Institut für Werkstofforientierte Technologien (IWT), Bremen
Leibniz Universität Hannover: Institut für Festkörperphysik, Hannover
Leibniz Universität Hannover: Institut für Werkstoffkunde, Hannover
Ludwig-Maximilians-Universität (LMU): Fakultät für Chemie und Pharmazie, München
Max-Planck-Institut für Chemische Energiekonversion, Mülheim a. d. Ruhr
Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden
Max-Planck-Institut für Festkörperforschung, Stuttgart
Max-Planck-Institut für Innovation und Wettbewerb, München
Max-Planck-Institut für Intelligente Systeme, Stuttgart
Max-Planck-Institut für Kohlenforschung, Mülheim a. d. Ruhr
Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam-Golm
Max-Planck-Institut für Polymerforschung, Mainz
Neue Materialien Fürth GmbH (NMF), Fürth
Ruhr-Universität Bochum: Institut für Experimentalphysik IV, Bochum
Ruhr-Universität Bochum: Institut für Geologie, Mineralogie und Geophysik, Bochum
Ruhr-Universität Bochum: Institut für Werkstoffe, Bochum
Ruhr-Universität Bochum: Interdiciplinary Centre for Advances Materials Simulation (ICAMS), Bochum
Ruhr-Universität Bochum: Lehrstuhl für allgemeine Mechanik, Bochum
Ruhr-Universität Bochum, Lehrstuhl für Analytische Chemie, Bochum
Ruhr-Universität Bochum: Lehrstuhl für Analytische Chemie II, Bochum
Ruhr-Universität Bochum: Lehrstuhl für Angewandte Festkörperphysik, Bochum
Ruhr-Universität Bochum: Lehrstuhl für Anorganische Chemie II, Bochum
Ruhr-Universität Bochum: Lehrstuhl für Informatik im Bauwesen, Bochum
Ruhr-Universität Bochum: Lehrstuhl für Physikalische Chemie I, Bochum
Ruhr-Universität Bochum: Lehrstuhl für Physikalische Chemie II, Bochum
Ruhr-Universität Bochum: Lehrstuhl für Technische Chemie, Bochum
Ruhr-Universität Bochum: Lehrstuhl für Theoretische Chemie, Bochum
Ruhr-Universität Bochum: Lehrstuhl für Theoretische Festkörperphysik, Bochum
Ruhr-Universität Bochum: Lehrstuhl für Werkstoffdesign, Bochum
Ruhr-Universität Bochum: Lehrstuhl für Werkstoffe der Mikrotechnik, Bochum
Ruhr-Universität Bochum: Lehrstuhl für Werkstofftechnik, Bochum

Ruhr-Universität Bochum: Lehrstuhl für Werkstoffwissenschaft, Bochum

Ruhr-Universität Bochum: Zentrum für Grenzflächendominierte Höchstleistungswerkstoffe (ZGH), Bochum

RWTH Aachen: Aachen Institute for Advanced Study in Computational Engineering Science (AICES), Aachen

RWTH Aachen: Gemeinschaftslabor für Elektronenmikroskopie (GFE), Aachen

RWTH Aachen: Gießerei-Institut (GI), Aachen

RWTH Aachen: Institut für Anorganische Chemie (IAC), Aachen

RWTH Aachen: Institut für Bildsame Formgebung (IBF), Aachen

RWTH Aachen: Institut für Eisenhüttenkunde (IEHK), Aachen

RWTH Aachen: Institut für Maschinenelemente und Systementwicklung (MSE), Aachen

RWTH Aachen: Institut für Metallkunde und Metallphysik (IMM), Aachen

RWTH Aachen: Institut für Physik, Aachen

RWTH Aachen: Institut für Werkstoffanwendungen im Maschinenbau (IWM), Aachen

RWTH Aachen: Klinik für Zahnärztliche Prothetik und Biomaterialien, Aachen

RWTH Aachen: Lehrstuhl für Werkstoffchemie (MCh), Aachen

Technische Universität Bergakademie Freiberg: Institut für Metallformung, Freiberg

Technische Universität Bergakademie Freiberg: Institut für Werkstoffwissenschaft, Freiberg

Technische Universität Bergakademie Freiberg: Lehrstuhl für Physikalische Chemie, Freiberg

Technische Universität Berlin: Lehrstuhl für Wirtschafts-, Unternehmens- und Technikrecht, Berlin

Technische Universität Chemnitz: Institut für angewandte Funktionalanalysis, Chemnitz

Technische Universität Clausthal: Institut für Metallurgie, Clausthal

Technische Universität Darmstadt: Fachbereich Material und Geowissenschaften, Darmstadt

Technische Universität Darmstadt: Fachgebiet Datenverarbeitung in der Konstruktion, Darmstadt

Technische Universität Darmstadt: Institut für Produktionstechnik und Umformmaschinen, Darmstadt

Technische Universität Dresden, Dresden

Technische Universität Kaiserslautern: Fachbereich Physik, Kaiserslautern

Technische Universität München: Fachgebiet Biogene Polymere, München

Technische Universität München: Friedrich-Schiedel-Lehrstuhl für Wissenschaftssoziologie, München

Technische Universität München: Heinz Maier-Leibnitz Zentrum, Garching

Technische Universität München: Lehrstuhl für effiziente Algorithmen, München

Technische Universität München: Munich Center for Technology in Society, München

Universität Bayreuth: Lehrstuhl Metallische Werkstoffe, Bayreuth

Universität Bielefeld: Fakultät für Physik, Bielefeld

Universität Bielefeld: Fakultät für Soziologie, Bielefeld

Universität Bremen: Institute for Advanced Energy Systems (AES), Bremen

Universität Clausthal: Fakultät für Natur- und Materialwissenschaften, Clausthal (MA)

Universität Duisburg-Essen, Duisburg

Universität Duisburg-Essen: Fakultät für Chemie, Duisburg

Universität Duisburg-Essen: Fakultät für Elektrotechnik, Duisburg

Universität Duisburg-Essen: Fakultät für Mathematik, Duisburg

Universität Duisburg-Essen: Fakultät für Mechanik, Duisburg

Universität Duisburg-Essen: Fakultät für Physik, Duisburg

Universität Duisburg-Essen: Institut für physikalische und theoretische Chemie, Essen

Universität Freiburg: Institut für Anorganische und Analytische Chemie, Freiburg

Universität Kassel: Institut für Werkstofftechnik, Kassel

Universität Konstanz: Fachbereich Physik - Hybrid Nanostructures, Konstanz

Universität Konstanz: Fachbereich Physik, Workgroup Soft Matter Physics, Konstanz

Universität Paderborn, Paderborn

Universität Regensburg: Fakultät für Mathematik, Regensburg

Universität Rostock: Institut für Experimentelle Chirurgie, Rostock

Universität Stuttgart: Institut für Mechanik, Stuttgart

Universität Ulm: Fakultät für Naturwissenschaften, Institut für Neurobiologie, Ulm

Universität Würzburg, Würzburg

Universität Würzburg: Center for Digital Fabrication, Würzburg

Westfälische Wilhelms-Universität (WWU) Münster: Institut für Materialphysik, Münster

## International:

Aalto University: Department of Applied Physics, Aalto, Finland

Aalto University: School of Chemical Technology, Aalto, Finland

Academia Sinica: Institute of Physics, Taipei, Taiwan

Academy of Sciences of the Czech Republic: Institute of Physics of Materials, Brno, Czech Republic

AGH University of Science and Technology, Krakow, Poland

Aix-Marseille University, Centre National de la Recherche Scientifique (CNRS): Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), Marseille, France

Austrian Academy of Sciences: Erich Schmid Institute of Materials Science, Leoben, Austria

Belgorod State University: Center of Nanostructured Materials and Nanotechnologies, Belgorod, Russia

Brown University, Providence, Rhode Island, USA

Brown University: Materials Engineering Faculty, Providence, Rhode Island, USA

California Institute of Technology, Pasadena, California, USA

Cardiff University, Cardiff, UK

Carnegie Mellon University: Materials Science & Engineering, Pittsburgh, Pennsylvania, USA

CEA Saclay, France

Center for Research and Advanced Studies of the National Polytechnic Institute (CINVESTAV), Queretaro, Mexico

Central South University: State Key Lab of Powder Metallurgy, Changsha, China

Centre de Mise en Forme des Matériaux (CEMEF), Nice, France

Centre de Recherches Metallurgiques C.M.R., Belgium

Centre National de la Recherche Scientifique (CNRS): Centre de Recherche sur l'Hétéro-Epitaxie et ses Applications (CRHEA), Sophia Antipolis, France

Centre National de la Recherche Scientifique (CNRS): Institut polytechnique de Grenoble (Grenoble INP), Grenoble, France

Centre National de la Recherche Scientifique (CNRS): Office National d'Etudes et de Recherches Aérospatiales (ONERA), Châtillon, France

Centro de Estudios e Investigaciones Tecnicas (CEIT), San Sebastián, Spain

Centro Ricerche Fiat S.c.p.A., Torino, Italy

Charles University Prague: Department of Physics of Materials, Prague, Czech Republic

Chimie-ParisTech - École nationale supérieure de chimie de Paris, Paris, Frankreich

Christian Michelsen Research AS, Bergen, Norway

Commissariat à l'énergie atomique et aux énergies alternatives (CEA), Saclay, France

Commissariat à l'énergie atomique et aux énergies alternatives (CEA), Grenoble and University of Grenoble: Institut of Nanosciences et Cryogénie, Grenoble, France

CTM Centre Tecnològic, Manresa, Spain

Dartmouth College: Thayer School of Engineering, Hanover, New Hampshire, USA

Deakin University: Institute for Frontier Materials, Geelong, Australia

Delft University of Technology: Department of Materials Science and Engineering, Delft, The Netherlands

Delft University of Technology: Department of Precision and Microsystems Engineering, Delft, The Netherlands

Delft University of Technology: Faculty of Aerospace Engineering, Delft, The Netherlands

Delft University of Technologyt: Faculty of Applied Sciences, FAME Group, Delft, The Netherlands

Delft University of Technology: Faculty of Mechanical, Maritime and Materials Engineering (3mE), Delft, The Netherlands

Ecole Polytechnique: Centre de PhysiqueThéorique, Paris, France

Eidgenössische Materialprüfungs- und Forschungsanstalt Thun, Thun, Switzerland

Eidgenössische Technische Hochschule Zürich, Zürich, Switzerland

Eindhoven University of Technology: Department of Mechanical Engineering, Eindhoven, The Netherlands

European Space Agency ESA, Noordwijk, The Netherlands

European Synchrotron Radiation Facility (ESRF), Grenoble, France

French Corrosion Institute, Brest, Frankreich

German University in Cairo, Egypt

Hasselt University, Hasselt, Belgium

Hasselt University: Institute for Materials Research, Diepenbeek, Belgium

Hokkaido University of Science: Department of Mechanical Engineering, Sapporo, Japan

Imperial College London: Department of Materials, Thomas Young Centre, UK

Indian Institute of Technology Madras, India

Indian Institute of Technology Roorkee: Department of Metallurgical Engineering, India

Institute for Metals and Technology (IMT), Ljubljana, Slovenia

Institute of Physics of Materials of the Academy of Sciences of the Czech Republic, Brno, The Czech Republic

Institute of Quantum Materials Science, Yekaterinburg, Russia

Iowa State University, Ames, Iowa, USA

Iwate University, Morioka, Japan

KAI Kompetenzzentrum Automobil- und Industrieelektronik GmbH, Villach, Austria

Katholieke Universiteit Leuven: Department of Materials Engineering and Department of Computer Science, Leuven, Belgium

KTH Royal Institute of Technology: Department of Materials Science and Engineering, Stockholm, Sweden

Kyushu University: Department of Mechanical Engineering, Fukuoka, Japan

Lawrence Livermore National Laboratory: Materials Science Division, Livermore, California, USA

Linköping University: Department of Physics and Measurement Technology (IFM), Linköping, Sweden

Los Alamos National Laboratory, New Mexico, USA

Los Alamos National Laboratory: Los Alamos Neutron Science Center (LANSCE), New Mexico, USA

Madrid Institute for Advanced Studies of Materials Institute (IMDEA), Madrid, Spain

Massachusetts Institute of Technology (MIT): Department of Materials Science and Engineering, Cambridge, Massachusetts, USA

McGill University: Department of Materials Engineering, Montreal, Canada

Michigan State University: Department of Chemical Engineering and Materials Science, East Lansing, Michigan, USA

Monash University: Department of Materials Science and Engineering, Melbourne, Australia

Montanuniversität Leoben, Leoben, Austria

Montanuniversität Leoben: Chair of Nonferrous Metallurgy, Leoben, Austria

Montanuniversität Leoben: Department of Material Physics, Leoben, Austria

Montanuniversität Leoben: Department of Physical Metallurgy and Materials Testing, Leoben, Austria

National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, California, USA

National Center for Metallurgical Research (CENIM-CSIC), Madrid, Spain

National Institute for Materials Science (NIMS), Japan

National Research Council of Italy, National Institute of Optics, Pisa, Italy

National University of Science and Technology (MISiS): Thermochemistry of Materials Scientific Research Centre, Moscow, Russia

Northwestern University: Department of Materials Science and Engineering, Illinois, USA

Norwegian University of Science and Technology (NTNU): Faculty of Engineering Science and Technology, Trondheim, Norway

Norwegian University of Science and Technology (NTNU): Department of Materials Science and Engineering, Trondheim, Norway

Oak-Ridge National Laboratory (ORNL): Manufacturing Demonstration Facility, Oak Ridge, Tennessee, USA

Oak Ridge National Laboratory (ORNL): Materials Science and Technology Division, Oak Ridge, Tennessee, USA

Ohio State University, Columbus, Ohio, USA

Oxford University: Department of Engineering Science, Oxford, UK

Pohang University of Science and Technology (POSTECH), Pohang, South Korea

Pohang University of Science and Technology (POSTECH): National Institute of Nanomaterials Technology (NINT), Pohang, South Korea

Polish Academy of Sciences: Institute of Metallurgy and Materials Science, Krakow, Poland

Polytechnic University of Catalonia: Department of Physics, Castelldefels, Spain

Russian Academy of Sciences: A.A. Baikov Institute of Metallurgy and Materials Science, Moscow, Russia

Sandia National Laboratories: Materials Science and Engineering Center, Albuquerque, New Mexico, USA

Seoul National University: Department of Materials Science and Engineering, Seoul, South Korea

Silesian University of Technology, Gliwice, Poland

Singapore University of Technology and Design, Singapore

Skolkovo Institute of Science and Technology, Moscow, Russia

Stiftelsen for industriell og teknisk forskning (SINTEF), Trondheim, Norway

Strategisch Initiatief Materialen (SIM), Flanders, Belgium

Swansea University, UK

Swerea KIMAB, Kista, Sweden

Technical University Liberec: Department of Material Science, Czech Republic

Technical University of Denmark (DTU), Lyngby, Denmark

Technion – Israel Institute of Technology: Department of Materials Engineering, Haifa, Israel

Technische Universität Wien, Vienna, Austria

Technische Universität Wien: Institute of Materials Science and Technology, Vienna, Austria

Technische Universität Wien: Institute Professor for Applied Interface Physics, Vienna, Austria

Texas A&M University: Department of Aerospace Engineering, College Station, Texas, USA

The Korean National Research Foundation (NRF), Daejeon, Korea

The Royal Institute of Technology (KTH), Stockholm, Sweden

The Royal Institute of Technology (KTH): Department of Materials Science and Engineering, Stockholm, Sweden

The University of Sydney, Sydney, Australia

Tokyo Institute of Technology: Department of Materials Science and Engineering, Japan

Tokyo Institute of Technology: School of Materials and Chemical Technology, Tokyo, Japan

Tsinghua University: Department of Engineering Mechanics, Center for Mechanics and Materials, Beijing, China

United Kingdom Atomic Energy Authority, UK

Universidad Nacional Autónoma de México (UNAM), Mexico City, Mexico

Universidade Federal do Rio de Janeiro (Coppe/UFRJ): Laboratório Nacional de Tecnologia da Soldagem, Soldagem, Brazil

Università Degli Studi Roma Tre: Department of Engineering, Rome, Italy

Università degli Studi di Torino (UNITO), Torino, Italy

Universität Wien: Department of Lithospheric Research, Vienna, Austria

Université de Metz: Laboratoire d'Étude des Microstructures (LEM3), Metz, France

Université de Rouen, France

Université de Strasbourg: Institut de Physique et Chimie de Matériaux de Strasbourg (IPCM), Department of Magnetic Objects on the NanoScale (DMONS), Strasbourg, France

Université Grenoble Alpes: Laboratoire de Science et Ingénierie des Matériaux et Procédés (SIMaP), France

Universiteit Gent, Gent, Belgium

University Lisboa, Portugal

University of Amsterdam (UvA), Amsterdam, The Netherlands

University of Amsterdam: Van't Hoff Institute for Molecular Sciences, Amsterdam, The Netherlands

University of Applied Sciences Upper Austria, Wels, Austria

University of Birmingham, Edgbaston Campus, UK

University of British Columbia: Department of Materials Engineering, Vancouver, Canada

University of California, Davis, California, USA

University of California: Department of Chemical Engineering and Materials Science, Irvine, California, USA

University of California: Department of Materials, Santa Barbara, California, USA

University of California: Department of Materials Science and Engineering, Berkeley, California, USA

University of Chicago, Chicago, Illinois, USA

University of Florida: Department of Materials Science and Engineering, Gainesville, Florida, USA

University of Illinois: Department of Materials Science and Engineering, Urbana, Illinois, USA

University of Manchester: School of Materials, Manchester, UK

University of North Texas: Department of Materials Science and Engineering, Denton, Texas, USA

University of Oulu: Faculty of Technology, Oulu, Finland

University of Oxford: Department of Chemistry, Oxford, UK

University of Oxford: Department of Materials, Oxford, UK

University of Pretoria, Pretoria, South Africa

University of Science and Technology Beijing, Beijing, China

University of Science and Technology Beijing: State Key Laboratory for Advanced Metals and Materials, Beijing, China

University of Sheffield, Sheffield, UK

University of Twente: Department of Mechanics of Solids, Surfaces & Systems, Enschede, The Netherlands

University of Ulsan: Department of Materials Science and Engineering, Ulsan, Korea

University of Vienna: Faculty of Physics, Vienna, Austria

University of Zurich, Zurich, Switzerland

Vrije Universiteit Brussel (VUB): Research Group on Electrochemical and Surface Engineering (SURF), Brussles, Belgium

West Virginia University, Morgantown, West Virginia, USA

Zhejiang University: Department of Materials Science and Engineering, Hangzhou, China

# Collaborating Industrial Partners and Patents

## Collaborating Industrial Partners

### National:

Airbus Group Innovations, München/Ottobrunn

Akademie für Elektronenmikroskopie und Analytik GmbH, Münster

Avantys engineering GmbH & Co. KG, Bad Lippspringe

Betriebsforschungsinstitut des VDEh (BFI), Düsseldorf, Deutschland

BGH Edelstahl Freital GmbH, Freital

Biochem Zusatzstoffe Handels- und Produktionsgesellschaft mbH, Lohne

BMW Group, München

Bruker EAS GmbH, Hanau

Bruker Nano GmbH, Berlin

Daimler AG, Düsseldorf

Deloro Wear Solutions GmbH, Koblenz

Deutsche Nanoschicht GmbH, Rheinbach

Dr. Kochanek Entwicklungsgesellschaft, Neustadt an der Weinstraße

Dr. Kurt Wolff GmbH & Co. KG, Bielefeld

Eickhoff Antriebstechnik GmbH, Bochum

Henkel AG & Co. KGaA, Düsseldorf

Hydro Aluminium Rolled Products GmbH, Research & Development, Bonn

Innovationsgesellschaft für fortgeschrittene Produktionssysteme GmbH (inpro), Berlin

Karanto Corrosion Protection Technologies GmbH, Düsseldorf

Kirchhoff Automotive, Iserlohn

NANOVAL GmbH & Co. KG, Berlin

Oerlikon Leybold Vacuum GmbH, Köln

Outokumpu Nirosta GmbH, Düsseldorf

Robert Bosch GmbH, Stuttgart

Salzgitter Mannesmann Forschung GmbH, Duisburg

Schaeffler Technologies AG & Co. KG, Herzogenaurach

Schott AG, Mainz

Siemens AG, Berlin

Siemens AG Industry Sector, Industry Automation Division, Erlangen

ThermProTEC GmbH, Offenburg

ThyssenKrupp Electrical Steel UGO S.A.S, Gelsenkirchen

ThyssenKrupp Steel Europe AG, Duisburg/Dortmund

TK VDM, Werdohl

TLS Technik GmbH & Co Spezialpulver KG, Bitterfeld-Wolfen

Umicore AG & Co. KG, Hanau

VDM Metals International GmbH, Werdohl

VDM Metals, Research and Development, Werdohl

Voestalpine Böhler Welding Germany GmbH, Hamm

## International:

ABB Turbo Systems AG, Baden, Switzerland

AMAG Austria Metall GmbH, Ranshofen, Austria

ArcelorMittal Maizières SA, Maizières-lès-Metz, France

Baekert, Kortrijk, Belgium

Centre de mise en forme des matériaux – MINES ParisTech, Paris, France

GE Avio, Torino, Italy

Infineon Technologies Austria AG, Villach, Austria

JFE Steel Corporation, Hiroshima, Japan

Johnson Matthey PLC, UK

Kobe Steel Ltd, Hyogo, Japan

LS Instruments AG, Fribourg, Switzerland

Molycorp Silmet AS, Sillamäe, Estonia

Moroccan Agency for Sustainable Energy (MASEN), Rabat, Morocco

Nippon Steel & Sumitomo Metal Corporation (NSSMC), Chiyoda, Japan

NIZO Food Research, Ede, The Netherlands

Norsk Titanium Components AS, Oslo, Norway

OCAS Belgium, Belgium

Outokumpu Stainless AB, Stockholm, Sweden

Renishaw plc, Wotton-under-Edge, UK

Rolls-Royce plc, London, UK

Sandvik Coromant R&D, Stockholm, Sweden

Senvion SE, Luxembourg, Luxembourg

Solinus, Green Bay, USA

Swerea KIMAB, Kista, Sweden

Tata Steel Europe, IJmuiden, The Netherlands

Tata Steel Nederland Technology BV, IJmuiden, The Netherlands

Tata Steel UK, Wednesfield, UK

Technical Research Laboratories POSCO, Pohang, Korea

Toyota Central R&D Labs., Inc., Nagakute, Japan

TWI Ltd., Cambridge, UK

Vallourec Research Center France, Aulnoye-Aymeries, France

Wärtsila Finland Oy, Vaasa, Finland

Wärtsila Netherlands BV, Drunen, The Netherlands

Winterthur Gas & Diesel Ltd, Winterthur, Switzerland

# Patents

## Patents issued in the given time schedule

| Date of Issue | Description | Inventors |
|---|---|---|
| June 07, 2018 | **Fabrication of nanoporous carbide membranes**<br>Joint invention with Universitat Politecnica de Catalunya<br>(EP 2 664 683) | Renner, Frank, Dr.<br>Duarte-Correa, Maria Jazmin, Dr.<br>Lengsfeld, Julia<br>Bruna, Pere, Dr., BarcelonaTech |
| utility patent<br>August 18, 2016 | **Multi purpose method cell**<br>(20 2016 104 543.6) | Kerger, Philip<br>Rohwerder, Michael, Dr. |
| March 03, 2016 | **Nanoelektroden-Partikelfalle für empfindliche spektroskopische und elektronische Analyse**<br>Joint invention with Academia Sinica Taipe<br>(TWI490487) | Erbe, Andreas, Dr.<br>Chu, Chia-Fu, PhD, Academia Sinica Taipe<br>Chu, Ming-Li, PhD, Academia Sinica Taipe<br>Lesser-Rojas, Leonardo, Academia Sinica Taipe |

## Patents filed in the given time schedule

| Date of Pending | Description | Inventors |
|---|---|---|
| January 20, 2016 | **Flat steel product and method for the production thereof**<br>Joint invention with ThyssenKrupp Steel Europe AG<br>(PCT/EP2016/051109) | Palm, Martin, Dr.<br>Ponge, Dirk, Dr.<br>Leitner, Andreas<br>Hofmann, Harald, Dipl.-Ing., ThyssenKrupp Steel Europe<br>Schirmer, Matthia, Dipl.-Ing. ThyssenKrupp Steel Europe<br>Grövert, Michael, ThyssenKrupp Steel Europe<br>Ferkel, Hans, Prof. Dr., Thyssen-Krupp Steel Europe |
| August 31, 2016 | **Hochduktile Mg-Al-Ca-Legierung**<br>(10 2016 116 244.2) | Neugebauer, Jörg, Prof.<br>Raabe, Dierk, Prof.<br>Sandlöbes, Stefanie, Dr.<br>Friak, Martin, Dr.<br>Pei, Zongrei, Dr. |
| October 25, 2016 | **Process for recycling of noble metals**<br>(PCT/ DE2016/ 100498) | Mayrhofer, Karl, Dr.<br>Hodnik, Nejc, Dr.<br>Baldizzone, Claudio, Dr. |

| Date of Pending | Description | Inventors |
|---|---|---|
| February 02, 2018 | **Hydroxylapatit**<br>Joint invention with Dr. Kurt Wolff GmbH & Co. KG<br>(10 2018 102 365.0) | Fabritius, Helge, Dr.<br>Enax, Joachim, Dr., Firma Wolff<br>Klenk, Adolf, Dr., Firma Wolff |
| September 2018 | **Heizung für Mikro-Verformungseinrichtung**<br>(18199374.2) | Argela, Viswanath Gowtham<br>Kirchlechner, Christoph, Dr.<br>Gonzalez, Iwan<br>Kölling, Michael |

# Conferences, Symposia and Meetings Organized by the Institute

## 2015 (not included in the Scientific Report 2013 - 2015)

*A. Erbe, C. Arckel and C.D. Fernández-Solis* organized the training course “Career Development” for fellows of the Marie Curie Initial Training Network “SOMATAI” at the MPIE, Düsseldorf (Germany), Dec 2015

*M. Palm* co-organized and chaired the session “Frontiers in Intermetallics” within the framework of the international conference „Advances in Materials & Processing Technologies - AMPT 2015“ in Madrid (Spain), Dec 2015

## 2016

*G. Dehm, C. Scheu, and S. Brinckmann* organized the “Mechanics meets Energy IV” symposium at Akademie Biggesee in Attendorn (Germany), 18 - 21 Jan 2016

*G. Dehm* co-organized the Symposium “In situ Microscopy with Electrons, X-Rays and Scanning Probes in Materials Science” at DPG Spring Meeting 2016 in Regensburg (Germany), 06 - 11 Mar 2016

*J. Neugebauer* co-organized the Topical Session “Integrated computational materials engineering for design of new materials” at the Spring Meeting of the German Physical Society (DPG) in Regensburg (Germany), 06 - 11 Mar 2016

*M. Palm and F. Stein together with F. Pyczak* (Helmholtz-Zentrum Geesthacht) co-organized and co-chaired the priority topic “Hochtemperaturwerkstoffe“ (high temperature materials) at the 62. Metallkunde Kolloquium in Lech am Arlberg (Austria), Apr 2016

*F. Archie* organized the 26$^{th}$ GLADD Meeting held at the MPIE, Düsseldorf (Germany), 16 Apr 2016

*F. Roters* co-organized the Mini-Symposium “Fourier-based Methods for Computing the Behavior of Heterogeneous Materials Developments, Extensions and Applications” during the European Congress on Computational Methods in Applied Sciences and Engineering ECCOMAS 2016 in Kreta (Greece), 05 - 10 May 2016

*B. Gault* was Co-Chair at the Biannual „NRW-APT User Meeting“ at the MPIE, Düsseldorf (Germany), 18 May 2016 and 15 Nov 2016

*M. Todorova* co-organized the 2$^{nd}$ German-Dutch Workshop on “Computational Materials Science” in Domburg (The Netherlands), 26 - 29 Jun 2016

*E. A. Jägle* organized the event “Alloys for Additive Manufacturing Workshop 2016” held at the MPIE in Düsseldorf (Germany) with 80 participants, 04 - 05 Jul 2016

*F. Roters* organized the 5$^{th}$ International Symposium on “Computational Mechanics of Polycrystals, CMCn 2016” and the “1$^{st}$ DAMASK User Meeting” held at the MPIE, Düsseldorf (Germany), 01 - 02 Sep 2016

*S. Brinckmann* co-organized the symposium „Tribology across length-scales: Experiments and simulations“ at the Materials Science Engineering in Darmstadt (Germany), 27 - 29 Sep 2016

*M. Rohwerder* organized the Symposium C06 “Metallic, Organic and Composite Coatings for Corrosion Protection” at the 230$^{th}$ Meeting of the Electrochemical Society - PRiME2016 in Hawaii (USA), Oct 2016

*T. Hickel and J. Neugebauer* organized the ADIS 2016 Workshop “Ab initio Description of Iron and Steel: Mechanical properties” at Ringberg Castle, Kreuth (Germany), 03 - 07 Oct 2016

*J. Neugebauer* co-organized the Symposium „Materials design: where condensed-matter physics and big-data informatics meet” at the MMM 2016 Conference in Dijon (France), 09 - 14 Oct 2016

*F. Roters* co-organized the Symposium “Microstructure evolution in materials: mechanisms, properties, manufacture” during the 8$^{th}$ International Conference on Multiscale Materials Modeling, Dijon (France), 09 - 14 Oct 2016

*J. Neugebauer* co-organized the Symposium “Design, Discovery, and Understanding of Materials Guided by Theory, Computation and Data Mining” at the MRS Fall Meeting 2016 in Boston (USA), 27 Nov - 02 Dec 2016

*K. Hübel, M. Rohwerder, C. Scheu and M. Todorova* organized the workshop “Status and Future Challenges in Characterisation of Interfaces for Electrochemical Applications - Part 1” at the MPIE, Düsseldorf (Germany), 05 Dec 2016

## 2017

*G. Dehm, C. Scheu,* and *S. Brinckmann* organized the “Mechanics meets Energy V” symposium at Ringberg Castle, Kreuth (Germany), 08 - 12 Jan 2017

*C. Scheu* organized the “Hydrogen Technology” Meeting at the MPIE, Düsseldorf (Germany), 25 Jan 2017

*T. Hickel* co-organized the Symposium “Advanced High-Strength Steels” at the TMS Meeting in San Diego (USA), 26 Feb - 2 Mar 2017

*J. Neugebauer* co-organized the Topical Session “Data driven materials design” at the Spring Meeting of the German Physical Society (DPG) in Dresden, 19 - 24 Mar 2017

*B. Gault* was Co-Chair at the “International workshop: high electric fields in electrochemistry and in atom probe tomography” at Ringberg Castle, Kreuth (Germany), 29 Mar - 1 Apr 2017

*M. Todorova, J. Neugebauer, S. Wippermann and G. Gault* organized the Workshop “High electric fields in electrochemistry and in atom probe tomography” at Ringberg Castle, Kreuth (Germany), 29 Mar - 1 Apr 2017

*S. Brinckmann* co-organized the „Frontiers in Material Science & Engineering: Hydrogen Interaction in Metals“ Workshop at the MPIE, 11 Apr 2017

*G. Dehm* co-organized the topic day “Lokale Charakterisierungsmethoden in der Werkstoffforschung“ at the Metallkundekolloquium/Arlbergkolloquium in Lech (Austria), 19 - 21 Apr 2017

*G. Dehm* co-organized the symposium “Mechanical Properties and Adhesion” at the 44th ICMCTF (International Conference on Metallurgical Coatings and Thin Films) in San Diego (USA), 24 - 28 April 2017

*T. Hickel* organized the “Fe-X French-German discussion meeting” at the MPIE, Düsseldorf (Germany), 15 - 16 May 2017

*K. Hübel, K. Mayrhofer, M. Rohwerder, C. Scheu and M. Todorova* organized the workshop “Status and Future Challenges in Characterisation of Interfaces for Electrochemical Applications - Part 2” at the MPIE, Düsseldorf (Germany), 16 Aug 2017

*G. Dehm* co-organized the symposium “Environmental, in-situ and time-resolved microscopy” at MC 2017 (Microscopy Conference 2017) in Lausanne (Switzerland), 21 - 25 Aug 2017

*S. Zaefferer and T. Griffiths* organized and chaired the workshop “3D Materials characterization on all length scales and its applications to iron and steel” held at the MPIE in Düsseldorf (Germany) with 75 participants, 29 Aug 2017

*M. Todorova* co-organized the CM - ICAMS Workshop in Ebernburg (Germany), 04 - 07 Sep 2017

*B. Gault* was Symposium Chair at the special symposium for the 50th Anniversary of the “Atom Probe, Microscopy & Microanalysis 2017” in Saint Louis (USA), 06 - 10 Sep 2017

*E. A. Jägle* co-organized the conference “Alloys for Additive Manufacturing Symposium 2017” with 120 participants, held at EMPA, in Dübendorf (Switzerland), 11 - 12 Sep 2017

*C. Kirchlechner* co-organized the “Summer School on Experimental Nano- and Micromechanics” at the MPIE, Düsseldorf (Germany), 11 - 15 Sep 2017

*M. Rohwerder* co-organized the Symposium C04 “Coatings and Inhibitors” at the 232nd Meeting of the Electrochemical Society in National Harbor (USA), Oct 2017

*M. Palm and F. Stein* co-organized the international conference “Intermetallics 2017” at the Educational Center Kloster Banz, Bad Staffelstein (Germany), 02 - 06 Oct 2017

*C. Scheu* organized the “100 year MPIE Anniversary Colloquium” at the MPIE, Düsseldorf (Germany), 5 Oct 2017

*B. Gault* was Co-Chair at the Biannual „NRW-APT User Meeting“ at the MPIE, Düsseldorf (Germany), 16 May 2017 and 23 Nov 2017

## 2018

*D. Raabe* chaired and *E. A. Jägle* coordinated the work group “Additive Manufacturing and 3D printing” of the National Academy of Sciences Leopoldina, 2018

*J. Janßen and J. Neugebauer* organized a 1st Pyiron-Workshop at the MPIE, Düsseldorf (Germany), 09 Jan 2018

*M. Todorova* co-organized the 3rd Austrian-German Workshop “Computational Materials Science on Complex Energy Landscapes” in Kirchdorf (Austria), 15 - 19 Jan 2018

*G. Dehm* co-organized the symposium “Fundamentals of mechanical response” at the “Conference on Electronic and Advanced Materials” in Orlando (USA), 17 - 19 Jan 2018

*C. Scheu* co-organized the symposium “Experimental and Theoretical insights on Interfaces of Ceramics” at the “Conference on Electronic and Advanced Materials” in Orlando (USA), 17 - 19 Jan 2018

*G. Dehm, C. Scheu,* and *S. Brinckmann* organized the “Mechanics meets Energy VI” symposium at Kloster Steinfeld, Kall (Germany), 29 Jan - 2 Feb 2018

*G. Dehm* co-organized the topic day “Dislocation based plasticity - experiment vs. simulation” at “The Schöntal Symposium Dislocation-based Plasticity” of the DFG Forschergruppe FOR 1650 in Schöntal (Germany), 25 Feb - 02 Mar 2018

*T. Hickel* co-organized the Symposium “Advanced High-strength Steels” at the TMS 2018 Annual Meeting & Exhibition in Phoenix (USA), 11-15 Mar 2018

*G. Dehm* co-organized the topical session “Mechanical Properties at Small Scales” at the DPG-Spring Meeting 2018 in Berlin, 11 - 16 Mar 2018

*T. Hickel* co-organized the Topical Session “Hydrogen in Materials” at the Spring Meeting of the German Physical Society (DPG) in Berlin (Germany), 11 - 16 Mar 2018

*T. Hickel* co-organized the Topical Session “Magnetism in Materials Science: Thermodynamics, Kinetics and Defects” at the Spring Meeting of the German Physical Society (DPG) in Berlin (Germany), 11 - 16 Mar 2018

*C. Kirchlechner* co-organized a session on “Experimental Nanomechanics” at the “16th European Mechanics of Materials Conference” in Nantes (France), 26 - 28 Mar 2018

*G. Dehm* co-organized the topic day “Novel materials and alloy design - microstructure property relationship” at the Metallkundekolloquium/Arlbergkolloquium in Lech (Austria), 09 - 11 Apr 2018

*J. Neugebauer* co-organized the “BigMax Workshop 2018” on “Big-Data-Driven Materials Science” in Kloster Irsee (Germany), 10 - 13 Apr 2018

*G. Dehm* co-organized the symposium “Mechanical Properties and Adhesion 45th ICMCTF” (International Conference on Metallurgical Coatings and Thin Films) in San Diego (USA), 23 - 27 Apr 2018

*T. Hickel* organized the “Fe-X French-German discussion meeting” at the MPIE, Düsseldorf (Germany) from 15 – 16 May 2017

*M. Herbig* organized a conference session of Correlative Methods at the Atom Probe Tomography & Microscopy conference in Washington (USA), 10 - 15 Jun 2018

*F. Roters* co-organized the Mini-Symposium “Computational modeling and experimental investigations of metallic materials across scales” during the 6th European Conference on Computational Mechanics in Glasgow (Scotland), 11 - 15 Jun 2018

*G. Dehm* co-organized the mini-symposium “Experimental Micromechanics and Nanomechanics” at the “10th edition of the European Solids Mechanics Conference” in Bologna (Italy), 02 - 06 Jul 2018

*G. Dehm* co-organized the Gordon Research Conference "Thin Film and Small Scale Mechanical Behavior" in Lewiston (USA), 15 - 20 Jul 2018

*C. Scheu co*-organized the symposium "PS12 - Materials for Energy Production, Storage and Catalysis" at the "19th International Microscopy Congress" in Sydney (Australia), 09 - 14 Sep 2018

*F. Roters* organized the 6th International Symposium on "Computational Mechanics of Polycrystals, CMC*n* 2018" and the "2nd DAMASK User Meeting" held at the MPIE, Düsseldorf (Germany), 17 - 19 Sep 2018

*R. Hadian* co-organized the Symposium "Predicting Interface Structure and Dynamics - From Atomic- to Meso-Scale" at the MSE 2018 Congress in Darmstadt, 26 - 28 Sep 2018

*S. Brinckmann* co-organized the symposium „Experiments and Simulations Towards Understanding Tribology Across Length-Scales" at the Materials Science Engineering in Darmstadt (Germany), 26 - 28 Sep 2018

*E. A. Jägle* co-organized the symposium "Additive Manufacturing - Composites and Complex Materials" at MS&T conference in Columbus (USA), Oct 2018

*M. Herbig* organized a MPIE Workshop 'Mechanisms of White Etching Matter Formation' held at the MPIE, Düsseldorf (Germany), 23 Oct 2018

*M. Kühbach and M. Diehl* organized the symposium "From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing" at the Multiscale Materials Modeling (MMM) conference in Osaka (Japan), 28 Oct - 02 Nov 2018

*T. Hickel* co-organized the Symposium „Data-Driven and Physics-Informed Materials Discovery and Design" at the 9th Multiscale Materials Modelling Conference (MMM 2018) in Osaka (Japan), 28 Oct - 02 Nov 2018

*T. Hickel and J. Neugebauer* organized the ADIS 2018 Workshop "Ab initio Description of Iron and Steel: Thermodynamics, Kinetics and Defects" at Ringberg Castle, Kreuth (Germany), 04 - 09 Nov 2018

*G. Dehm, B. Gault, D. Raabe and C. Scheu* organized the "Opening symposium for advanced (S)TEM and APT facilities" at the MPIE, Düsseldorf (Germany), 05 - 06 Nov 2018

*J. Neugebauer, S. Wippermann, E.Gattermann and R. Groever* organized the "Topical Joint Workshop IMPRS-SurMat & IMPRS RECHARGE about Catalysis and Corrosion: Towards an Atomistic Understanding of Reactions at Interfaces" at the MPIE, Düsseldorf (Germany), 20 Nov 2018

# Institute Colloquia and Invited Seminar Lectures

## 2016

*S. Biermann*, Centre de Physique Theorique, Ecole Polytechnique, France: Spectral Properties of Correlated Electron Materials from First Principles - Where Do We Stand? (07 Jan 2016)

*I. Eremin*, Institute for Theoretical Physics III, Ruhr-University Bochum, Germany: Superconductivity in Fe-based Superconductors: Competing Orders and Pairing Fluctuations (12 Jan 2016)

*O. Glushko*, Erich Schmid Institute of Materials Science, Leoben, Austria: Strain-induced Room Temperature Grain Coarsening: Side Effect or Major Energy Dissipation Mechanism? (14 Jan 2016)

*G. Hummer*, MPI for Biophysics, Frankfurt/Main, Germany: Extracting Accurate Free Energy Surfaces and Rates from Single-Molecule Pulling Experiments (18 Jan 2016, Colloquium)

*J. Haubrich*, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany: Ti-Interfaces for Aging-resistant Bonding between Metals and Thermoplastics (18 Jan 2016)

*T. F. Kelly*, Division Vice President for Innovation and New Technologies, CAMECA Instruments, Inc., Madison, WI, USA: Atomic-Scale Tomography: An Achievable Vision (29 Jan 2016)

*P. R. Rios*, Universidade Federal Fluminense, Rio de Janeiro, Brazil: Grain Boundary, Triple Junction and Quadruple Point Mobility Controlled Normal Grain Growth (01 Feb 2016)

*L. Dezerald*, Institut Jean Lamour, Université de Lorraine, Nancy, France: Plastic Anisotropy and Dislocation Glide in bcc Metals (03 Feb 2016)

*X. Fang*, Tsinghua University, Beijing, China: Stress and Diffusion Coupling during Oxidation at High Temperature (16 Feb 2016)

*A. Winkelmann*, Bruker Nano GmbH, Berlin, Germany: Applications of Dynamical Electron Diffraction Simulations in the SEM (10 Mar 2016)

*M. Gouné*, Métallurgie et Matériaux Fonctionnels, ICMCB-CNRS, France: New Insights into Alloying Elements Interaction with α-Ferrite/γ-Austenite Migrating Interface in Fe-C-Mn System (18 Mar 2016)

*F. Danoix*, Université de Rouen, France: Combined Atom Probe Tomography and Electron Microscopy Investigation of Intermediate Carbides Precipitation from Supersaturated Virgin Fe-Ni-C Martensites (07 Apr 2016)

*A. Ektarawong*, Department of Physics, Linköping University, Linköping, Sweden: Theoretical Study of Configurational Disorder in Boron Carbide Modeled by the Superatom-Special Quasirandom Structure Approach (11 Apr 2016)

*O. Gutfleisch*, TU Darmstadt, Germany: Re-thinking Rare Earth Magnets for Energy Applications: Demand, Sustainability and the Reality of Alternatives (12 Apr 2016, Colloquium)

*B.W.J. Clegg*, University of Cambridge, UK: Softening Non-Metallic Crystals by Inhomogeneous Elasticity (04 May 2016, Colloquium)

*A. Deschamps*, *Frederic De Geuser*, Grenoble Institute of Technology, France: Precipitation in Al-Alloys (04 May 2016)

*P. A. van Aken*, MPI for Solid State Research, Stuttgart, Germany: Structural Defects and Local Interfacial Chemistry of Complex Oxide Heterointerfaces (23 May 2016, Colloquium)

*P. Pant*, Indian Institute of Technology-Bombay, Mumbai, India: Role of Orientation and Grain Interactions on the Deformation of Ti64 (23 May 2016)

*U. Dahmen*, National Center for Electron Microscopy, Molecular Foundry, LBNL, Berkeley, CA, USA: Atomic Resolution Observations of Step Structure and Dynamics in Grain Boundaries (24 May 2016, Colloquium)

*I. Vrejoiu*, Institute of Physics II, University of Cologne, Germany: Driving Forces and Challenges of Interfacing Functional Oxide Perovskites (13 Jun 2016)

*S. Ahmadi*, University of Erlangen-Nuremberg, Germany: Stochastic KMC-FEM Modelling of Avalanche Phenomena in Creep Deformation of Bulk Metallic Glasses (14 Jun 2016)

*K. Lejaeghere*, Center for Molecular Modeling, Ghent University, Belgium: Error Overload? Dealing with DFT Uncertainty (14 Jun 2016)

*D. Blavette*, Normandie University, Rouen, France: Phase Transformations: Atom-Probe Tomography versus Modeling (23 Jun 2016, Colloquium)

*G. Kresse*, Faculty of Physics, University of Vienna, Austria: The Relation between RPA and GW - Forces and Singles (05 Jul 2016)

*M. Huang*, The University of Hong Kong, China: Deformation Mechanisms of TWIP Steel: From Micro-pillars to Bulk Samples (06 Jul 2016)

*C. C. Fu*, DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, France: Diffusion Mechanisms of Solutes in α-Iron Systems (08 Jul 2016)

*X. Maeder*, Empa, Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland: *In Situ* HR-EBSD Characterization during Micromechanical Testing (12 Jul 2016)

*M. Kabel*, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik (ITWM), Kaiserslautern, Germany: Composite Voxels for Nonlinear Mechanical Problems (21 Jul 2016)

*S. Singh*, MPI for Chemical Physics of Solids, Dresden, Germany: Nature and Origin of Structural Modulation in $Ni_2MnGa$ Magnetic Shape Memory Alloy (19 Jul 2016)

*M.Beetz*, Ludwig-Maximilians-University Munich, Germany: Parameter Analysis and Performance Improvement of Discrete Iterative Reconstruction Techniques in Electron Tomography (20 Jul 2016)

*K. Hameyer*, RWTH Aachen University, Germany: Magnetic Material Modeling for Numerical Simulation of Electrical Machines (22 Jul 2016)

*M. Zamanzade*, Saarland University, Germany: Environmental Effects on the Mechanical Properties of Metals (22 Jul 2016)

*M. Elhebeary*, University of Illinois at Urbana-Champaign, IL, USA: A Pull-to-Bend Testing Technique for Testing Single Crystal Silicon (03 Aug 2016)

*G. M. Stocks*, Materials Theory Group, Oak Ridge National Laboratory, TN, USA: Tuning Materials Properties through Extreme Chemical Complexity (24 Aug 2016, Colloquium)

*A. Linscheid*, Department of Physics, University of Florida, USA: From the Crystal Structure to the Superconducting $T_C$: The Role of First Principles Calculations in Computing Superconducting Properties of Real Materials (31 Aug 2016)

*L. Mädler*, Foundation Institute of Materials Science (IWT), Department of Production Engineering, University of Bremen, Germany: High-Throughput with Particle Technology (05 Sep 2016, Colloquium)

*N. Rolland*, Université de Rouen, France: Some New Ideas to Model Artefacts in Atom Probe Tomography: Application to 3D Reconstruction (08 Sep 2016)

*M. Schroeder,* Ruhr-University Bochum, Germany: Lattice Dynamics in Hybrid Perovskite $MAPbI_3$ (29 Sep 2016)

*M. Chandross*, Materials Science and Engineering Center, Sandia National Laboratories, Albuquerque, NM, USA: Linking Microstructural Evolution and Tribology in Metallic Contacts (30 Sep 2016)

*I. Baker*, Dartmouth College, Hanover, NH, USA: Microstructures and Mechanical Behavior of FeNiMnAl(Cr) Alloys (06 Oct 2016, Colloquium)

*H.-H. Heyn*, Norwegian University of Science and Technology, Trondheim, Norway: Molecular Dynamics Simulation of Nanoindentation of fcc and bcc Systems: Influence of Hydrogen and Vacancies (18 Oct 2016)

*K. Haenen*, Hasselt University, Belgium: Doping Induced Properties of Nanocrystalline CVD Diamond Films and Particles (08 Nov 2016, Colloquium)

*C. W. Sinclair*, The University of British Columbia, Vancouver, Canada: Predicting Solute Segregation Kinetics and Properties in Binary Alloys from a Dynamical Variational Gaussian Model (09 Nov 2016)

*O. Prymak*, Inorganic Chemistry and Center for Nanointegration Duisburg-Essen (CeNIDE), Germany: Investigation of Nanostructural Materials by means of X-Ray Powder Diffraction (16 Nov 2016)

*S. Kölling*, Technische Universiteit Eindhoven, The Netherlands: Disassembling Nanostructures Atom by Atom (17 Nov 2016)

*T. Wang*, Interdisciplinary Centre For Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany: Calculation of Phonon Scattering and Thermal Conductivity at Atomistic Scale (21 Nov 2016)

*M. Eberhart*, Molecular Theory Group, Colorado School of Mines, CO, USA: The Search for Charge Density Based Structure-Property Relationships (07 Dec 2016, Colloquium)

*I. MacLaren*, University of Glasgow, Scotland: Quantitative Analysis of Nanoscale Carbonitrides in High-Mn Steel (07 Dec 2016)

*D. G. Sangiovanni*, Interdisciplinary Centre For Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany and Department of Physics, Chemistry, and Biology (IFM), Linköping University, Linköping, Sweden: Mass Transport in Solid Crystals: Equilibrium and Accelerated Molecular Dynamics Investigations (07 Dec 2016)

## 2017

*O. Waseda*, MATEIS Lab. INSA de Lyon, France: Atomic Scale Investigation of Cottrell Atmospheres in Steel (09 Jan 2017)

*Y. Funakawa*, Head of the research department for automotive steel, JFE Steel Corporation, Chiyoda, Tokyo, Japan: NANO-HITEN - Development of High Strength Hot-rolled Sheet Steel Consisting of Ferrite and Nanometer-sized Carbides (19 Jan 2017)

*K. D. Molodov*, RWTH Aachen University, Germany: Plasticity in Magnesium: Twinning and Slip Transmission (23 Jan 2017)

*M. Hu*, RWTH Aachen University, Germany: Phonons beyond Lattice Vibration: From Intrinsic to Atomic Complexity (31 Jan 2017)

*A. Stukowski*, TU Darmstadt, Germany: From Large-scale Atomistic Simulations to Insights: Powerful Data Analysis and Transformation Tools (06 Feb 2017)

*S. Siebentritt*, University of Luxembourg, Belvaux, Luxembourg: Solar Cells, Defects and Recombination – News from CIGS (08 Feb 2017)

*W. Ludwig*, The European Synchrotron ESRF, Grenoble / MATEIS Lab. INSA de Lyon, France: Recent Developments in Synchrotron X-Ray Diffraction Imaging (10 Feb 2017)

*D. Dye*, Imperial College London, UK: Adventures in Alloys (10 Feb 2017)

*R. Woracek*, European Spallation Source ESS AB, Lund, Sweden: Probing the Meso- and Macroscale with Advanced Neutron Imaging Techniques (16 Feb 2017)

*V. Uhlenwinkel*, Institut für Werkstofftechnik, Bremen, Germany: Hot Gas Atomization of Glass Forming Alloys (23 Mar 2017)

*D. Trinkle*, University of Illinois at Urbana-Champaign, IL, US: Computing Mass Transport in Crystals: Theory, Computation, and Applications (27 Mar 2017, Colloquium)

*G. Richter*, MPI for Intelligent Systems, Stuttgart, Germany: Filamentary Growth of Magnetic and Alloy Nanowhiskers (28 Mar 2017)

*P. Schaaf*, TU Ilmenau, Germany: Complex Nanostructures and Nanocomposites for Plasmonic and Photonic Applications (04 Apr 2017, Colloquium)

*M. Leitner*, Physics Department, TU Munich, Germany: Experimental Determination of Vibrational Dynamics in the Solid State (05 Apr 2017)

*B. Cantor*, University of Bradford, UK: Multicomponent and High-Entropy Alloys (06 Apr 2017)

*B. Berkels*, RWTH Aachen University, Germany: Variational Image Processing for Electron Microscopy (12 Apr 2017)

*D. Lehmhus*, University of Bremen, Germany: Cellular Metals - from Aluminium Foams to Steel Matrix Syntactic Foams (19 Apr 2017)

*A. Bergman*, Department of Physics and Astronomy, Uppsala University, Sweden and CEA Saclay, France: Atomistic Spin Simulations beyond the Heisenberg Model (26 Apr 2017)

*A. Tehranchi*, EPFL Lausanne, Switzerland: Atomistic Study of Hydrogen Embrittlement (11 May 2017)

*M. G. Willinger*, Fritz-Haber-Institut der MPG, Berlin, Germany: The Dynamics of Active Metal Catalysts Revealed by *In Situ* Electron Microscopy (23 May 2017, Colloquium)

*J. A. Francis*, University of Manchester, UK: Phase Transformation Effects on Residual Stress Development in Welding (13 Jun 2017)

*K. Woll*, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany: Phase Transformations under Rapid Heating in Metallic Micro- and Nanolaminates (19 Jun 2017)

*K. Tschulik*, Ruhr-University Bochum, Germany: New Concepts in Electrochemistry – From Magnetic Structuring of Macroscopic Layers to Single Nanoparticle Analysis (28 Jun 2017, Colloquium)

*M. J. Demkowicz*, Department of Materials Science and Engineering, Texas A&M University, College Station, TX, USA: Some Methods and Applications of Data-driven Inference in Materials Science (29 Jun 2017, Colloquium)

*M. G. D. Geers*, Technische Universiteit Eindhoven, The Netherlands: Size Effects in Metals: On the Role of Internal Boundaries across the Scales (04 Jul 2017, Colloquium)

*S. Ishibash*, AIST, Tsukuba, Japan: Calculation of Positron States and Annihilation Parameters for Vacancy-type Defects (24 Aug 2017)

*M. Militzer*, University of British Columbia, Vancouver, Canada: Next Generation Phase Transformation Models for Advanced Low-carbon Steels (31 Aug 2017)

*K. Chattopadhyay*, Indian Institute of Science, Bangalore, India: Introducing High Temperature Intermetallic Eutectic as Potential Structural Materials (08 Sep 2017)

*A. Bagdasaryan*, Sumy State University, Sumy Oblast, Ukraine: Nitride Coatings based on High-Entropy Alloys (12 Sep 2017)

*N. Sridharan*, Oak Ridge National Labs, USA: Strain Induced Transformations and Additive Manufacturing - A Pathway to Develop Multiphase Materials (14 Sep 2017)

*L. Lilensten*, IRCP Institut de Recherche de Chimie Paris – CNRS-Chimie-Paristech, France: Complex Multicomponent Alloys: Coupled Structural and Mechanical Study of a bcc Model Alloy, and Possible Improvement Path (21 Sep 2017)

*U. Dahmen*, National Center for Electron Microscopy (NCEM), Berkeley, USA: Electron Microscopy of Atomic Structure and Mechanisms in Crystalline Interfaces (05 Oct 2017, 100 years MPIE anniversary colloquium)

*J. Cairney*, University Sydney, Australia: Nanometre-scale Materials Characterisation: New Applications and Techniques (05 Oct 2017, 100 years MPIE anniversary colloquium)

*C. Volkert*, University of Göttingen, Germany: Why So Much Friction? Probing Dissipation at the Nanoscale in Materials with Tailored Electronic and Phononic Degrees of Freedom (05 Oct 2017, 100 years MPIE anniversary colloquium)

*C. Schuh*, Massachusetts Institute of Technology (MIT), Boston, USA: How Grain Boundary Segregation Enables 3D Printing of Bulk Nanostructured Metals (05 Oct 2017, 100 years MPIE anniversary colloquium)

*M. Asta*, University Berkeley, USA: Computational Materials Science: an Enabling Framework for Accelerated Materials Discovery and Design (05 Oct 2017, 100 years MPIE anniversary colloquium)

*P. Gumbsch*, Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany: Triboanalytic and –simulation (05 Oct 2017, 100 years MPIE anniversary colloquium)

*F. Schüth*, Max-Planck-Institut für Kohlenforschung, Mühlheim a. d. Ruhr, Germany: Materials Challenges for a Hydrogen Economy (05 Oct 2017, 100 years MPIE anniversary colloquium)

*K. Mayrhofer*, Helmholtz-Institute Erlangen-Nürnberg for Renewable Energy, Erlangen, Germany: Dissolution of Noble Metals and Metal Oxide (05 Oct 2017, 100 years MPIE anniversary colloquium)

*L. Gránásy*, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary: Phase-field Modeling of Polycrystalline Structures: From Needle Crystals to Spherulites (10 Oct 2017, Colloquium)

*P. Junker*, Ruhr-University Bochum, Germany: Variational Methods in Material Modeling: Applications of Hamilton's Principle (10 Oct 2017)

*T. Hyodo*, Innovative Structural Materials Association (ISMA), Tokyo, Japan: Introduction to ISMA (16 Oct 2017)

*T. Murakami*, Kobe Steel LTD., Kobe, Japan: The Influence of Carbon Content Distribution in Retained Austenite on Elongation of TRIP Steel (16 Oct 2017)

*Y. Toji*, JFE Steel Co., Chiba, Japan: High Accuracy Determination of Carbon Content in Steel by FE-EPMA (16 Oct 2017)

*D. Gambino*, Department of Physics, Chemistry, and Biology (IFM), Linköping University, Sweden: Method Development for Defects in Magnetic Materials in the High Temperature Paramagnetic State (17 Oct 2017)

*S. V. Divinski*, Institute of Materials Physics, University of Münster, Germany: Diffusion and Segregation of Solutes in Grain Boundaries: From Pure Metals to High-Entropy Alloys (19 Oct 2017)

*P. Denis*, University of Ulm, Germany: Shear Bands in Metallic Glasses: What Are They, How to Find Them? (25 Oct 2017)

*R. E. Sanders, Jr.*, Chongqing University, China, and Novelis Global Research and Technology Center, Kennesaw, GA, USA: Application of Scientific Principles to Aluminium Automotive Sheet (06 Nov 2017)

*B. Appolaire*, Onera, CNRS, Chatillon, France: Insights into the Role of Mechanics on Diffusion-Controlled Phase Transformations using Phase Field Models (07 Nov 2017, Colloquium)

*M. Greiner*, Max-Planck Institute for Chemical Energy Conversion, Mülheim a. d. Ruhr, Germany: Combining Contemporary Methods for a Comprehensive Picture of Functional Materials (13 Nov 2017, Colloquium)

*P. Jenus*, Jožef Stefan Institute, Ljubljana, Slovenia: Synthesis and Characterization of Tungsten-based Composites for High-Temperature Applications (20 Nov 2017)

*S. Betzler*, University of Munich, Germany: Environmental Transmission Electron Microscopy Revealing the Effect of the Atmosphere on the Heat Induced Phase Transformation of Niobium Oxides (24 Nov 2017)

*L. Mädler*, Universität Bremen, Germany: High-Throughput with Particle Technology for Toxicology and Materials Discovery (29 Nov 2017, Reimar Lüst Lecture 2017)

*N. Le Biavan*, CNRS-CRHEA, Valbonne, France: Zinc Oxide Epitaxial Growth and Optoelectronic Applications (06 Dec 2017)

## 2018

*A. Schneider,* CEA Saclay, France: Interplay between magnetic and energetic properties in bcc Fe-Mn alloys from first principles (23 Jan 2018)

*C. Stephan-Scherb*, Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany: Early Stages of High Temperature Oxidation and Sulphidation Studied by Synchrotron X-Ray Diffraction and Spectroscopy (08 Feb 2018)

*B. Curtin*, Institute of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, Switzerland: Mechanism of Enhanced Ductility in Mg Alloys (21 Feb 2018, Colloquium)

*Y. Champion*, Univ. Grenoble Alpes, Grenoble, France: Nanoindentation for Investigating Dynamics of Shear Bands in Metallic Glasses (01 Mar 2018, Colloquium)

*B. Klaes*, University of Rouen, France: Towards a New 3D Imaging and Analysis Method of Punctual and Clusters Defects in Metals (13 Mar 2018)

*P. Chakraborty*, S. N. Bose National Centre for Basic Sciences, Kolkata, India: Effect of Hydrogen on Degradation Mechanism of Zirconium: A Molecular Dynamics Study (19 Mar 2018)

*M. Krüger*, Forschungszentrum Jülich, Institute for Energy and Climate Research, Jülich, Germany: High Temperature Materials - Recent Developments for Future Challenges (17 Apr 2018, Colloquium)

*M. T. McDowell*, Georgia Institute of Technology/ G. W. Woodruff School of Mechanical Engineering/ School of Materials Science and Engineering - Atlanta, Georgia, USA: *In Situ* Investigation of the Dynamic Evolution of Materials and Interfaces in Energy Storage Systems (19 Apr 2018, Colloquium)

*A. Shapeev*, Skoltech Innovation Center, Moscow, Russia: Machine-Learning Interatomic Potentials (25 Apr 2018)

*K. O'Keeffe*, Swansea University, UK: Quantum-Path-Sensitive Extreme Ultraviolet Interferometry (07 May 2018)

*J. Grin*, MPI for Chemical Physics of Solids, Dresden, Germany: Quantum Chemistry in Position Space and Chemical Bonding in Intermetallic Compounds (08 May 2018, Colloquium)

*A. Rollett*, Carnegie Mellon Univ., Pittsburgh, PA, USA: Additive Manufacturing, 3D Printing, Porosity and Synchrotron Experiments (14 May 2018)

*V. Schnabel*, ETH Zürich, Switzerland: Active Materials by Design: Self-healing Metals and Structural Color Sensors with a Thermal Memory (14 May 2018)

*R. Kirchheim*, Georg-August_Universität Göttingen, Germany: Changing the Interfacial Composition of Carbide and Oxide Precipitates and Its Effect on Hydrogen Trapping (15 May 2018)

*R. K. W. Marceau*, Deakin University, Geelong, Victoria, Australia: APT Studies of Carbon-related Materials (18 May 2018)

*M. Ghidelli*, Politecnico di Milano, Milano, Italy: Novel Multifunctional Thin Films with Superior Mechanical and Functional Properties: Advances in Synthesis and Characterization (05 Jun 2018)

*L. Stegbauer*, Northwestern University, Evanston, IL, USA: Learning from Nature: Investigation of the High-tech Hybrid Nanocomposites of the Chiton Tooth towards 3d-Printable Materials (05 Jun 2018)

*A. M. Hodge*, University of Southern California, Los Angeles, USA: From Nanometallic Multilayers to Nanostructures: Processes and Mechanisms (06 Jun 2018)

*D. Banerjee*, Indian Institute of Science, Bangalore, India: Transformations, Recrystallization, Microtexture Texture and Plasticity in Titanium Alloys (08 Jun 2018)

*K. Hata*, Nippon Steel & Sumito Metal Corporation (NSSMC), Japan: Reconstruction of Three-Dimensional Ferrite-Austenite Microstructure and Crystallographic Analysis in an Early Stage of Alpha-Gamma Phase Transformation in Fe-Mn-low C Alloy (15 Jun 2018)

*S. Fähler*, Leibniz Institute for Solid State and Materials Research (IFW), Dresden, Germany: Martensitic Microstructure: Modern Art or Science? (19 Jun 2018, Colloquium)

*V. Subramanya Sarma*, Indian Institute of Technology Madras, Chennai, India: Role of Grain Boundary Character on Hot Corrosion and Liquation Cracking in a Ni Base Superalloy and Austenitic Stainless Steel (22 Jun 2018)

*H. Edongue,* University of Yaounde I, Cameroon: One-dimensional Simulations of Electrical Properties of $CuIn_{1-x}Ga_xSe_2$ Single Crystal Photo-absorbers (27 Jun 2018)

*S. Roy*, Indian Institute of Technology, Kharagpur, India: Orientation Dependent Spheroidization Response and α-phase Texture Evolution during Sub β-transus Annealing of Ti-6Al-4V Alloy (04 Jul 2018)

*T. Frolov*, Lawrence Livermore National Laboratory, USA: Predicting Phase Behavior of Grain Boundaries with Evolutionary Algorithms and Machine Learning (09 Jul 2018)

*V. I. Levitas*, Iowa State University, Ames, IA, USA: Phase Field Approach to Phase Transformations, Dislocations, and Their Interaction at Nano- and Microscales (09 Jul 2018)

*U. Hangen*, Bruker Nano GmbH, Aachen, Germany: Streamlined Nanoindentation Workflow for Testing Steels and Alloys: From the Experiment to the Publishable Result (12 Jul 2018)

*T. Sasaki*, National Institute for Materials Science (NIMS), Tsukuba, Japan: Development of Bake-hardenable Wrought Magnesium Alloys for Automotive Body Panel Applications (23 Jul 2018)

*S. Freakley*, Cardiff Catalysis Institute, Cardiff University, Wales, UK: Heterogeneous Catalysis: Not Always Supported Metallic Nanoparticles (25 Jul 2018, Colloquium)

*A. Leineweber*, TU Bergakademie Freiberg, Germany: Iron Nitrides and Carbides: Phase Equilibria, Crystallography, and Phase Transformations (07 Aug 2018, Colloquium)

*T. R. Bieler*, Michigan State University, East Lansing, MI, USA: Quantification and Simulation of Slip Transfer across Grain Boundaries in Near-cube Oriented Aluminum and Mesoscale Elastic Strain Heterogeneity in Titanium (09 Aug 2018)

*T. Bereau*, Max Planck Institute for Polymer Research, Mainz, Germany: Multiscale Simulations of Soft Matter Augmented by Data-driven Methods (09 Aug 2018)

*J. Ast*, Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland: *In-situ* Deformation and Fracture Experiments at Variable Temperatures in the SEM (23 Aug 2018)

*A. Dollmann*, Karlsruhe Institute of Technology KIT, Germany: High Entropy Alloy CoCrFeMnNi under mild tribological load (30 Aug 2018)

*S. Maier*, RWTH Aachen, Germany: Thermoelectric energy conversion - From waste heat to sustainable energy (11 Sep 2018)

*V. Oliveira*, Federal University of Rio de Janeiro (UFRJ), Brazil: Use of Computational and Physical Simulation on Arc Welding Heat Affected Zone Microstructure Evolution Studies (11 Sep 2018)

*S. Suwas*, Indian Institute of Science, Bangalore, India: Deformation micro-mechanisms and texture evolution in microcrystalline and nanocrystalline FCC materials: The role of stacking fault energy (19 Sep 2018)

*D. Dini*, Imperial College London, UK: Exploring Surface Interactions at the Molecular Scale in Tribological Applications (25 Sep 2018)

*K. Hemker*, Department of Mechanical Engineering, Johns Hopkins University, Baltimore, MD, USA: Topological Optimization and Textile Manufacturing of 3D Lattice Materials (25 Sep 2018)

*S. Barcikowski*, Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany: Metal and Alloy Nanoparticles from Ultrafast, Scalable Laser Synthesis and their Downstream Integration in Catalysis and Additive Manufacturing (02 Oct 2018, Colloquium)

*S. K. Kim*, University of Science and Technology (UST) and Korea Institute of Industrial Technology (KITECH), South Korea: ECO-Almag with no trade-off of strength and ductility: a practical approach to achieve ultra-high strength and ductility (12 Oct 2018)

*C. Ophus*, NCEM, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, USA: Atomic Electron Tomography Using Coherent and Incoherent Imaging in (Scanning) Transmission Electron Microscopy (18 Oct 2018, Colloquium)

*K. M. Kareh*, Nature Communications, Nature Research, London, UK: How to publish in Nature-branded journals (18 Oct 2018)

*G. Jeffrey Snyder*, Northwestern University, Department of Materials Science and Engineering, Evanston, IL, USA: Complex Thermoelectric Materials (15 Nov 2018)

*A. Baldi*, DIFFER - Dutch Institute for Fundamental Energy Research, Eindhoven, The Netherlands: Hydrogen Storage in Single Metal Nanocrystals (29 Nov 2018, Colloquium)

# Lectures and Teaching at Universities

## 2015 (not included in the Scientific Report 2013 - 2015)

*D. Raabe,* RWTH Aachen: Micromechanics of Materials, WS 2015/2016

*M. Rohwerder,* Ruhr-Universität Bochum: Surface Science and Corrosion, WS 2015/2016

*F. Roters*, RWTH Aachen: ICME for Steels, WS 2015/2016

*F. Roters*, RWTH Aachen: Prozess- und Werkstoffsimulation, WS 2015/2016

*M. Valtiner,* Ruhr-Universität Bochum: Physical Chemistry (joint lecture with C. Morgenstern), WS 2015/2016

## 2016

*S. Brinckmann, R. Janisch*, Ruhr-Universität Bochum: Assessment and Description of Material Properties, WS 2016/17

*G. Dehm*, Ruhr-Universität Bochum: Mechanische Eigenschaften in kleinen Dimensionen, SS 2016

*G. Dehm, C. Liebscher*, Ruhr-Universität Bochum: Transmissionselektronenmikroskopie für Fortgeschrittene, WS 2016/2017

*H.-O. Fabritius,* TU München: Bioinspirierte Materialien und Prozesse, WS 2016/2017

*B. Grabowski*, Universität Paderborn: Computerphysik, WS 2016/2017

*T. Hickel*, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2016/2017

*J. Neugebauer*, Ruhr-Universität Bochum: Application and implementation of electronic structure methods, SS 2016

*J. Neugebauer*, Ruhr-Universität Bochum, IMPRS-SurMat Lecture: Ab Initio Description of Surfaces: Fundamentals and Applications, WS 2016/2017

*D. Raabe,* RWTH Aachen: Micromechanics of Materials, SS 2016

*D. Raabe,* RWTH Aachen: Micromechanics of Materials, WS 2016/2017

*M. Rohwerder,* Ruhr-Universität Bochum: Surface Science and Corrosion, WS 2016/2017

*F. Roters*, RWTH Aachen: Prozess- und Werkstoffsimulation, WS 2016/2017

*C. Scheu,* RWTH Aachen: Electron Microscopy and Analytical Techniques, WS 2016/2017

*H. Springer*, RWTH Aachen: Applied micromechanics: multiphase and composite material design, Jun 2016

*H. Springer*, RWTH Aachen: Micromechanics of Materials Design and micromechanics of metal matrix composites and high-throughput mechanical testing for alloy design, SS 2016

*S. Wippermann,* Universität Paderborn: Advanced Topics in Quantum Mechanics, WS 2016/2017

*S. Zaefferer,* Deakin University, Geelong, Australia: Textures, Microstructures and Microscopy, WS 2016/2017

*S. Zaefferer,* Fachhochschule Münster, Akademie für Elektronenmikroskopie: EBSD – Grundlagen und Anwendungen, Spring Course 2016

*S. Zaefferer, T. Hickel, U. Prahl*, RWTH Aachen: Microstructures, Microscopy and Modelling, SS 2016

## 2017

*S. Brinckmann, R. Janisch*, Ruhr-Universität Bochum: Assessment and Description of Material Properties, WS 2017/18

*G. Dehm*, Ruhr-Universität Bochum: Mechanische Eigenschaften in kleinen Dimensionen, SS 2017

*G. Dehm, C. Liebscher*, Ruhr-Universität Bochum: Transmissionselektronenmikroskopie für Fortgeschrittene, WS 2017/2018

*H.-O. Fabritius,* TU München: Bioinspirierte Materialien und Prozesse, WS 2017/2018

*B. Grabowski*, Universität Paderborn: Atomistic Materials Modeling, WS 2017/2018

*T. Hickel*, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2017/2018

*E. A. Jägle,* Indian Institute of Technology Roorkee, India: Microstructural Aspects of Additive Manufacturing, Workshop "Microstructural Aspects of Additive Manufacturing", Dec 2017

*J. Neugebauer*, Ruhr-Universität Bochum, Application and implementation of electronic structure methods, SS 2017

*D. Raabe*, Max-Planck-Institut für Eisenforschung, IMPRS-SurMat Lecture: „Dislocations and crystals, interfaces in materials" March 2017

*D. Raabe,* RWTH Aachen: Micromechanics of Materials, SS 2017

*D. Raabe,* RWTH Aachen: Micromechanics of Materials, WS 2017/2018

*M. Rohwerder,* Ruhr-Universität Bochum: Surface Science and Corrosion, WS 2017/2018

*M. Rohwerder,* Ruhr-Universität Bochum, IMPRS-SurMat Lecture: „UHV surface analytics", WS 2017/2018

*M. Rohwerder,* Ruhr-Universität Bochum, IMPRS-SurMat Lecture: "Corrosion", WS 2017/2018

*F. Roters,* RWTH Aachen, ICME for Steels, SS 2017

*F. Roters*, RWTH Aachen: Prozess- und Werkstoffsimulation, WS 2017/2018

*C. Scheu,* RWTH Aachen: Advanced Characterisation, SS 2017

*C. Scheu,* RWTH Aachen: Electron Microscopy and Analytical Techniques, WS 2017/2018

*M. Todorova,* Max-Planck-Institut für Eisenforschung, IMPRS-SurMat Lecture: Phase diagrams and Phase Transformations, SS 2017

*S. Wippermann,* Universität Paderborn: Advanced Topics in Quantum Mechanics, WS 2017/2018

*S. Wippermann,* Max-Planck-Institut für Eisenforschung, IMPRS-SurMat Lecture: "Atomic Structure and Surface Thermodynamics", Oct 2017

S. *Zaefferer,* Institute of Metals and Technology (IMT), Ljubljana, Slovenia: Textures, Microstructures and Microscopy, Winter Course 2017

*S. Zaefferer,* Fachhochschule Münster, Akademie für Elektronenmikroskopie: EBSD – Grundlagen und Anwendungen, Spring Course, 2017

*S. Zaefferer, T. Hickel, U. Prahl,* RWTH Aachen: Microstructures, Microscopy and Modelling, SS 2017

## 2018

*S. Brinckmann, R. Spatschek*, RWTH Aachen: Dislocation Dynamics (Software Tools for Integrated Computational Materials Design), SS 2018

*G. Dehm*, Ruhr-Universität Bochum: Mechanische Eigenschaften in kleinen Dimensionen, SS 2018

*G. Dehm, C. Liebscher*, Ruhr-Universität Bochum: Transmissionselektronenmikroskopie für Fortgeschrittene, WS 2018/2019

*T. Hickel*, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2018/2019

*T. Hickel*, Max-Planck-Institut für Eisenforschung, IMPRS-SurMat Lecture: Understanding phase stabilities and microstructure formation with finite temperature ab initio methods, Jun 2018

*J. Neugebauer*, Ruhr-Universität Bochum: Application and implementation of electronic structure methods, SS 2018

*D. Raabe,* RWTH Aachen: Micromechanics of Materials, SS 2018

*C. Scheu,* RWTH Aachen: Advanced Characterisation, SS 2018

*M. Rohwerder,* Ruhr-Universität Bochum: Surface Science and Corrosion, WS 2018/2019

*S. Zaefferer*, Fachhochschule Münster, Akademie für Elektronenmikroskopie: EBSD – Grundlagen und Anwendungen, Spring Course 2018

*S. Zaefferer, T. Hickel, W. Song,* RWTH Aachen: Microstructures, Microscopy and Modelling, SS 2018

*S. Zaefferer,* University of Teheran, Iran: Textures, Microstructures and Microscopy, Autumn Course 2018, Oct 2018

# Invited Talks at Conferences and Colloquia

## 2015 (not included in the Scientific Report 2013 - 2015)

Dehm, G.; Imrich, P. J.; Malyar, N.; Kirchlechner, C.: *Differences in deformation behavior of bicrystalline Cu micropillars containing different grain boundaries*. (Materials Science & Technology (MS&T 2015), symposium entitled "Deformation and Transitions at Grain Boundaries". Columbus, OH, USA. 2015-10-12 to 2015-10-16).

Dehm, G.; Zhang, Z.; Völker, B.: *Structure and strength of metal-ceramic interfaces: New insights by Cs corrected TEM and advances in miniaturized mechanical testing*. (Materials Science & Technology (MS&T 2015), symposium entitled "Structures and Properties of Grain Boundaries: Towards an atomic-scale understanding of ceramics". Columbus, OH, USA. 2015-10-12 to 2015-10-16).

Dehm, G.: *New insights into the mechanical behavior of interface controlled metals*. (Colloquium Materials Modelling, Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre (IMWF). Universität Stuttgart, Germany. 2015-11-12).

Dehm, G.: *Mikromechanik: lokale Einblicke in die mechanischen Eigenschaften von Materialien.* (Opening of the Christian Doppler Laboratory for Lifetime and Reliability of Interfaces in Complex Multi-Material Electronics „RELAB". Vienna, Austria. 2015-12-09).

Erbe, A.; Schneider, P.; Sarfraz, A.; Iqbal, D.: *Neue Ergebnisse zur Bildung und Wirkung klassischer und moderner Vorbehandlungen*. (Gfkorr Jahrestagung. Frankfurt am Main, Germany. 2015-11-03 to 2015-11-04).

Fabritius, H.-O.: *Photonische Strukturen in der Natur: Wie Lebewesen Licht manipulieren*. (Meilensteintreffen - BMBF Nachwuchsgruppe morPHOx. Universität Paderborn, Germany. 2015-12-16).

Grabowski, B.; Wippermann, S.; Glensk, A.; Hickel, T.; Neugebauer, J.: *Random phase approximation up to the melting point: The impact of anharmonicity and non-local many-body effects on the thermodynamics of Au.* (MISIS Workshop. Moscow, Russia. 2015-10-26 to 2015-10-30).

Grabowski, B.; Ma, D.; Körmann, F.; Neugebauer, J.; Raabe, D.: *Ab initio thermodynamics of the CoCrFeMnNi high entropy alloy: Importance of entropy contributions beyond the configurational one.* (ICAMS Seminar, Ruhr-Universität Bochum, Germany. 2015-11-12).

Grabowski, B.: *Modern materials design from first-principles: Recent progress and future prospects.* (Seminar, Imperial College London, UK. 2015-11-25).

Hickel, T.; Glensk, A.; Zendegani, A.; Körmann, F.; Grabowski, B.; Neugebauer, J.: *Ab-intio based assessment of the thermodynamic stability of Al-based intermetallic phases.* (Intermetallics conference. Kloster Banz, Germany. 2015-09-28 to 2015-10-02).

Hickel, T.; Bleskov, I.; Zhang, X.; Körmann, F.; Sandlöbes, S.; Neugebauer, J.: *Ab-initio based understanding of deformation mechanisms in high-Mn steels.* (International Workshop on "Electronic Structure Theory for the Accelerated Design of Structural Materials". Moscow, Russia. 2015-10-26 to 2015-10-30).

Hickel, T.; Glensk, A.; Duff, A.; Körmann, F.; Grabowski, B.; Neugebauer, J.: *Ab-initio description of thermodynamic properties of unaries: A progress report.* (Unary SGTE Meeting. Stockholm, Sweden. 2015-11-10).

Hickel, T.; Dutta, B.; Körmann, F.; Neugebauer, J.: *Coupling of magnetic and lattice degrees of freedom in bulk materials.* (P@N seminars, King's College. London, UK. 2015-11-11).

Hickel, T.: *Ab-initio basierte Methoden der mechanismen-orientierten Werkstoffentwicklung.* (8. Nano und Material Symposium Niedersachsen. Salzgitter, Germany. 2015-11-25 to 2015-11-26).

Hickel, T.; Dutta, B.; Glensk, A.; Körmann, F.; Grabowski, B.; Neugebauer, J.: *Understanding complex materials at finite temperatures by ab inito methods.* (MRS Fall meeting. Boston, MA, USA. 2015-11-29 to 2015-12-04).

Iqbal, D.; Erbe, A.: *Chemie der kathodischen Delamination – welche Bindung bricht?* (Sitzung des Gfkorr Arbeitskreises "Korrosionsschutz durch Beschichtungen". Frankfurt am Main, Germany. 2015-11-03 to 2015-11-04).

Jägle, E. A.: *Alloys for and by Laser Additive Manufacturing – the basic research perspective*. (2nd European Scientific Steel Panel – Metal Additive Manufacturing, Steel Institute VdEH. Düsseldorf, Germany. 2015-11-23).

Kirchlechner, C.; Imrich, P. J.; Völker, B.; Jaya, B. N.; Raghavan, R.; Harzer, T. P.; Dehm, G.: *Small Scale Mechanical Testing and its Impact on Materials' Applications*. (Keynote Lecture, 14th International Union of Materials Research Societies-International Conference on Advanced Materials. Jeju Island, South Korea. 2015-10-25 to 2015-10-29).

Körmann, F.; Grabowski, B.; Hickel, T.; Neugebauer, J.: *Temperature-dependent coupling of atomic and magnetic degree of freedom from first-principles*. (Electronic Structure Theory for the Accelerated Design of Structural Materials. Moscow, Russia. 2015-10-26 to 2015-10-30).

Kuzmina, M.; Wang, M.; Herbig, M.; Ponge, D.; Tasan, C. C.; Sandlöbes, S.; Raabe, D.: *Segregation engineering enables nanostructured bulk steels by confined martensite-to-austenite reversion*. (Asia Steel International Conference 2015 (Asia Steel 2015). Yokohama, Japan. 2015-10-05 to 2015-10-08).

Kuzmina, M.; Herbig, M.; Ponge, D.; Stoffers, A.; Sandlöbes, S.; Raabe, D.: *Nanostructuring metallic alloys through confined phase transformations*. (Colloquium Lecture - GDCh (Gesellschaft Deutscher Chemiker). Bielefeld, Germany. 2015-10-29).

Kuzmina, M.; Herbig, M.; Ponge, D.; Stoffers, A.; Sandlöbes, S.; Raabe, D.: *Atomic Scale Analysis of Interfaces: Gibbs Adsorption Revisited*. (Colloquium at Physics Department, Friedrich-Alexander-Universität Erlangen-Nürnberg. Erlangen, Germany. 2015-11-02).

Kuzmina, M.; Herbig, M.; Ponge, D.; Choi, P.-P.; Stoffers, A.; Sandlöbes, S.; Raabe, D.: *Segregation engineering enables nanostructured dual-phase laminates via solute decoration and phase transformation at lattice defects*. (Colloquium lecture at Department of Mechanical Engineering, Technische Universiteit Eindhoven, The Netherlands. 2015-11-26).

Liebscher, C.: *High Resolution (Scanning) Transmission Electron Microscopy*. (MPIE-DLR Workshop. German Aerospace Center (DLR) Cologne, Germany, 2015-10-26).

Lymperakis, L.; Neugebauer, J.: *Interplay of kinetics and thermodynamics of epitaxially grown wide bandgap semiconductors.* (10th Asian-European Conference on Plasma Surface Engineering. Jeju Island, Korea. 2015-09-20 to 2015-09-24).

Mayrhofer, K. J. J.: *Novel in situ in operando methods*. (66th Meeting of the International Society of Electrochemistry, Symposium “Novel in situ in operando methods”. Taipei, Taiwan. 2015-10-04 to 2015-10-09).

Neugebauer, J.: *Towards automated toolsets for computing high-precision free energies by ab initio approaches*. (Materials Science & Technology (MS&T 205). Columbus, OH, USA. 2015-10-04 to 2015-10-08).

Neugebauer, J.: *Design of structural materials by ab initio guided multiscale simulations*. (CMRI Symposium. Sendai, Japan. 2015-10-13 to 2015-10-14).

Neugebauer, J.: *Stand ICMPE in Wissenschaft und Industrie*. (VDI-GME Werkstoffdialog. Maria Laach, Germany. 2015-10-16).

Neugebauer, J.: *Mastering the structural and thermodynamic complexity of modern materials*. (ESTADSM Conference. Moskau, Russia. 2015-10-25 to 2015-10-30).

Neugebauer, J.: *Materials design and discovery on the computer: Prospects and challenges*. (Colloquium at Universität Braunschweig, Germany. 2015-12-15).

Scheu, C.: *Dewetting of epitaxial Al thin films on (0001) single crystalline sapphire substrates*. (Materials Science & Technology (MS&T 2015). Columbus, OH, USA. 2015-10-04 to 2015-10-08).

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Brinckmann, S.: *Multiscale Simulations of Microstructure Evolution*. (Fracture & Fatigue, Mikromechanische Materialmodellierung. Technischen Universität Bergakademie Freiberg, Germany. 2016-05).

Cereceda, D.; Diehl, M.; Roters, F.; Raabe, D.; Marian, J.: *Unraveling the temperature dependence of the yield strength in BCC metals from atomistically-informed crystal plasticity calculation*. (Dislocations 2016, Purdue University. West Lafayette, IN, USA. 2016-09-19 to 2016-09-23).

Dehm, G.: *Unexpected stress induced martensite formation in ultra-strong pearlitic steel*. (TMS 2016, Symposium: Advanced Characterization Techniques for Quantifying and Modeling Deformation. Nashville, USA, 2016-02-14 to 2016-02-18).

Dehm, G.: *Deformation and Adhesion of Metallic Thin Films*. (International Conference on Metallurgical Coatings and Thin Films, 43rd ICMCTF. San Diego, CA, USA. 2016-04-25 to 2016-04-29).

Dehm, G.: *Mechanically driven martensite formation in ultra-strong pearlitic steel*. (Thermec 2016. Graz, Austria. 2016-05-29 to 2016-06-03).

Dehm, G.: *Stability of nanocrystalline metals: Cu-Cr as a case study*. (PICS meeting. Marseilles, France. 2016-06-14 to 2016-06-17).

Dehm, G.: *Mechanical Testing at Microscopic Length Scale*. (EMMC 15 - 15th European Mechanics of Materials Conference. Brussels, Belgium. 2016-09-07 to 2016-09-09).

Dehm, G.: *Resolving the interplay of nanostructure and mechanical properties by advanced electron microscopy*. (MSE Conference, Materials Science and Engineering. Darmstadt, Germany. 2016-09-27 to 2016-09-29).

Dehm, G.; Harzer, T. P.; Dennenwaldt, T.; Freysoldt, C.; Liebscher, C.: *Chemical demixing and thermal stability of supersaturated nanocrystalline CuCr alloys: Insights from advanced TEM*. (Materials Science & Technology (MS&T 2016). Salt Lake City, UT, USA. 2016-10-23 to 2016-10-27).

Dehm, G.: *Fracture testing of thin films: insights from synchrotron XRD and micro-cantilever experiments*. (2016 MRS Fall Meeting. Boston, MA, USA. 2016-11-27 to 2016-12-02).

Diehl, M.; Cereceda, D.; Wong, S. L.; Reuber, J. C.; Roters, F.; Raabe, D.: *From Phenomenological Descriptions to Physics-based Constitutive Models EPSRC Workshop on Multiscale Mechanics of Deformation and Failure in Materials*. (EPSRC Workshop on Multiscale Mechanics of Deformation and Failure in Materials. Aberdeen, Scotland. 2016-11-23).

Diehl, M.; Shanthraj, P.; Reuber, J. C.; Cereceda, D.; Wong, S. L.; Eisenlohr, P.; Roters, F.; Raabe, D.: *DAMASK - the Düsseldorf Advanced Material Simulation Kit Engineering of Advanced Materials*. ("Engineering of Advanced Materials: Numerische Optimierung basierend auf Vorhersagemodellen" Meeting. Erlangen, Germany. 2016-12-20).

Djaziri, S.; Li, Y.; Goto, S.; Raabe, D.; Dehm, G.: *Unexpected Stress Induced Martensite Formation in Ultra-strong Pearlitic Steel*. (TMS 2016, Symposium: Advanced Characterization Techniques for Quantifying and Modeling Deformation. Nashville, TN, USA. 2016-02-14 to 2016-02-18).

Duarte, M. J.: *Chemical analysis at the atomic scale: increasing our knowledge of the materials behavior*. (Talk at CINVESTAV-Unidad Queretaro. Queretaro, Mexico. 2016-03-15).

Duarte, M. J.; Kostka, A.; Crespo, D.; Dehm, G.; Springer, H.; Aparicio-Fernández, R.; Renner, F. U.: *Tailoring microstructures from amorphous precursors: crystallization and corrosion in Fe-based amorphous alloys*. (EMN Meeting on Metallic Glasses 2016. Kuala Lumpur, Malaysia. 2016-09-12 to 2016-09-16).

Fabritius, H.-O.; Schwind, B.; Wu, X.: *Broadband reflecting fibers with tailored structures inspired by desert ants*. (SPP 1839 Kick-off and Networking Meeting, Wilhelm-Conrad-Roentgen Campus (Bessy II). Berlin, Germany. 2016-02-26).

Fabritius, H.-O.; Enax, J.; Wu, X.: *Structure-property relations in biological composite materials: An inspiration source for synthetic materials*. (8th Indo-German Frontiers of Engineering Symposium 2016, Alexander von Humboldt Foundation. Potsdam, Germany. 2016-05-19 to 2016-05-22).

Gault, B.; De Geuser, F.: *A perspective on the ion projection in field ion & atom probe microscopy*. (Atom Probe Tomography & Microscopy 2016. Gyeongju, South Korea. 2016-06-12 to 2016-06-17).

Gault, B.; Herbig, M.; Liebscher, C.; Kuzmina, M.; Dehm, G.; Mayer, J.; Ponge, D.; Scheu, C.; Stoffers, A.; Sandlöbes, S.; Neugebauer, J.; Raabe, D.: *Defect Segregation studied by Correlative Atom Probe Tomography and Electron Microscopy*. (Japan-Germany Joint Symposium on Advanced Characterization of Nanostructured Materials for Energy and Environment. Düsseldorf, Germany. 2016-06-29).

Gault, B.: *Full determination of 3D atomic position by combining APT & EM*. (Scientific Directions for Future TEM, Forschungszentrum Jülich, Germany. 2016-07).

Gault, B.; Herbig, M.; Povstugar, I.; Liebscher, C.; Kuzmina, M.; Cojocaru-Mirédin, O.; Dehm, G.; Nematollahi, G. A.; Ponge, D.; Scheu, C.; Stoffers, A.; Sandlöbes, S.; Neugebauer, J.; Raabe, D.: *Atoms, ions, electrons: simulated, measured and manipulated*. (Workshop on Scientific Directions for Future Transmission Electron Microscopy. Jülich, Germany. 2016-07-13 to 2016-07-15).

Gault, B.; Katnagallu, S.: *Atom probe microscopy: a new playground for big data analysis?* (Workshop Big-Data-Driven Materials Science. Ringberg Castle, Kreuth, Germany. 2016-07-27 to 2016-07-30).

Gault, B.; Herbig, M.; Stoffers, A.; Yao, M.; Cojocaru-Mirédin, O.; Liebscher, C.; Raabe, D.: *Correlative Atom Probe Microscopy: Recent Progress and Possibilities*. (European APT Workshop. St Catherine College, Oxford, UK. 2016-09-21 to 2016-09-23).

Gault, B.; Stoffers, A.; Cojocaru-Mirédin, O.; Liebscher, C.; Li, Y.; Herbig, M.; Raabe, D.: *Materials for energy generation probed at the nanoscale*. (European Energy Resarch Alliance Conference 2016, EERA. Birmingham, UK. 2016-11-24 to 2016-11-25).

Grabowski, B.: *Modern materials design from first-principles: Recent progress and future prospects*. (Spring Meeting of the German Physical Society (DPG ). Regensburg, Germany. 2016-03-07 *to 2016-03-11*).

Grabowski, B.: *Entwicklung von quantenmechanischen Simulationsmethoden für das Design moderner metallischer Werkstoffe*. (Seminar, Universität Paderborn, Germany. 2016-05-09).

Grabowski, B.; Rogal, L.; Körmann, F.: *Discovery of an ordered hexagonal superstructure in an Al-Hf-Sc-Ti-Zr high entropy alloy.* (Seminar, University of Münster, Germany. 2016-07-12).

Hadian, R.*: Grain boundary dynamics* (Seminar, Imperial College London, Thomas-Young Center. London, UK. 2016-11-03).

Herbig, M.; Kuzmina, M.; Haase, C.; Molodov, D. A.; Marceau, R. K. W.; Gutiérrez-Urrutia, I.; Goto, S.; Zaefferer, S.; Choi, P.-P.; Raabe, D.: *Measurement of grain boundary chemistry and crystallography by atom probe tomography and correlated electron microscopy*. (Thermec 2016. Graz, Austria. 2016-05-29 to 2016-06-03).

Herbig, M.: *Investigation of Segregation Phenomena in Steels by Correlative Transmission Electron Microscopy and Atom Probe Tomography*. (International Conference on Atom Probe Tomography & Microscopy 2016. Gyeongju, South Korea. 2016-06-12 to 2016-06-17).

Herbig, M.: *How correlative transmission electron microscopy and atom probe tomography could benefit from a 3D nanobeam diffraction orientation mapping technique*. (Workshop on Scientific Directions for Future Transmission Electron Microscopy. Forschungszentrum Jülich, Germany. 2016-07-14 to 2016-07-16).

Herbig, M.: *Joint Characterization of Crystallography and Chemistry on the Nanometer Scale by Correlative Electron Microscopy and Atom Probe Tomography*. (Interdisciplinary Symposium on 3D Microscopy. Congress Center, Les Diablerets. Switzerland. 2016-10-18 to 2016-10-21).

Hickel, T.; Dutta, B.; Glensk, A.; Körmann, F.; Grabowski, B.; Neugebauer, J.: *Ab initio predicted phase stabilities of complex materials at finite temperatures.* (Materials Chain Conference. Bochum, Germany. 2016-05-30 to 2016-06-01).

Hickel, T.; Glensk, A.; Nazarov, R.; Dey, P.; Puchakayala, A.; Grabowski, B.; Neugebauer, J.: *Ab initio thermodynamics of point defects in metals: Hydrogen, vacancies and their interaction.* (2nd International Workshop on Models and Data for Plasma-Materials Interaction in Fusion Devices. Loughborough, UK. 2016-06-22 to 2016-06-24).

Hickel, T.; Mrovec, M.; DiStefano, D.; Elsässer, C.; McEniry, E.; Nazarov, R.; Neugebauer, J.: *New Insights into H trapping and Diffusion in Metallic Microstructures Obtained from Atomistic Simulations.* (2016 International Hydrogen Conference. Jackson Lake Lodge, Moran, USA. 2016-09-11 to 2016-09-14).

Hickel, T.; Zhang, X.; Rogal, J.; Neugebauer, J.: *The role of interfaces for structural transformations among austenite, ferrite and cementite in steels.* (Seminar on occasion of the 25th anniversary of OCAS research centre Gent, Belgium. 2016-10-27).

Hickel, T.; Dutta, B.; Körmann, F.; Zhang, X.; Sözen, H.; Neugebauer, J.: *Coupling of magnetic and lattice degrees of freedom in ab initio materials design. (Physics Seminar, Warwick, UK. 2016-12-01).*

Jägle, E. A.: *Precipitation Reactions in Age-Hardenable Alloys During Laser Additive Manufacturing*. (Seminar, EMPA (Eidgenössische Materialprüfungs- und Forschungsanstalt). Dübendorf, Switzerland. 2016-02-05).

Jägle, E. A.: *Alloys for Laser Additive Manufacturing: general considerations and precipitation reactions*. (Seminar, Institut für Werkstoff-Forschung, DLR Köln 2016. Köln, Germany. 2016-03-21).

Jägle, E. A.: *Small variations in powder composition lead to strong differences in part properties*. (Alloys for Additive Manufacturing Workshop 2016. Düsseldorf, Germany. 2016-07-05).

Jägle, E. A.: *Alloy design for Additive Manufacturing*. (DARE Annual Workshop 2016. University of Sheffield, UK. 2016-09-02).

Jägle, E. A.: *Atomsondentomographie - Chemische Analyse von Grenzflächen mit sub-nm Auflösung*. (19. Arbeitstagung Angewandte Oberflächenanalytik, Fraunhofer-Institut AWZ. Soest, Germany. 2016-09-06).

Jägle, E. A.: *Alloys for Additive Manufacturing*. (Research Seminar, Voestalpine Additive Manufacturing Research Center. Düsseldorf, Germany. 2016-09-23).

Jägle, E. A.: *Alloys for Additive Manufacturing*. (Verfahrenstechnisches Kolloquium, Universität Bremen, Germany. 2016-10-20).

Jägle, E. A.: *Hot cracking in SLM-produced Inconel 738LC: origins and remedy*. (Materials Science and Technology 2016. Salt Lake City, UT, USA. 2016-10-26).

Jägle, E. A.: *Phase transformations in alloys produced by Laser Additive Manufacturing*. (Spezialseminar, Fakultät für Werkstoffwissenschaft und Werkstofftechnologie, TU Bergakademie Freiberg, Germany. 2016-11-02).

Jägle, E. A.: *Phase transformation phenomena in additively produced alloys*. (Werkstoffkolloquium 2016, Deutsches Zentrum für Luft- und Raumfahrt Köln, Germany. 2016-12-06).

Kirchlechner, C.; Malyar, N.; Imrich, P. J.; Dehm, G.: *X-ray µLaue diffraction to understand plasticity at interfaces*. (Spring Meeting of the German Physical Society (DPG ), Regensburg, Germany. 2016-03-06 to 2016-03-11).

Kirchlechner, C.: *Synchrotron based µLaue diffraction to probe plasticity at interfaces*. (IRSP 2016, 14th International Conference Reliability and Stress-Related Phenomena in Nanoelectronics – Experiment and Simulation. Dresden, Germany. 2016-05-30 to 2016-06-01).

Kirchlechner, C.; Malyar, N.; Dehm, G.: *Insights into dislocation grain-boundary interaction by X-ray µLaue diffraction*. (Dislocations 2016. West Lafayette, IN, USA. 2016-09-19 to 2016-09-23).

Kirchlechner, C.: *What can you learn from a µLaue experiment?* (8th International Conference on Multiscale Materials Modeling - MMM 2016. Dijon, France. 2016-10-09 to 2016-10-14).

Kirchlechner, C.: *Brillantes Licht für unser Leben*. (KopfSalat - zu Gast bei Max Planck, MPI für Eisenforschung. Düsseldorf, Germany. 2016-10-20).

Körmann, F.; Grabowski, B.; Hickel, T.; Neugebauer, J.: *Lattice excitations in magnetic alloys: Recent advances in ab initio modeling of coupled spin and atomic fluctuations*. (TMS 2016. Nashville, TN, USA. 2016-02-14 to 2016-02-18).

Körmann, F.; Alling, B.; Grabowski, B.; Dutta, B.; Hickel, T.; Neugebauer, J.: *Parameter-free Computational Design of Magnetic Materials – Recent Advances in Ab Initio Techniques of Coupled Lattice and Spin Fluctuations*. (MRS Fall Meeting 2016. Boston, MA, USA. 2016-11-26 to 2016-12-02).

Kuzmina, M.; Gault, B.; Herbig, M.; Ponge, D.; Sandlöbes, S.; Raabe, D.: *From grains to atoms: ping-pong between experiment and simulation for understanding microstructure mechanisms*. (Res Metallica Symposium, Department of Materials Engineering, KU Leuven, The Netherlands. 2016-05-11).

Li, Z.; Raabe, D.; Ponge, D.; Springer, H.; Tasan, C. C.; Sandlöbes, S.: *Designing and understanding novel alloys towards superior properties*. (2016 European Workshop on Materials Design. Grenoble, France. 2016).

Liebscher, C.: *Complex Alloys down to atomic resolution*. (Materials Day. Ruhr-Universität Bochum, Germany. 2016-10-25).

Liebscher, C.: *Correlative atomic resolution STEM and atom probe tomography*. (Workshop on Scientific Directions for Future Transmission Electron Microscopy. Jülich, Germany. 2016-10-25).

Liebscher, C.: *Atomic structure of complex engineering materials and interfaces.* (Seminar Engineering Alloys Group, Imperial College, UK. 2016-11-16).

Lymperakis, L.: *Epitaxial Growth of III-Nitrides: Insights from Density Functional Theory Calculations.* (Seminar, Physics Department, University of Crete, Greece. 2016-07-21).

Lymperakis, L.; Freysoldt, C.; Schulz, T.; Maisel, S.; Albrecht, M.; Neugebauer, J.: *Ordering Phenomena in InGaN Alloys – An Ab-Initio Thermodynamics Study*. (International Workshop on Nitride Semiconductors (IWN 2016). Orlando, FL, USA. 2016-10-02 to 2016-10-07).

Marx, V. M.; Palm, M.: *The wet and hot corrosion behavior of iron aluminides*. (THERMEC 2016 – Int. Conf. on Processing & Manufacturing of Advanced Materials. Graz, Austria. 2016-05-29 to 2016-06-03).

Mayrhofer, K. J. J.: *In-situ investigation of catalyst degradation*. (Keynote Lecture, 18th Topical Meeting of the International Society of Electrochemistry. Gwangju, South Korea. 2016-03-08 to 2016-03-11).

Mayrhofer, K. J. J.: *Electrochemical Energy Conversion – the key for sustainable utilization of solar energy*. (Keynote Lecture, Integration of Sustainable Energy Conference (iSEneC). Nürnberg, Germany. 2016-07-11 to 2016-07-12).

Neugebauer, J.*: Mechanical properties and finite temperatures.* (CECAM Conference Lausanne. Switzerland, 2016-01-25 to 2016-01-27).

Neugebauer, J.: *Describing Hydrogen Embrittlement by ab initio guided multiscale modeling – status, perspectives and challenges.* (I²CNER Annual Symposium: Computational Solutions to Fundamental Problems in Carbon-Neutral Energy Research. Fukuoka, Japan. 2016-02-01 to 2016-02-02).

Neugebauer, J.; Glensk, A.; Grabowski, B.; Hickel, T.; Körmann, F.: *Ab Initio thermodynamics: Understanding the fundamental mechanisms behind H embrittlement in metals: An ab initio guided multiscale approach.* (Hydrogenius Workshop. Fukuoka, Japan. 2016-02-03 to 2016-02-04).

Neugebauer, J.: *Understanding the fundamental mechanisms behind H embrittlement in metals: An ab initio guided multiscale approach.* (Joint Hydrogenius and I²CNER International Workshop on Hydrogen-Materials Interactions. Kyushu University, Fukuoka, Japan. 2016-02-04).

Neugebauer, J.; Glensk, A.; Grabowski, B.; Hickel, T.: *Inclusion of Phonon-Phonon and Magnon-Phonon couplings in the thermodynamic description of materials: An ab initio approach.* (Hume-Rothery Award Symposium, TMS 2016. Nashville, TN, USA. 2016-02-14 to 2016-02-19).

Neugebauer, J.*: The digital transformation in Materials Science from a Modellers Perspective.* (VDI Workshop „Digitale Transformation in der Werkstofftechnik". Düsseldorf, Germany. 2016-02-24).

Neugebauer, J.: *Database concepts and ICME links for atomistic simulations.* (Plenary talk, 2nd International Workshop on Software Solutions for Integrated Computational Materials Engineering ICME 2016. Barcelona, Spain. 2016-04-12 to 2016-04-15).

Neugebauer, J.; Grabowski, B.; Hickel, T.; Ruban, A.V.; Gong, Y.; Reed, R.C.; Koermann, F.: *Ab initio determination of lattice stabilities and comparison to CALPHAD.* (Plenary talk, CALPHAD XLV Conference. Awaji Island, Japan. 2016-05-29 to 2016-06-03).

Neugebauer, J.: *Hydrogen embrittlement research at the MPIE. (Max-Planck-Institut für Eisenforschung).* (SNEAC Workshop Environmental Assisted Cracking. Trondheim, Norway. 2016-06-08 to 2016-06-10).

Neugebauer, J.: *HPC-Based Quantum Mechanical Design of Engineering Materials.* (Exascale Computing Workshop during ICS 2016. Frankfurt, Germany. 2016-06-19 to 2016-06-23).

Neugebauer, J.: *Ab initio description of defects in materials under extreme conditions.* (2016 Joint ICTP-CAS-IAEA School and Workshop on Plasma-Material Interaction in Fusion Devices. Hefei, China. 2016-07-18 to 2016-07-22).

Neugebauer, J.: *Stahl: Wie ein alter Werkstoff sich immer wieder neu erfindet und damit Wissenschaft und Wirtschaft beflügelt.* (Plenary talk, 129. Versammlung der Gesellschaft der deutschen Naturforscher und Ärzte. Greifswald, Germany. 2016-09-09 to 2016-09-12).

Neugebauer, J.; Glensk, A.; Körmann, F.; Grabowski, B.; Hickel, T.: *Ab initio thermodynamic description of advanced structural materials: Status and challenges.* (Plenary talk, Workshop "Ab-initio Based Modeling of Advanced Materials". Yekaterinburg, Russia. 2016-09-22 to 2016-09-24).

Neugebauer, J.; Glensk, A.; Grabowski, B.; Hickel, T.: *Modelling structural materials in extreme environments by ab initio guided multiscale simulations.* (International Workshop "Theory and Modelling of Materials in Extreme Environment". Abingdon, UK. 2016-09-25 to 2016-09-28).

Neugebauer, J.: *Collective variable description of crystal anharmonicity.* (IPAM Workshop II: Collective Variables in Classical Mechanics. Los Angeles, CA, USA. 2016-10-24 to 2016-10-28).

Neugebauer, J.; Glensk, A.; Grabowski, B.; Hickel, T.: *Point Defects at Finite Temperatures.* (Bunsen Colloquium - Defects and Diffusion in Solids. RWTH Aachen, Germany. 2016-11-10 to 2016-11-11).

Neugebauer, J.; Todorova, M.: *Solvent-controlled single atom dissolution, surface alloying and Wulff shapes of nanoclusters; Electrocatalysis at electrocodes in the dry.* (RESOLV Workshop Research Area III, ZEMOS. Bochum, Germany. 2016-11-24).

Palm, M.: *Development and processing of advanced iron aluminide alloys for application at high temperatures*. (62. Metallkunde Kolloquium. Lech am Arlberg, Austria. 2016-04-11 to 2016-04-13).

Ponge, D.; Sandlöbes, S.; Millán, S. J.; Choi, P.-P.; Wang, M.; Inden, G.; Dmitrieva, O.; Kuzmina, M.; Herbig, M.; Raabe, D.: *Segregation engineering in medium manganese steels*. (Workshop Integrated Computational Grain Boundary Engineering: The role of segregation. Graz, Austria. 2016-05-29).

Ponge, D.; Kuzmina, M.; Sandlöbes, S.; Herbig, M.; Raabe, D.: *Austenite formation along dislocations in medium manganese steels*. (Thermec 2016, Intl. Conf. on Processing & Manufacturing of Advanced Materials. Graz, Austria. 2016-05-29 to 2016-06-03).

Ponge, D.; Roters, F.; Diehl, M.; Shanthraj, P.; Herbig, M.; Tasan, C. C.; Raabe, D.: *Integrated experimental and simulation analysis of lattice defects and micromechanics in steels*. (Materials Modeling Colloquium, Universität Stuttgart, Germany. 2016-06-23).

Ponge, D.; Gault, B.; Herbig, M.; Liebscher, C.; Kuzmina, M.; Dehm, G.; Welsch, E. D.; Yao, M.; Hickel, T.; Li, Z.; Tasan, C. C.; Neugebauer, J.; Scheu, C.; Stoffers, A.; Sandlöbes, S.; Raabe, D.: *Chemo-Mechanics at Lattice Defects: from Mechanisms to Bulk Alloys*. (Gordon Research Conference on Thin Film & Small Scale Mechanical Behavior. Lewiston, ME, USA. 2016-07-24 to 2016-07-29).

Ponge, D.; Wang, M.; Dutta, A.; Kwiatkowski da Silva, A.; Sandlöbes, S.; Millán, S. J.; Choi, P.-P.; Tasan, C. C.; Leyson, G. P. M.; Inden, G.; Dmitrieva, O.; Kuzmina, M.; Herbig, M.; Raabe, D.: *Austenite Reversion in Medium Manganese Steels*. (The 3rd International Conference on High Manganese Steels. Chengdu, China. 2016-11-16 to 2016-11-18).

Ponge, D.; Kuzmina, M.; Herbig, M.; Sandlöbes, S.; Raabe, D.: *Segregation and Austenite Reversion at Dislocations in a Binary Fe–9%Mn Steel Studied by Correlative TEM-atom Probe Tomography.* (The 3rd International Conference on High Manganese Steels. Chengdu, China. 2016-11-16 to 2016-11-18).

Raabe, D.: *Materials Engineering through the Ages: from the Battle of Kadesh to Atomic Scale Materials Design*. (Elite Network of Bavaria (ENB) Forum in Erlangen: Focus on Materials Engineering. Erlangen, Germany. 2016-05-30).

Raabe, D.; Choi, P.-P.; Gault, B.; Ponge, D.; Yao, M.; Herbig, M.: *Segregation engineering for self-organized nanostructuring of materials - from atoms to properties?* (APT&M 2016 - Atom Probe Tomography & Microscopy 2016 (55th IFES). Gyeongju, South Korea. 2016-06-12 to 2016-06-17).

Raabe, D.; Ponge, D.; Gault, B.; Herbig, M.; Liebscher, C.; Dey, P.; Dehm, G.; Welsch, E. D.; Yao, M.; Wong, S. L.; Hickel, T.; Lipinska-Chwalek, M.; Neugebauer, J.; Prahl, U.; Madivala, M.; Scheu, C.; Bleck, W.: *Ab-Initio Guided Design of Twinning Induced Plasticity and Weight Reduced Austenitic Steels*. (MRS Fall Meeting. Boston, MA, USA. 2016-11-27 to 2016-12-02).

Raabe, D.; Ponge, D.; Gault, B.; Herbig, M.; Liebscher, C.; Kuzmina, M.; Leyson, G.; Wang, M.; Tasan, C. C.; Nematollahi, G. A.; Springer, H.; Belde, M. M.; Neugebauer, J.; Sandlöbes, S.: *Segregation Engineering - Solute Decoration, Complexions and Transformations for Self-Organized Metallurgical Bulk Nanostructures*. (MRS Fall Meeting. Boston, MA, USA. 2016-11-27 to 2016-12-02).

Raabe, D.; Li, Z.; Tasan, C. C.; Yao, M.; Ma, D.; Grabowski, B.; Körmann, F.; Neugebauer, J.: *Thermodynamics and Mechanical Properties of Non-Equiatomic CoCrFeMnNi Alloys*. (2016 MRS Fall Meeting. Boston, MA, USA. 2016-11-27 to 2016-12-02).

Rohwerder, M.: *Conducting Polymers for Intelligent Self-Healing Coatings*. (Energy Materials Nanotechnology (EMN) Meeting on Polymer. Hongkong, Hongkong. 2016-01-12 to 2016-01-15).

Rohwerder, M.: *Characterization of Oxides in the Heat Affected Zone*. (Welding Workshop “Guidelines for use of welded stainless steel in corrosive environments” at TWI, Granta Park. Cambridge, UK. 2016-01-26).

Rohwerder, M.: *Nanokapseln für den intelligenten Korrosionsschutz – eine kritische Übersicht.* (GfKORR- Nanoskalige Korrosionsschutzsysteme – Anspruch und Wirklichkeit, Dechema. Frankfurt, Germany. 2016-06-02 to 2016-06-03).

Rohwerder, M.: *Die Rasterkelvinsonde: neue Entwicklungen für die Charakterisierung von Korrosionsschutzbeschichtungen*. (7. Korrosionsschutz-Symposium. Kloster Irsee, Germany. 2016-06-22 to 2016-06-24).

Rohwerder, M.: *Metal/Nano-Container Composite Coatings for Long-Term Reliable Self-Healing Capability*. (6th Annual World Congress of Nano Science & Technology – Nano S&T 2016. Singapur, Singapur. 2016-10-26 to 2016-10-28).

Scheu, C.: *Atomic arrangement and defects in $Nb_3O_7(OH)$ and $TiO_2$ nanoarrays and their effect on functional properties*. (Talk at Institut für Anorganische und Analytische Chemie, Universität Freiburg, Germany. 2016-01-27).

Scheu, C.: *The role of defects in $Nb_3O_7(OH)$ and $TiO_2$ nanoarrays*. (Energy Materials Nanotechnology (EMN). Dubrovnik, Croatia. 2016-05-04 to 2016-05-07).

Scheu, C.: *New insights into HTPEM fuel cells using electron microscopy techniques*. (THERMEC'2016: 9th International Conference on Processing & Manufacturing of Advanced Materials. Graz, Austria. 2016-05-29 to 2016-06-03).

Scheu, C.: *Interface structure of Kappa-Carbides in high Mn Steels*. (PICS meeting. Luminy, Marseille, France. 2016-06-14 to 2016-06-17).

Scheu, C.: *Correlative STEM & Atom Probe Tomography (ATP): Insights in the k-carbide/austenite interface*. (Workshop on "New trends in electron microscopy", Ringberg Castle. Kreuth am Tegernsee, Germany. 2016-06-22 to 2016-06-24).

Scheu, C.: *Insights into structural and functional properties of nano-structured electrodes for energy and fuel generating devices*. (Talk at Helmholtz-Zentrum Geesthacht, Germany. 2016-06-22 to 2016-06-30).

Scheu, C.: *Transmission electron microscopy – a versatile tool to study the microstructure of HT-PEMFC*. (Materials Science 2016. Atlanta, GA, USA. 2016-09-12 to 2016-09-14).

Scheu, C.: *Insights into structural and functional properties of $Nb_3O_7(OH)$ and $TiO_2$ nanoarrays*. (European Materials Research Society's (EMRS) Fall Meeting. Warsaw, Poland. 2016-09-12 to 2016-09-15).

Scheu, C.: *Thermal stability and phase transformation of nanostructured $Nb_3O_7(OH)$ photocatalyst*. (Materials Science & Technology (MS&T 2016). Salt Lake City, USA. 2016-10-23 to 2016-10-27).

Schwarz, T.; Choi, P.-P.; Cojocaru-Mirédin, O.; Mousel, M.; Redinger, A.; Siebentritt, S.; Raabe, D.: *Formation of nano-sized Cu–Sn–Se particles in $Cu_2ZnSnSe_4$ thin-films and their effect on solar cell efficiency*. (Seminar, Katholieke Universiteit Leuven/IMEC, Belgium. 2016-11-16).

Šlapáková, M.; Stein, F.; Liebscher, C.; Voß, S.; Kumar, S.: *TEM Analysis of Deformation Structure in $Fe_2Nb$ Laves Phase*. (Seminar on Metal Materials. Prague, Czech Republic. 2016-05-18).

Springer, H.: *Leichtbau durch Kombinatorische Metallurgie und Prozesstechnik*. (VDI Forum Warmmassivumformung. Düsseldorf, Germany. 2016-02-03).

Stein, F.; Horiuchi, T.: *Discontinuous Precipitation of the Complex Intermetallic Phase $Nb_2Co_7$ from Supersaturated Co Solid Solution*. (Thermec 2016. Graz, Austria. 2016-05-29 to 2016-06-03).

Stein, F.: *Stability Competition between Laves Phase Polytypes*. (Seminar, Escola Politécnica da Universidade de São Paulo, Brazil. 2016-09-12).

Todorova, M.; Vatti, A.K.; Yoo, S.; Neugebauer, J.: *Oxide stability and defect chemistry in an electrochemical environment: an ab initio perspective.* (Workshop 2016 der DFG-Forschergruppe 1376 "Elementary reaction steps in electrocatalysis: Theory meets experiment". Reisensburg, Günzburg, Germany. 2016-05-01 to 2016-05-04).

Todorova, M.; Vatti, A.K.; Yoo, S.; Neugebauer, J.: *New Insights into Corrosion Mechanisms from Ab Initio Concepts.* (GRC "Corrosion – Aqueous". New London, NH, USA. 2016-07-10 to 2016-07-15).

Todorova, M.; Neugebauer, J.: *Formation and dissolution of protective oxide layers in a wet electrochemical environment*. (MMM 2016 Conference. Dijon, France. 2016-10-09 to 2016-10-14).

Valtiner, M.: *Direct measurement of single molecular interaction free energies at solid/liquid interfaces based on non-equilibrium force spectroscopy.* (Colloquium, TU Berlin, Germany. 2016-01-12)

Valtiner, M.: *Resolving non-specific and specific adhesive interactions of catechols at solid/liquid interfaces at the single molecular scale.* (Keynote talk, AICHE meeting. San Francisco, CA, USA. 2016-11-17)

Valtiner, M.: *Measuring single molecule interaction free energies and ion structuring at solid/liquid interfaces.* (INM. Saarbrücken, Germany. 2016-12-02)

Valtiner, M.: *Quantification of Single Molecular Interactions at Solid/Liquid Interfaces.* (Colloquium, Twente University. Twente, The Netherlands. 2016-12-15)

Wippermann, S.: *Interface-controlled materials for solar energy conversion: semiconducting nanocrystal solids*. (Colloquium, Tsinghua University. Beijing, China. 2016-07)

Wippermann, S.: *Entropy stabilizes Peierls condensate: phonon-driven charge density wave formation and adatom-induced early condensation.* (IBS conference on surface atomic wires. Pohang, South Korea. 2016-08-29)

Zaefferer, S.: *Boundary characterisation using correlative ECCI and EBSD.* (ACMM pre-conference workshop, Geelong, Australia. 2016-01-29).

Zaefferer, S.: *Correlation of 5-parameter GB character with GB properties.* (ACMM pre-conference workshop, Geelong, Australia. 2016-01-29).

Zaefferer, S.: *Exploring microstructure-property-relationships of crystalline materials by application of diffraction techniques (electron backscatter diffraction, EBSD, and electron channelling, ECCI) in the SEM.* (Australian conference on microscopy and microanalysis. Melbourne, Australia. 2016-01-31 to 2016-02-04).

Zaefferer, S.: *Introduction to ECCI.* (EBSD Training Tutorial Workshop. Manchester, UK. 2016-03-22 to 2016-03-23).

Zaefferer, S.: *Electron channelling contrast imaging (ECCI) – Recent advances and new applications.* (RMS-EBSD conference. Manchester, UK. 2016-03-23 to 2016-03-25).

Zaefferer, S.: *Electron channelling contrast imaging (ECCI): an amazing tool for observations of crystal lattice defects in bulk samples*. (SCANDEM. Trondheim, Norway. 2017-06-07 to 2016-06-10).

Zaefferer, S.: *Electron backscatter diffraction (EBSD) –possibilities and limits.* (European Mineralogy Union workshop 2016. Vienna, Austria. 2016-06-19 to 2016-06-20).

Zaefferer, S.: *Investigations on the relationship between crystallographic character of grain boundaries and their functional and mechanical properties in various engineering materials*. (24th International conference on materials and technology. Portorož, Slovenia. 2016-09-27 to 2016-09-29).

Zaefferer, S.: *Direkte Beobachtung von Kristalldefekten in Massivproben mittels Electron-Channelling Contrast Imaging (ECCI) im REM*. (Workshop „Von Nano bis Makro“, der EFDS. Dresden, Germany. 2016-11-07 to 2016-11-09).

Zaefferer, S.: *Electron channelling contrast imaging (ECCI) – an amazing tool for observations of crystal lattice defects in bulk samples*. (Micromat IX. Belo Horizonte, Brazil. 2016-11-22 to 2016-11-25).

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Archie, F. M. F.; Zaefferer, S.: *Investigations on the origin of crack initiation and propagation susceptibility of prior austenite grain boundaries in DP and martensitic steels*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Brinckmann, S.; Fink, C.; Dehm, G.: *Severe Microscale Deformation of Pearlite and Cementite*. (2017 MRS Spring Meeting & Exhibits. Phoenix, AZ, USA. 2017-04-17 to 2017-04-21).

Brinckmann, S.: *Microscale Materials Tribology: Severe Deformation of Pearlite*. (Talk at Institut für Konstruktionswissenschaften und Technische Logistik, Technische Universität Wien, Austria. 2017-11).

Brinckmann, S.: *Severe Deformation of Pearlite during Microscale Tribology*. (Talk at Erich Schmid Institute für Materialwissenschaft. Leoben, Austria. 2017-11).

Cojocaru-Mirédin, O.; Schwarz, T.; Mainz, R.; Abou-Ras, D.: *Understanding the defects in Cu(In,Ga)$Se_2$ solar cell: a correlative microscopy approach*. (Spring Meeting of the German Physical Society (DPG ), Dresden, Germany. 2017-03-19 to 2017-03-24).

Dehm, G.; Malyar, N.; Kirchlechner, C.: *Towards probing the barrier strength of grain boundaries for dislocation transmission*. (Electronic Materials and Applications 2017. Orlando, FL, USA. 2017-01-18 to 2017-01-20).

Dehm, G.: *Resolving the interplay of nanostructure and mechanical properties in advanced materials*. (Karlsruher Werkstoffkolloquium im Wintersemester 2016/2017. Karlsruhe, Germany. 2017-02-07).

Dehm, G.; Harzer, T. P.; Liebscher, C.; Raghavan, R.: *High Temperature Plasticity of Cu–Cr Nanolayered and Chemically Nanostructured Cu–Cr Films*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Dehm, G.; Duarte, M. J.: *Structure and Micro-/Nanomechanics of Materials*. (DLR Cologne. Köln, Germany. 2017-05-23).

Dehm, G.; Malyar, N.; Kirchlechner, C.: *Do we understand dislocation transmission through grain boundaries?* (PICS meeting. Luminy, Marseille, France. 2017-05-30 to 2017-06-02).

Dehm, G.: *Resolving the mechanical performance of materials in microelectronic components with µm spatial resolution*. (FIMPART - Frontiers in Materials Processing Applications, Research and Technology. Bordeaux, France. 2017-07-09 to 2017-07-12).

Dehm, G.: *Towards thermally stable nanocrystalline alloys with exceptional strength: Cu–Cr as a case study*. (16th International Conference on Rapidly Quenched and Metastable Materials (RQ16). Leoben, Austria. 2017-08-27 to 2017-09-01).

Dehm, G.: *Aktuelle Einblicke in den Nanokosmos von Werkstoffen*. (Physikalisches Kolloquium, Bergische Universität Wuppertal, Germany. 2017-11-27).

Dey, P.; Timmerscheidt, T.A.; von Appen, J.; Hickel, T.; Dronskowski, R.; Neugebauer, J.: *Ab initio investigation of the interaction of hydrogen with carbides in advanced high-strength steels.* (Southern University of Science and Technology. Shenzhen, China. 2017-03-20).

Diehl, M.; Naunheim, Y.; Morsdorf, L.; An, D.; Roters, F.; Raabe, D.: *Crystal Plasticity Simulations on Real Data: Towards Highly Resolved 3D Microstructures*. (MRS Spring Meeting 2017. Phoenix, Arizona, USA. 2017-04-17 to 2017-04-21).

Duarte, M. J.; Fang, X.; Brinckmann, S.; Dehm, G.: *In-situ nanoindentation of hydrogen bcc Fe–Cr charged surfaces: Current status and future perspectives*. (Frontiers in Material Science & Engineering workshop: Hydrogen Interaction in Metals, MPIE. Düsseldorf, Germany. 2017-04-11).

Dutta, B.; Hickel, T.; Neugebauer, J.: *Ab initio modelling of phase diagrams in magnetic Heusler alloys: achievements and future challenges*. (SUSTech Global Scientists Forum. Shenzhen, China. 2017-03-18 to 2017-03-20).

Dutta, B.; Hickel, T.; Neugebauer, J.: *Finite temperature excitation mechanisms and their coupling in magnetic shape memory alloys*. (The Materials Research Centre (MRC), Indian Institute of Science (IISc). Bangalore, India. 2017-06-27).

Dutta, B.; Körmann, F.; Hickel, T.; Neugebauer, J.: *Temperature-driven effects in functional materials: Ab initio insights*. (Talk at University Pierre and Marie CURIE (UPMC). Paris, France. 2017-11-21).

Fabritius, H.-O.; Wu, X.: *Mechanochromic photonic crystals based on cuticular scales of the weevil Entimus imperialis*. (IOP Conference "Optical Biomimetics". Imperial College London, UK. 2017-02-22).

Fabritius, H.-O.: *How living organisms manipulate light: Photonic structures in nature*. (Spring School of the SPP 1839 „Tailored Disorder". Karlsruhe, Germany. 2017-05-15 to 2017-05-17).

Fabritius, H.-O.: *In-vitro-Untersuchungen zur Wechselwirkung von synthetischen Hydroxylapatit-Partikeln mit der Zahnschmelzoberfläche*. (Biorepair-Symposium. Bielefeld, Germany. 2017-05-20).

Fabritius, H.-O.: *Broadband reflecting fibers with tailored structures inspired by desert ants*. (SPP 1839 – Retreat. Kostanz, Germany. 2017-09-18 to 2017-09-20).

Fabritius, H.-O.; Fabritius-Vilpoux, K.; Enax, J.: *Quantitative Interaktion von HAP-Partikeln mit standardisierten Schmelzoberflächen in vitro und ultrastrukturelle Untersuchungen von Milchzähnen*. (Biorepair-Symposium. Bielefeld, Germany. 2017-12-01 to 2017-12-02).

Freysoldt, C.; Mishra, A.; Neugebauer, J.: *Ab initio simulations of charged surfaces*. (57th Sanibel Meeting. St. Simons Island, GA, USA. 2017-02-19 to 2017-02-24).

Freysoldt, C.; Mishra, A.; Neugebauer, J.: *Ab initio simulations of charged surfaces.* (Workshop "High electric fields in electrochemistry and atom probe tomography". Ringberg Castle, Kreuth, Germany. 2017-03-29 to 2017-04-01).

Gault, B.; Dagan, M.; Katnagallu, S.; De Geuser, F.; Vurpillot, F.; Raabe, D.; Moody, M. P.: *Revisiting Field Ion Microscopy*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Gault, B.; De Geuser, F.; Katnagallu, S.; Nematollahi, G. A.; Dagan, M.; Parviainen, S.; Rusitzka, A. K.; Johnson, E.; Sundell, G.; Andersson, M.; Stephenson, L.; Neugebauer, J.; Moody, M. P.; Vurpillot, F.; Raabe, D.: *Reconstructing field ion microscopy and atom probe data*. (Australian Atom Probe Workshop. Magnetic Island, Australia. 2017-06).

Gault, B.; Chang, Y.; Kwiatkowski da Silva, A.; Zhao, H.; Kontis, P.; Breen, A. J.; Ponge, D.; Raabe, D.: *Interfaces and defect composition at the near-atomic scale*. (MRS Fall Meeting 2017. Boston, MA, USA. 2017-11-26 to 2017-12-01).

Glensk, A.; Grabowski, B.; Hickel, T.; Neugebauer, J.; Leitner, M.; Neuhaus, J.; Petry, W.: *Ab initio determination of phonon lifetimes up to the melting point*. (EMRS Spring 2017. Strasbourg, France. 2017-05-22 to 2017-05-24).

Grabowski, B.: *Development and application of quantum mechanics based simulation tools for the design of modern metallic materials.* (Seminar, RWTH Aachen, Germany. 2017-03-14).

Grabowski, B.: *Data driven engineering of advanced materials: Combining high precision and scale bridging.* (Colloquium, Forschungszentrum Jülich, Germany. 2017-07-20).

Grabowski, B.: *Knowledge driven engineering of metals: Development and application of ab initio based scale bridging methods.* (Seminar, TU Delft, Netherlands. 2017-12-04).

Grabowski, B.: *Knowledge driven engineering of materials: Development and application of ab initio based scale bridging methods.* (Seminar, University Stuttgart, Germany. 2017-12-06).

Hadian, R: *Complexions and dewetting.* (Keynote talk, Workshop: Mechanics Meets Energy 2017. Ringberg Castle, Germany. 2017-01-08 to 2017-01-12).

Hadian, R.; Grabowski, B.; Race, C.; Neugebauer, J.: *Atomistic Simulations on Grain Boundary Migration.* (Keynote talk, Materials Science & Technology (MS&T 2017). Pittsburgh, PN, USA. 2017-10-08 to 2017-10-12).

Hengge, K.: *TEM Tomography: Insights into the degradation of Pt/Ru fuel cell catalysts*. (3D materials characterization at all length scales and its application to iron and steel, MPIE. Düsseldorf, Germany. 2017-08-29).

Herbig, M.: *Spatially correlated electron microscopy and atom probe tomography*. (Klausurtagung des Erlanger Lehrstuhls für Werkstoffwissenschaften WW1. Erlangen, Germany. 2017-09-27 to 2017-09-29).

Herbig, M.: *Materials Science Using Correlative Microscopy*. (National Institute for Materials Science (NIMS). Tsukuba, Japan. 2017-11-08).

Herbig, M.: *Materials Science Using Correlative Microscopy*. (Nippon Steel & Sumitomo Metals Corporation. Kimitsu, Japan. 2017-11-09).

Herbig, M.: *Materials Science Using Correlative Microscopy*. (JFE steel corporation. Chiba, Japan. 2017-11-10).

Herbig, M.; Parra, C. D.; Lu, W.; Toji, Y.; Liebscher, C.; Li, Y.; Goto, S.; Dehm, G.; Raabe, D.: *Where does the carbon atom go in steel? – Insights gained by correlative transmission electron microscopy and atom probe tomography*. (International Symposium on Steel Science 2017. Kyoto, Japan. 2017-11-13 to 2017-11-16).

Herbig, M.: *Atomare Einsichten in Struktur und Zusammensetzung von Stählen durch korrelative Elektronenmikroskopie/ Atomsondentomographie*. (25. Werkstoffkolloquium des Technischen Beirats. Hannover, Germany. 2017-11-24).

Hickel, T.; Dey, P.; Mrovec, M.; McEniry, E.; Neugebauer, J.: *Ab initio insights into interface in steels: Fundamentals, recent results & outlook.* (Retreat of the SN department, Tegernsee, Germany, 2017-01-09 to 2017-01-12).

Hickel, T.; McEniry, E.; Dey, P.; Neugebauer, J.; Mrovec, M.; Di Stefano, D.; Elsässer, C.: *The first principles approach: Insights into hydrogen trapping by microstructures in steels.* (Royal Society Discussion Meeting "The challenges of hydrogen and metals". London, UK. 2017-01-16 to 2017-01-18).

Hickel, T.; Bleskov, I.; Aydin, U.; Körmann, F.; Grabowski, B.; Neugebauer, J.: *Quantum mechanically guided materials design*. (Summer school "Materials 4.0 - The digitally enabled atom to system revolution". Dresden, Germany. 2017-09-11 to 2017-09-15).

Jägle, E. A.: *Phase transformation phenomena in additively produced alloys*. (Seminar „Materials Science and Technology". Ruhr-Universität Bochum, Germany. 2017).

Jägle, E. A.: *Metallische Werkstoffe in der Additiven Fertigung*. (Workshop "Steels for Additive Manufacturing". Stahlinstitut VDEh, Düsseldorf, Germany. 2017-02-21).

Jägle, E. A.: *Alloys for Additive Manufacturing, Alloys by Additive Manufacturing*. (Seminar, Institut für Umformtechnik und Leichtbau, TU Dortmund, Germany. 2017-06-02).

Jägle, E. A.: *Alloys for Additive Manufacturing, Alloys by Additive Manufacturing*. (Laser-Kolloquium, Fraunhofer Institut für Lasertechnik. Aachen, Germany. 2017-07-13).

Jägle, E. A.: *Alloys for Additive Manufacturing, Alloys by Additive Manufacturing*. (Seminar, Culham Center for Fusion Energy, Oxford, UK. 2017-08-10).

Jägle, E. A.: *Exploiting the Intrinsic Heat Treatment during Laser Additive Manufacturing to trigger Precipitation Reactions*. (International Mechanical Engineering Congress & Exposition (IMECE). Tampa, FL, USA. 2017-11-09).

Jägle, E. A.: *Alloys for Additive Manufacturing, Alloys by Additive Manufacturing*. (Plenary talk, Advances in Materials & Processing: Challenges and Opportunities. Indian Institute of Technology Roorkee, India. 2017-11-30).

Jägle, E. A.: *Additive Manufacturing and 3D Printing - What's beyond the hype?* (Institute Lecture, Indian Institute of Technology Roorkee, India. 2017-12-03).

Jägle, E. A.: *Ex-situ and in-situ heat treatment of alloys during Laser Additive Manufacturing*. (AWT Kolloquium, Institut für Werkstofftechnik. Bremen, Germany. 2017-12-13).

Jaya, B. N.; Kirchlechner, C.; Dehm, G.: *Fracture Behavior of Nanostructured Heavily Cold Drawn Pearlite: Influence of the Interface*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Kirchlechner, C.; Malyar, N.; Peter, N. J.; Dehm, G.; Micha, J.-S.: *New Insights into Plasticity at Grain Boundaries by Nano- and Micromechanics*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Kirchlechner, C.: *Using nano- and micromechanics to understand interface plasticity*. (Hysitron Nanobrücken 2017. University of Manchester, UK. 2017-04-04 to 2017-04-06).

Kirchlechner, C.: *Insights into dislocation grainboundary interactions by in situ micromechanics*. (Seminar, FAU Erlangen/Nürnberg. Erlangen, Germany. 2017-06-29).

Kirchlechner, C.; Kirchlechner, I.; Soler, R.; Du, C.; Schneider, J. M.; Dehm, G.: *In situ small scale fracture experiments*. (RQ16, Microstructural Kinetics Group, Department of Materials Science & Metallurgy. Leoben, Austria. 2017-08-27 to 2017-09-01).

Körmann, F.; Bleskov, I.; Grabowski, B.; Dutta, B.; Hickel, T.; Neugebauer, J.: *Parameter-free Finite-temperature Computations of Stacking Fault Energies for Magnetic Materials*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Li, Z.: *Designing and understanding novel high-entropy alloys towards superior properties*. (Talk at Universität Kassel, Institut für Werkstofftechnik. Kassel, Germany. 2017-06-06).

Li, Z.; Raabe, D.: *Designing novel high-entropy alloys towards superior properties*. (Frontiers in Materials Processing Applications, Research and Technology (FiMPART'2017). Bordeaux, France. 2017-07-09 to 2017-07-12).

Liebscher, C.: *Atomic structure and chemistry of complex energy materials and interfaces*. (Seminar, Lawrence Livermore Laboratory, USA. 2017-03-07).

Liebscher, C.: *Atomic structure and chemistry of complex energy materials and interfaces.* (63. Metallkunde Kolloquium. Lech am Arlberg, Austria. 2017-04-18 – 2017-04-21).

Liebscher, C.: *Correlative aberration-corrected STEM and 3D-APT study of coherent interfaces in low density steel*. (Symposium on Advanced Mechanical and Microstructural Characterization Methods for SX Ni- and Co-based alloys. Ruhr-Universität Bochum, Germany. 2017-09-14).

Lymperakis, L.; Freysoldt, C.; Neugebauer, J.: *Elastically frustrated rehybridization of InGaN surfaces: Implications on growth temperature and alloy ordering.* (Spring school on short period superlattices. Warsaw, Poland. 2017-03-21 to 2-17-03-24).

Lymperakis, L.: *Physics, growth mechanisms, and peculiarities of III-N surfaces from ab-initio.* (Institute for solid state physics, TU Berlin, Germany. 2017-06-28).

Malyar, N. V.; Imrich, P. J.; Micha, J.-S.; Dehm, G.; Kirchlechner, C.: *Quantifying dislocation slip transfer by in situ micromechanics*. (MRS Fall Meeting 2017. Boston, MA, USA. 2017-11-26 to 2017-12-01).

Marian, J.; Cereceda, D.; Raabe, D.; Roters, F.; Zhao, Y.; Diehl, M.: *Predicting Materials Strength in BCC Alloys using parameter-less mesoscale approaches*. (MRS Spring Meeting 2017. Phoenix, AZ, USA. 2017-04-17 to 2017-04-21).

Mayrhofer, K. J. J.: *Understanding Electrocatalysis in Fuel Cells and Electrolyzers*. (Keynote Lecture, Recent Advances in Renewable Energy Technology, Education City. Doha, Quatar. 2017-04-02 to 2017-04-03).

Mayrhofer, K. J. J.: *High-throughput methods with online analytics – from fundamental electrocatalysis to real applications*. (Keynote Lecture, 6th Regional Symposium on Electrochemistry for South-East Europe. Balatonkenese, Hungary. 2017-06-11 to 2017-06-15).

Neugebauer, J.; Zhang, X.; Körmann, F.; Grabowski, B.; Hickel, T.; Leyson, G.: *Ab Initio Guided Design of High Strength Steels: Where Do We Stand?* (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Neugebauer, J.: *Ab initio guided design of structural materials with superior mechanical properties*. (APS Meeting 2017. New Orleans, LA, USA. 2017-03-13 to 2017-03-17).

Neugebauer, J.: *How to achieve interoperability - a modeler's perspective*. (1st EMMC International Workshop. Wien, Austria. 2017-04-05 to 2017-04-07).

Neugebauer, J.: *From Semiconductors to High-Strength Steels and Back Again*. (10 years of the Laboratory for Photovoltaics & Semiconductor Physics. Luxembourg, Luxembourg. 2017-05-05).

Neugebauer, J.; Aydin, U.; Grabowski, B.; Hickel, T.: *Machine learning as tool to enhance ab initio based alloy design*. (International workshop on machine learning and data analytics in advanced metals processing. Manchester, UK. 2017-05-23).

Neugebauer, J.; Lymperakis, L.; Freysoldt, C.: *Fundamental compositional limitations in the thin film growth of metastable alloys*. (Keynote Lecture, Rapidly Quenched & Metastable Materials 16. Leoben, Austria. 2017-08-29).

Neugebauer, J.; Hickel, T.; Grabowski, B.; Koermann, F.; Janssen, J.: *Modelling structural materials in realistic environments by ab initio thermodynamics.* (EUROMAT 2017. Thessaloniki, Greece. 2017-09-22).

Neugebauer, J.; Hickel, T.; Grabowski, B.; Pei, Z.; Janssen, J.: *Materials Discovery and Design at Finite Temperatures*. (Materials Science & Technology (MS&T 2017). Pittsburgh, PA, USA. 2017-10-09).

Neugebauer, J.: *Free energy sampling strategies for structurally complex materials.* (IPAM Long Program "Complex High-Dimensional Energy Landscapes" (2017-09-11 to 2017-12-15) Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, IPAM, UCLA. Los Angeles, CA, USA. 2017-10-16 to 2017-10-20).

Neugebauer, J.; Surendralal, S.; Todorova, M.: *A first principles approach to model electrochemical reactions in an electrolytic cell.* (Workshop: The Electrode Potential in Electrochemistry - A Challenge for Electronic Structure Theory Calculations. Schloß Reisensburg, Günzburg, Germany. 2017-11-26 to 2017-11-29).

Palm, M.: *Iron aluminides: Recent Alloy Developments and Industrial Processing*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Peter, N. J.: *Exploring Grain Boundaries: Structure, Chemistry and Nanomechanics.* (Seminar, National Institute for Electron Microscopy. Berkeley, CA, USA. 2017-09-05).

Ponge, D.; Kuzmina, M.; Sandlöbes, S.; Herbig, M.; Raabe, D.: *Austenite Formation along Dislocations in Medium Manganese Steels*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Ponge, D.; Han, J.; Kwiatkowski da Silva, A.; Raabe, D.; Lee, S.-M.; Lee, Y.-K.; Lee, S.-I.; Hwang, B.: *Relationship between Impact Toughness, Prior Austenite Grain Boundaries and Microstructural Morphology in Medium Mn Steel*. (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Ponge, D.; Kuzmina, M.; Kwiatkowski da Silva, A.; Wang, M.; Sandlöbes, S.; Herbig, M.; Raabe, D.: *Segregation Engineering in Medium Manganese Steels*. (TMS2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Ponge, D.; Tarzimoghadam, Z.; Klöwer, J.; Raabe, D.: *Hydrogen-assisted Failure in Ni-base Superalloy 718 Studied under In-situ Hydrogen Charging: The Role of Localized Deformation in Crack Propagation.* (TMS 2017. San Diego, CA, USA. 2017-02-26 to 2017-03-02).

Ponge, D.; Tasan, C. C.; Springer, H.; Koyama, M.; Kuzmina, M.; Wang, M.; Morsdorf, L.; Gault, B.; Seol, J. B.; Liebscher, C.; Yao, M.; Li, Z.; Gutiérrez-Urrutia, I.; Wang, H.; Neugebauer, J.; Scheu, C.; Raabe, D.: *Metastability Alloy Design*. (16th Intern. Conference on Rapidly Quenched and Metastable Materials (RQ16). Leoben, Austria. 2017-08-31).

Ponge, D.; Tasan, C. C.; Springer, H.; Gutiérrez-Urrutia, I.; Koyama, M.; Kuzmina, M.; Wang, M.; Morsdorf, L.; Gault, B.; Seol, J. B.; Choi, P.-P.; Liebscher, C.; Yao, M.; Li, Z.; Wang, H., H.; Neugebauer, J.; Scheu, C.; Raabe, D.: *1 Billion Tons of Nanostructure - Metastability Alloy Design and Segregation Engineering*. (38th Risø Intern. Symp. Materials Science Advanced Metallic Materials by Microstructural Design. Roskilde, Denmark. 2017-09-04 to 2017-09-08).

Raabe, D.; Gault, B.; Breen, A. J.; Chang, Y.; Yao, M.; Ponge, D.; Herbig, M.; Liebscher, C.; Dehm, G.; Scheu, C.; Stoffers, A.; Neugebauer, J.: *A Brief History of Metals*. (Public Named Max Planck Lecture, MPIE. Düsseldorf, Germany. 2017).

Raabe, D.; Gault, B.; Breen, A. J.; Chang, Y.; Yao, M.; Ponge, D.; Herbig, M.; Liebscher, C.; Dehm, G.; Scheu, C.; Stoffers, A.; Neugebauer, J.: *Atomic Scale Characterization of Complex Materials*. (Physikalisches Kolloquium, Fakultät für Mathematik und Physik, Universität Freiburg, Germany. 2017-02-06).

Raabe, D.; Gault, B.; Breen, A. J.; Chang, Y.; Yao, M.; Ponge, D.; Herbig, M.; Liebscher, C.; Dehm, G.; Scheu, C.; Stoffers, A.; Neugebauer, J.: *Advanced Atom Probe Tomography*. (25th Annual Meeting of the German Crystallographic Society. Karlsruhe, Germany. 2017-03-27 to 2017-03-30).

Raabe, D.; Gault, B.; Yao, M.; Scheu, C.; Liebscher, C.; Herbig, M.: *Correlated and simulated electron microscopy and atom probe tomography*. (Workshop on Possibilities and Limitations of Quantitative Materials Modeling and Characterization 2017. Bernkastel, Germany. 2017-05-16).

Raabe, D.; Gault, B.; Breen, A. J.; Chang, Y.; Yao, M.; Ponge, D.; Herbig, M.; Liebscher, C.; Tarzimoghadam, Z.; Dehm, G.; Scheu, C.; Stoffers, A.; Neugebauer, J.: *Multiprobe and Multiscale Characterisation of complex Materials*. (Fraunhofer Conference 'The Future of Materials – Materials Future'. Halle, Germany. 2017-06-19).

Raabe, D.: *Seeing Hydrogen*. (2017 Hydrogen Metal Systems Gordon Research Conference, Stonehill College. Easton, MA, USA. 2017-07-16 to 2017-07-21).

Raabe, D.; Tasan, C. C.; Diehl, M.; Yan, D.; Zambaldi, C.; Zaefferer, S.; Shanthraj, P.; Roters, F.: *Integrated experimental and simulation analysis of stress and strain partitioning in dual phase steel*. (Nanomechanical Testing in Materials Research and Development VI. Dubrovnik, Croatia. 2017-10-01 to 2017-10-06).

Raabe, D.; Gault, B.; Breen, A. J.; Chang, Y.; Yao, M.; Ponge, D.; Herbig, M.; Liebscher, C.; Scheu, C.: *Atomic- and multiscale observation of segregation*. (Eindhoven Multiscale Institute (EMI) Symposium, Eindhoven University. Eindhoven, The Netherlands. 2017-10-30 to 2017-10-31).

Raabe, D.; Gault, B.; Breen, A. J.; Yao, M.; Zhao, H.; Ponge, D.; Stoffers, A.: *Textures Studied at Near Atomic-Scale*. (18th International Conference on Textures of Materials (ICOTOM-18). St. George, UT, USA. 2017-11-06 to 2017-11-10).

Rohwerder, M.: *A Novel Potentiometric Approach to a Quantitative Characterization of Oxygen Reduction Kinetics at Buried Interfaces and under Ultrathin Electrolyte Layers*. (Second International Conference on Electrochemical Science and Technology – ICONEST 2017. Indian Institute of Science, Bangalore, India. 2017-08-10 to 2017-08-12).

Rohwerder, M.: *A Novel Potentiometric Approach to a Quantitative Characterization of Oxygen Reduction Kinetics at Buried Interfaces and under Ultrathin Electrolyte Layers*. (ECASIA 2017. Montpellier, France. 2017-09-24 to 2017-09-29).

Rohwerder, M.; Tran, T. H.: *Novel zinc-nanocontainer composite coatings for intelligent corrosion protection*. (11th Intrenational Conference on Zinc And Zinc Alloy Coated Steel Sheet - GALVATECH 2017. Tokyo, Japan. 2017-11-12 to 2017-11-16).

Scheu, C.: *In-situ Transmission Electron Microscopy Observation of Heat-Induced Structural Changes of 3D $Nb_3O_7(OH)$ Networks*. (Electronic Materials and Applications 2017 (EMA). Orlando, FL, USA. 2017-01-18 to 2017-01-20).

Scheu, C.: *Grain growth and dewetting of thin Al films on (0001) $Al_2O_3$ substrates*. (3 Phase, Interface, Component Systems (PICS), Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), France. 2017-05-30 to 2017-06-02).

Scheu, C.: *Structural and functional properties of $Nb_3O_7(OH)$ nanoarrays and their modification via doping and thermal annealing*. (Talk at Institut für Werkstofftechnik, Technische Universität Ilmenau, Gemany. 2017-07-26).

Scheu, C.; Betzler, S. B.: *$Nb_3O_7(OH)$ – a promising candidate for photocatalyst: synthesis, nanostructure and functionality*. (International Conference on Functional Nanomaterials and Nanodevices. Budapest, Hungary. 2017-09-24 to 2017-09-25).

Scheu, C; Hieke, S. W.; Willinger, M. G.; Wang, Z.-J.; Richter, G.; Dehm, G.: *In-situ electron microscopy: Insights in solid state dewetting of epitaxial Al thin films on sapphire*. (13th Multinational Congress on Microscopy. Rovinj, Croatia. 2017-09-26 to 2017-09-29).

Scheu, C.; Hieke, S. W.; Willinger, M. G.; Wang, Z.-J.; Richter, G.; Dehm, G.: *Evolution of faceted voids and fingering instabilities in a model thin film system - Insights by in-situ environmental scanning electron microscopy*. (Symposium - In situ Microscopy with Electrons, X-rays and Scanning Probes. Universität Erlangen-Nürnberg. Erlangen, Germany. 2017-10-09).

Schwarz, T.: *Untersuchung von Defekten in polykristallinen Dünnschichten mittels Atomsondentomographie*. (gmr2 – Gesellschaft für Materialografie Rhein-Ruhr e.V., MPIE. Düsseldorf, Germany. 2017-11-16).

Soler, R.; Venkatesan, S.; Kirchlechner, C.; Dehm, G.; Rainer, H.; Bartosik, M.; Mayrhofer, P. H.: *Can superlattice structures enhance the fracture toughness of ceramic coating?* (TMS 2017. San Diego, CA, USA. 2017-02-27 to 2017-03-03).

Springer, H.; Raabe, D.: *Rapid Alloy Prototyping – High Throughput Bulk Metallurgy at the MPIE*. (Workshop on machine learning and data analytics in advanced metals processing. RollsRoyce Institute Manchester, UK. 2017).

Springer, H.: *Innovative Stähle*. (Handelsblatt Tagung. Düsseldorf, Germany. 2017-02).

Stockem, I.: *The interaction of spin dynamics and lattice vibrations of CrN in the paramagnetic state*. (BIfAM Seminar. Bielefeld, Germany. 2017-11-14).

Taniguchi, S.; Soler, R.; Kirchlechner, C.; Liebscher, C.; Taniyama, A.; Dehm, G.: *In-situ TEM Study of Mechanical Size Effects in TiC Strengthened Steels*. (Microscopy & Microanalysis 2017. St. Louis, MO, USA. 2017-08-06 to 2017-08-10).

Todorova, M.; Neugebauer, J.: *From semiconductor defect chemistry to electrochemistry: Gaining new insights from computational physics tools*. (ICCP10 Conference. Macao, China. 2017-01-16 to 2017-01-20).

Todorova, M.; Neugebauer, J.: *From semiconductor defect chemistry to electrochemistry: Insight into corrosion mechanisms from ab initio concepts.* (57. Sanibel Symposium. St. Simon Island, GA, USA. 2017-02-21).

Todorova, M.; Vatti A.K.; Yoo, S.; Neugebauer, J.: *Ab initio description of oxides in an electrochemical environment*. (TMS 2017. San Diego, CA, USA. 2017-02-28).

Todorova, M.: *From weakened chemical bonds to materials breakdown: An ab initio perspective*. (Spring Meeting of the German Physical Society (DPG ), Dresden, Germany. 2017-03-19 to 2017-03-24).

Todorova, M.; Vatti, A.K.; Yoo, S.; Neugebauer, J.: *Ab-initio modelling of electrochemical processes: Challenges and insights.* (Workshop: Fundamental Electrochemistry: Theory Meets Experiment. Lorentz Center, Leiden, Netherlands. 2017-06-26 to 2016 -06-30).

Todorova, M.; Vatti, A.K.; Yoo, S.; Neugebauer, J.: *Free energy sampling for electrochemical systems.* (Workshop II: Stochastic Sampling and Accelerated Time Dynamics on Multidimensional Surfaces, IPAM, UCLA. Los Angeles, CA, USA. 2017-10-16 to 2017-10-20).

Todorova, M.; Yoo, S.; Neugebauer, J.: *Selective stabilization of polar oxide surfaces in electrochemical environment.* (Workshop: The Electrode Potential in Electrochemistry - A Challenge for Electronic Structure Theory Calculations. Schloß Reisensburg, Günzburg, Germany. 2017-11-26 to 2017-11-29).

Valtiner, M.: *Combining X-Ray Reflectivity and white light interferometry in a surface forces apparatus.* (DESY4 workshop. Hamburg, Germany. 2017-03-10 to 2017-03-14)

Valtiner, M.: *In-situ tracking of the dynamic structure evolution in nanometer confined liquids by combining X-Ray Reflectivity and white light interferometry in a surface forces apparatus.* (Keynote talk, TIN‘17. Trieste, Italy. 2017-06-25 to 2017-06-30)

Valtiner, M.: *Dynamic structure evolution in nanometer confined liquids.* (Keynote talk, World Tribology Conference in Beijing, China. 2017-09-17 to 2017-09-22)

Valtiner, M.: *Peter Mark Memorial Award Lecture.* (65th AVS conference and symposium. Tampa, FL, USA. 2017-10-29 to 2017-11-03)

Wippermann, S.: *Exotic forms of silicon for photovoltaic applications*. (E-MRS spring meeting. Strasbourg, France. 2017-02)

Wippermann, S.: *Optical fingerprints of electrochemical solid/liquid interfaces*. (Resolv Klausurtagung. Velen, Germany. 2017-02)

Wippermann, S.: *Novel silicon phases and nanostructures for solar energy conversion*. (ICFSI-16. Hannover, Germany. 2017-07)

Wippermann, S.: *Light-Matter Interactions at Interfaces: From Analysis Techniques to Applications in Solar Energy Conversion*. (Workshop “Internal Interfaces – Perspectives and Challenges for Theory”. Marburg, Germany. 2017-11)

Zaefferer, S., An D., Wang Z.: *Experimental investigations on the relationship between crystallographic character of grain boundaries and their functional and mechanical properties in various engineering materials.* (Spring Meeting of the German Physical Society (DPG ). Dresden, Germany. 2017-03-20 to 2017-03-24).

Zaefferer, S.: *Measurement and observation of elastic stresses and plastic strain phenomena at a local scale using SEM-based diffraction techniques.* (DAAD workshop Recent Trends in Advanced Microstructure Characterization. Universität des Saarlandes, Saarbrücken, Germany. 2017-04-03 to 2017-04-05).

Zaefferer, S.: *Electron channelling contrast imaging (ECCI) For quantitative analysis of crystal lattice defects in bulk samples.* (Canadian Microscopy and Cytometry Symposium. Montreal, Canada. 2017-05-09 to 2017-05-11).

Zaefferer, S.: *Electron Channelling Contrast Imaging (ECCI): An Amazing Tool for Observations of Crystal Lattice Defects in Bulk Samples.* (M&M 2017. St. Louis, MO, USA. 2017-08-06 to 2017-08-11).

Zaefferer, S.: *3D materials investigations – an overview on techniques, applications and limi*. (MPIE-workshop 3D Materials characterization on all length scales and its applications to iron and steel. Düsseldorf, Germany. 2017-08-29).

Zaefferer, S.: *Observation and quantification of elastic and plastic strain using SEM-based diffraction methods*. (Summerschool Micro- and Nanomechanics. Düsseldorf, Germany. 2017-09-11 to 2017-09-15).

Zaefferer, S., L. Schemmann, G. Stechmann, F. Ram, F. Archie: *Using orientation microscopy to explore the correlation of materials properties and microstructures.* (25th International conference on materials and technology. Portorož, Slovenia. 2017-10-16 to 2017-10-19).

Zaefferer, S.: *Observation and quantification of elastic and plastic strain using SEM-based diffraction methods, Part 1.* (7th international conference deformation and fracture of materials and nanomaterials. Moscow, Russia. 2017-11-07 to 2017-11-10).

Zaefferer, S.: *Observation and quantification of elastic and plastic strain using SEM-based diffraction methods, Part 2.* (7th international conference deformation and fracture of materials and nanomaterials. Moscow, Russia. 2017-11-07 to 2017-11-10).

## 2018

Baron, C.; Springer, H.; Raabe, D.: *Design of cost-efficient high modulus steels as innovative lightweight materials*. (Advanced Composite Materials Congress. Stockholm, Sweden. 2018-06-03 to 2018-06-06).

Brinckmann, S.: *Using Simulations to Investigate the Apparent Fracture Toughness of Microcantilevers*. (STKS-ICAMS-Seminar. Bochum, Germany. 2018-06).

Brinckmann, S.: *Understanding the fracture toughness for brittle and ductile materials at the microscale.* (Materials Science and Engineering. Darmstadt, Germany. 2018-09-26 to 2018-09-28).

Dehm, G.: *"Mechanical microscopy": Resolving the mechanical behavior and underlying mechanisms of materials with high spatial resolution*. (Keynote Lecture, IMEC18 / The 18th Israel Engineering Conference. Dead Sea, Israel. 2018-02-06 to 2018-02-08).

Dehm, G.: *Advanced TEM/STEM – a powerful tool to guide materials design*. (Inauguration Symposium, Institut für Metallphysik. Rheinisch-Westfälische Universität Münster, Münster, Germany. 2018-02-15).

Dehm, G.: *Dislocation – grain boundary interactions: Insights and challenges from micromechanical testing*. (3rd Schöntal Symposium on Dislocation- based Plasticity (DFG Forschergruppe FOR 1650). Schöntal, Germany. 2018-02-25 to 2018-03-02).

Dehm, G.; *Correlating the state and properties of grain boundaries*. (PICS meeting. Luminy/Marseilles, France. 2018-05-22 to 2018-05-25).

Dehm, G.; Peter, N.J.; Liebscher, C.H.; Kirchlechner, C.: *Ag-induced phase transformation of a sigma 5 grain boundary in copper*. (THERMEC'2018. Paris, France. 2018-07-18 to 2018-07-13).

Dehm, G.: *Changing material properties by grain-boundary phase transformation*. (Seminar, University of New South Wales, School of Materials Science and Engineering, Sydney, Australia. 2018-09-17).

Dehm, G.: *Probing the strength and atomic structure of individual grain boundaries in Cu*. (Seminar, The University of Sydney, Faculty of Engineering & Information Technologies, Sydney, Australia. 2018-09-18).

Dehm, G.: *Probing dislocation - grain boundary interactions and grain boundary phase transformations: New experiments on Cu bicrystals*. (Seminar, Nanyang Technological University, School of Mechanical & Aerospace Engineering, Singapore. 2018-09-21).

Dehm, G.: *Structure and Nano-/Micromechanics of Materials*. (Seminar, Beijing Institute of Technology, Beijing, China. 2018-09-24).

Dehm, G.: *Coexistence of different atomic motifs in a <111> Cu tilt grain boundary resolved by STEM*. (3rd Sino-German Symposium on Advanced Electron Microscopy of Interface Structures and Properties of Materials Tsinghua University. Beijing, China. 2018-09-24 to 2018-09-27).

Dehm, G.: *Plasticity and Stresses in Thin Films*. (GDRi MECANO General School 2018. Cargèse, Corsica, France. 2018-10-02).

Dey, P.; Hickel, T.; Neugebauer, J.: *Understanding Hydrogen Embrittlement based on ab initio methods.* (Linköping University, Sweden. 2018-02-15).

Dey, P.: *Materials design based on ab initio methods: Coherent microstructure & its impact on real application.* (TU Delft, Netherlands. 2018-04-05).

Diehl, M.; Shanthraj, P.; Eisenlohr, P.; Roters, F.; Raabe, D.: *DAMASK – From Crystal Plasticity to Multi-Physics*. (Seminar of the Centre des Matériaux. Paris, France. 2018-06-08).

Diehl, M.; Shanthraj, P.; Eisenlohr, P.; Roters, F.; Raabe, D.: *DAMASK - Düsseldorf Advanced Material Simulation Kit*. (Seminar of the Department of Mechanical Engineering, Villanova University, PA, USA. 2018-07-19).

Diehl, M.; Shanthraj, P.; Eisenlohr, P.; Roters, F.; Raabe, D.: *DAMASK - Düsseldorf Advanced Material Simulation Kit*. (Seminar of the Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, PA, USA. 2018-07-20).

Dutta, B.; Körmann, F.; Hickel, T.; Neugebauer, J.: *Role of temperature dependent excitations and the coupling between them in functional materials: Ab-initio insight.s* (IFM, Linköping University, Sweden. 2018-02-15).

Fabritius, H.-O.: *Small-scale structure-property relations in biological hard tissues by nanoindentation*. (Indentation 2018. Liège, Belgium. 2018-09-11 to 2018-09-14).

Fabritius, H.-O.: *Exploring biomimetic oral care concepts using advanced electron microscopy.* (The Goettingen Spirit Summer School "Symposium on mineralization and biometric concepts in dental research." Göttingen, Germany. 2018-09-18 to 2018-09-19).

Freysoldt, C.; Mishra, A. Ashton, M.; Neugebauer, J.: *Density-functional modelling of field evaporation.* (Atom probe tomography and microscopy conference 2018. NIST, Gaithersburg, USA. 2018-06-10 to 2018-06-16).

Garzón-Manjón, A.; Meyer, H.; Grochla, D.; Ludwig, A.; Scheu, C.: *Insights in the structure and composition of nanoparticles for energy applications*. (Advanced Structural and Functional Materials. Krakow, Poland. 2018-08-20 to 2018-08-24).

Gault, B.; Kontis, P.; Zhao, H.; Kwiatkowski da Silva, A.; Makineni, S. K.; Chang, Y.; Ponge, D.; Raabe, D.: *Segregations at defects and interfaces and their relations to properties*. (TMS 2018. Phoenix, AZ, USA. 2018-03-11 to 2018-03-15).

Gault, B.; Kontis, P.; Cormier, J.; Raabe, D.: *From systematic characterisation to the next generation of high performance materials.* (THERMEC 2018. Paris, France. 2018-07-08 to 2018-07-13).

Glensk, A.: *From Thermodynamics to phonon lifetimes: Anharmonic calculations with ab initio accuracy.* (CECAM workshop: Anharmonicity and thermal properties of solids. Paris, France. 2018-01-10 to 2018-01-12).

Grabowski, B.; Hadian, S.; Nematollahi, A.; Kirchlechner, C.; Dehm, G.; Neugebauer, J.; Ko, W.S.; Jeon, J.B.: *Dislocation-twin boundary interactions in nanoscale Cu bi-crystals: Simulation versus experiment.* (Schöntal Symposium - Dislocation based Plasticity, Schöntal. Germany. 2018-02-26 to 2018-02-01).

Grabowski, B.; Zhu, L.; Neugebauer, J.: *Efficient and Accurate Computation of Melting Temperatures and Enthalpies and Entropies of Fusion from Ab Initio.* (TMS 2018. Phoenix, USA. 2018-03-12 to 2018-03-15).

Grabowski, B.: *Knowledge driven engineering of materials: Development and application of ab initio based scale bridging methods.* (Seminar. HSU Hamburg, Germany. 2018-05-18).

Hadian, R.: *Grain boundary dynamics.* (Multiscale Materials Modeling (MMM 2018). Osaka, Japan2018-10-28 to 2018-11-02).

Hengge, K.: *Insight into the degradation of polymer based fuel cells*. (3rd international conference on Battery and Fuel Cell Technology. London, UK. 2018-09-10 to 2018-09-11).

Herbig, M.; Li, Y.; Kumar, A.; Morsdorf, L.; Qin, Y.; Mayweg, D.; Goto, S.; Sietsma, J.; Petrov, R.; Raabe, D.: *The role of carbon in the formation of white etching cracks*. (THERMEC 2018 Annual Meeting & Exhibition. Paris, France. 2018-07-08 to 2018-07-13).

Hickel, T.; Neugebauer, J.; Körmann, F.; Grabowski, B.; Todorova, M.: *Modelling Structural Materials in Realistic Environments by Ab Initio Thermodynamics.* (TMS 2018. Phoenix, Arizona. 2018-03-11 to 2018-03-15).

Hickel, T.; Bleskov, I.; Dey, P.; Körmann, F.; Grabowski, B.; Neugebauer, J.: *Strengthening mechanisms in a precipitation hardened high-Mn lightweight steel.* (6th ESISM Workshop on “Fundamental Issues of Structural Materials”. Kyoto, Japan. 2018-02-26 to 2018-02-28).

Hickel, T.; Lochner, F.; Ahn, F.; Eremin, I.: *Electronic properties, low-energy Hamiltonian and superconducting instabilities in $CaKFe_4As_4$.* (APS March Meeting 2018. Los Angeles, CA. 2018-03-05 to 2018-03-09).

Hickel, T.; Glensk, A.; Nazarov, R.; Aydin, U.; Hegde,O:; Grabowski, B.; Neugebauer, J.: *Ab initio thermodynamics of point defects in metals: Hydrogen, vacancies and their interaction.* (2018 Joint ICTP-IAEA School and Workshop on Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments. Miramare, Trieste, Italy. 2018-04-16 to 2018-04-20).

Hickel, T.: *Characterizing complex materials by ab initio methods.* (Abteilungskolloquium 8. Zerstörungs freie Prüfung. BAM Berlin, Germany, 2018-06-01).

Hickel, T.; Grabowski, B.; Körmann, F.; Glensk, A.: *Understanding phase stabilities and microstructure formation with finite temperature ab initio methods.* (MPIE Lecture Series. Düsseldorf, Germany. 2018-06-14).

Hickel, T.; Dey, P.; Dutta, B.; Friak, M.; Neugebauer, J.: *Phase stability and chemical composition of nano precipitates: A first principles study for the example of kappa carbides.* (Thermec2018. Paris, France. 2018-07-09 to 2018-07-13).

Huber, L.; Grabowski, B.; Neugebauer, J.; Rottler, J.; Militzer, M.: *High-throughput calculations and modelling of solute-GB segregation* (Thermec 2018 Conference. Paris, France. 2018-07-08 to 2018-07-13).

Jägle, E. A.: *New steels for and by Additive Manufacturing.* (JFE Steel Research Seminar. Chiba, Japan. 2018-03-15).

Jägle, E. A.: *Alloys and Additive Manufacturing: Conflict or Synergy?* (Seminar, IMDEA Madrid. Spain. 2018-05-18).

Jägle, E. A.: *Hot cracking in alloys produced by additive manufacturing.* (THERMEC 2018. Paris, France. 2018-07-08 to 2018-07-13).

Jägle, E. A.: *Impact of the process gas atmosphere in Laser Additive Manufacturing – desired and undesired effects*. (Alloys for Additive Manufacturing Symposium 2018. Sheffield, UK. 2018-09-03 to 2018-09-04).

Kirchlechner, C.: *Beyond Hall-Petch: Mechanism based description of dislocation grain-boundary interactions.* (Spring Meeting of the German Physical Society (DPG ), Berlin, Germany. 2018-03-11 to 2018-03-16).

Kirchlechner, C.; Malyar, N. V.; Dehm, G.: *Dislocation - Grain Boundary Interactions Probed by In-Situ Micromechanical Experiments*. (55th Annual Technical Meeting, SES2018. Madrid, Spain. 2018-10-10 to 2018-10-12).

Kontis, P.; Raabe, D.; Gault, B.: *The role of systematic characterization on the development of new nickel-based superalloys*. (Industrial Colloquium - SFB/TR 103 „From Atoms to Turbine Blades“. Fürth, Germany. 2018-03-06 to 2018-03-07).

Kontis, P.; Makineni, S. K.; Stephenson, L.; Chang, Y.; Cormier, J.; Ponge, D.; Raabe, D.; Gault, B.: *The Role of Atom Probe Tomography on the Development of the Next Generation of High Performance Materials*. (4th International Congress on 3D Materials Science (3DMS 2018). Helsingør (Elsinore), Denmark. 2018-06-10 to 2018-06-13).

Kühbach, M.; Roters, F.; Imran, M.; Bambach, M.; Breen, A. J.; Gault, B.; Bajaj, P.; Zhao, H.: *Scalable Quantifying of Evolving Descriptive Spatial Statistics in Full-Field Crystal Plasticity and Atom Probe Tomography.* (Institut für Metallkunde und Metallphysik, RWTH Aachen University, Germany. 2018-06-30).

Lee, S.; Liebscher, C.; Dehm, G.: *In-situ TEM study on deformation behaviors of CrMnFeCoNi single crystal high entropy alloys*. (European Solid Mechanics Conference (ESMC). Bologna, Italy. 2018-07-02 to 2018-07-06).

Lee, S.; Duarte, M. J.; Soler, R.; Kirchlechner, C.; Liebscher, C.; Oh, S. H.; Dehm, G.: *In-situ TEM Study of Dislocation Plasticity of a Single Crystal FeCoCrMnNi HEA*. (IAMNano 2018, The International Workshop on Advanced and In-situ Microscopies of Functional Nanomaterials and Devices. Hamburg, Germany. 2018-10-14 to 2018-10-17).

Lee, S.; Duarte, M. J.; Soler, R.; Kirchlechner, C.; Liebscher, C.; Oh, S. H.; Dehm, G.: *In-situ TEM Study of Dislocation Plasticity of a Single Crystal FeCoCrMnNi HEA*. (ENGE 2018, 5th International Conference on Electronic Materials and Nanotechnology for Green Environment. Jeju, South Korea. 2018-11-11 to 2018-11-14).

Li, Z.; Raabe, D.: *Carbon and Nitrogen Co-doping in an Equiatomic High-entropy Alloy.* (TMS 2018. Phoenix, AZ, USA. 2018-03-11 to 2018-03-15).

Li, Z.; Raabe, D.: *Interstitially alloyed high-entropy alloys with improved mechanical properties*. (THERMEC 2018. Paris, France. 2018-07-08 to 2018-07-13).

Liebscher, C.: *Complex interfaces at the atomic scale: insights from aberration-corrected STEM*. (Inauguration colloquium Titan Themis G3 300. Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany. 2018-02-15).

Liebscher, C.: *Experimental insights into atomic scale phase transitions in metallic grain boundaries*. (International Workshop on Grain Boundaries and Dislocations towards High Performance Metals and Alloys. Beijing University of Technology, China. 2018-06-22).

Liebscher, C.: *Digitalization in materials characterization*, (9. Brazilian-German Frontiers of Science and Technology Symposium. Florianopolis, Brasil, 2018-10-08 to 2018-10-11).

Liebscher, C.: *Transmission Electron Microscopy: A tool to decipher the atomic structure of complex materials.* (Inauguration ceremony Talos F200X G2, Chair of Nonferrous Metallurgy, Montanuniversität Leoben, Leoben, Austria, 2018-10-31).

Lymperakis, L; Freysoldt C.; Neugebauer J.: *Elastically Frustrated Rehybridization: Implications in Alloy Ordering and Strong Compositional Limitations in Epitaxial InGaN Films.* (1st German Austrian Conference of Crystal Growth. Vienna, Austria. 2018-02-14 to 2018-02-16).

Malyar, N.V.; Micha, J.-S.; Dehm, G.; Kirchlechner C.: *Quantifying dislocation slip transmission by in situ micromechanics* (18th International Conference on the Strength of Materials (ICSMA18). Ohio State University. Columbus, OH, USA. 2018-07-15 to 2018-07-19).

Malyar, N. V.; Kirchlechner, C.; Dehm, G.: *Dislocation Transmission Through Grain Boundaries: Insights from In-Situ Micromechanical Experiments*. (Materials Science & Technology (MS&T 2018). Columbus, OH, USA. 2018-10-14 to 2018-10-18).

Molin, J.-B.; Renversade, L.; Malyar, N. V.; Ulrich, O.; Micha, J.-S.; Kirchlechner, C.: *Nondestructive 3D information on dislocation density and elastic strain in deforming micro-fatigue specimen*. (ESMC 2018. Bologna, Italy. 2018-07-02 to 2018-07-06).

Mouton, I.; Katnagallu, S.; Schwarz, T.; Makineni, S. K.; Printemps, T.; Grenier, A.; Barnes, J. P.; Cojocaru-Mirédin, O.; Raabe, D.; Gault, B.: *Calibration of Atom Probe Tomography Reconstructions from Correlation with Electron Tomograms or Micrographs*. (APT&M 2018, NIST. Gaithersburg, MD, USA. 2018-06-10 to 2018-06-15).

Neugebauer, J.; Todorova, M.; Grabowski, B.; Hickel, T.; Leyson, G.: *Understanding the fundamental mechanisms behind H embrittlement: An ab initio guided multiscale approach.* (Seminar, E2M (“Wall Forum”). Max-Planck-Institut für Plasmaphysik, Garching, Germany. 2018-02-26).

Neugebauer, J.; Janssen, J.; Körmann, F.; Grabowski, B.; Hickel, T.: *Exploration of large ab initio data spaces to design structural materials with superior mechanical properties.* (Hume-Rothery Award Symposium, TMS 2018. Phoenix, AZ, USA. 2018-03-11 to 2018-03-15).

Neugebauer, J.; Zhu, L.-F.; Koermann, F.; Grabowski, B.; Hickel, T.: *From electrons to the design of structurally complex materials.* (SFB ViCoM conference EPT 2018: From electrons to phase transitions. Vienna, Austria. 2018-04-03 to 2018-03-06).

Neugebauer, J.; Freysoldt, C.; Lymperakis, L.: *Understanding fundamental doping and stoichiometry limits in semiconductors by ab initio modelling.* (Plenary talk, EDS 2018 Conference. Thessaloniki, Greece. 2018-06-24 to 2018-06-29).

Neugebauer, J.; Hadian, S.; Huber, L.; Race, C.; Grabowski, B.: *Modelling thermodynamics and kinetics of general grain boundaries: Challenges and successes* (Thermec 2018 Conference. Paris, France. 2018-07-08 to 2018-07-13).

Neugebauer, J.; Freysoldt, C.: *First-principles approaches for charged defects in low dimensional systems.* (Conference on Physics of Defects in Solids: Quantum Mechanics meets Topology. Trieste, Italy. 2018-07-09 to 2018-07-13).

Neugebauer, J.; Lymperakis, L.; Freysoldt, C.: *Fundamental compositional limitations in the thin film growth of metastable alloys.* (Keynote lecture, 3rd Conference on Advanced Functional Materials. Vildmarkshotellet Kolmården, Norrköping, Sweden. 2018-08-21 to 2018-08-23).

Neugebauer, J.; Zhu, L.; Körmann, F.; Grabowski, B.; Hickel, T.: *Data driven approaches in materials design: theory meets experiment.* (RCTP-2018 Conference. Moscow, Russia. 2018-10-15 to 2018-10-19).

Neugebauer, J.; Janssen, J.; Koermann, F.; Grabowski, B.; Hickel, T.: *Exploration of large ab initio data spaces to design structural materials with superior mechanical properties.* (MMM 2018 Conference, Osaka, Japan. 2018-10-28 to 2018-11-02).

Neugebauer, J.: *Electronic structure and computational metallurgy.* (Workshop Coupling and linking simulations - EMMC expert meeting and roadmap, CECAM-HQ-EPFL, Lausanne, Switzerland. 2018-11-08 to 2018-11-09).

Neugebauer, J.; Ikeda, Y.; Körmann, F.; Grabowski, B.; Hickel, T.: *High entropy alloys beyond configurational entropy.* (MRS 2018 Conference. Boston, USA. 2018-11-25 to 2018-12-01).

Ponge, D.; Tarzimoghadam, Z.; Klöwer, J.; Raabe, D.: *Hydrogen-assisted Failure in Ni-base Superalloy 718 Studied under In-situ Hydrogen Charging: The Role of Localized Deformation in Crack Propagation*. (Spring Meeting of the German Physical Society (DPG ), Berlin, Germany. 2018-03-11 to 2018-03-16).

Ponge, D.; Dutta, A.; Sandlöbes, S.; Raabe, D.: *Strain partitioning in medium manganese steels.* (THERMEC 2018, Intl. Conf. on Processing & Manufacturing of Advanced Materials. Paris, France. 2018-07-09 to 2018-07-13).

Raabe, D.; Ponge, D.; Kwiatkowski da Silva, A.; Herbig, M.; Makineni, S. K.; Liebscher, C.; Yao, M.; Scheu, C.; Gault, B.: *Chemo-Mechanics in Metallic Alloys*. (16th Edition of the European Mechanics of Material Conference. Nantes, France. 2018-03-25 to 2018-03-28).

Raabe, D.; Ponge, D.; Kwiatkowski da Silva, A.; Herbig, M.; Makineni, S. K.; Katnagallu, S.; Stephenson, L.; Scheu, C.; Liebscher, C.; Gault, B.: *From Seeing Atoms Toward Understanding Atoms: Methods, Results and Challenges of Advanced Atom Probe Tomography.* (Hausdorff Lecture. Hausdorff Center for Mathematics, Rheinische Friedrich-Wilhelms-Universität Bonn, Germany. 2018-06-18).

Raabe, D.; Ponge, D.; Kwiatkowski da Silva, A.; Herbig, M.; Makineni, S. K.; Wu, X.; Katnagallu, S., Stephenson, L.; Zhao, H.; Koyama, M.; Kontis, P.; Scheu, C.; Liebscher, C.; Eggeler, G. F.; Spiecker, E.; Gault, B.: *Advancing Alloys by Segregation Engineering*. (18th International Conference on the Strength of Materials (ICSMA18), Ohio State University. Columbus, OH, USA. 2018-07-15 to 2018-07-19).

Raabe, D.; Ponge, D.; Kwiatkowski da Silva, A.; Makineni, S. K.; Katnagallu, S.; Stephenson, L.; Kontis, P.; Wu, X.; Freysoldt, C.; Neugebauer, J.; Gault, B.: *Segregation and Transformation at Lattice Defects as Microstructure Design Toolbox.* (Materials Science and Engineering Congress. Darmstadt, Germany. 2018-09-26 to 2018-09-28).

Rohwerder, M.: *Delamination of organic coatings: unraveling the underlying mechanisms.* (69th Annual Meeting of the International Society of Electrochemistry. Bologna, Italy. 2018-09-02 to 2018-09-07).

Rohwerder, M.: *High-throughput approaches in Corrosion Research by Scanning Flow Cell and Scanning Kelvin Probe.* (2nd Forum of Materials Genome Engineering in Beijing, China. 2018-10-14 to 2018-10-16).

Roters, F.; Sharma, L.; Diehl, M.; Shanthraj, P.: *Including Damage Modelling into Crystal Plasticity Simulations using the Düsseldorf Advanced Material Simulation Kit DAMASK*. (Symposium Nano and Micro Scale Damage in Metals. Utrecht, The Netherlands. 2018-02-08).

Roters, F.; Wong, S. L.; Shanthraj, P.; Diehl, M.; Raabe, D.: *Multi-physics simulation of advanced high strength steels.* (THERMEC 2018. Paris, France. 2018-07-11).

Scheu, C.: *3D $Nb_3O_7(OH)$ Nanoarrays – Structure, Stability and Functional Properties*. (Talk at Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, Germany. 2018-01-10).

Scheu, C.: *Defects in $AgSbTe_2$ thermoelectrics*. (3 Phase, Interface, Component Systems (PICS), Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), France. 2018-05-23 to 2018-05-25).

Scheu, C.: *Combining ultimate resolution: Cs corrected STEM and 3D atom probe tomography*. (Grand Opening of UC Irvine Materials Research Institute (IMRI) & the First International Symposium on Advanced Microscopy and Spectroscopy, University of California. Irvine, CA, USA. 2018-06-06 to 2018-06-08).

Scheu, C.; Folger, A.: *Tuning the properties of $TiO_2$ nanowires by heat treatment in various atmospheres*. (THERMEC 2018 – International conference on processing and manufacturing of advanced materials. Paris, France. 2018-07-09 to 2018-07-13).

Scheu, C.: *Electron Energy-Loss Spectroscopy in a Scanning Transmission Electron Microscope Fundamentals and Applications.* (Talk, New Technology Research Centre, University of West Bohemia. Pilsen, Czech Republic. 2018-07-17).

Scheu, C.: *Unraveling the secrets of interfaces and grain boundaries*. (Seminar, University of New South Wales, School of Materials Science and Engineering, Sydney, Australia. 2018-09-17).

Scheu, C.: *Insights in interfaces by combining Cs corrected STEM and APT experiments with atomistic simulations*. (Seminar, The University of Sydney, Faculty of Engineering & Information Technologies, Sydney, Australia. 2018-09-18).

Scheu, C.: *Nanostructured photocatalyst based on transition metal oxides*. (Seminar, National University of Singapore, Dept. of Materials Science and Engineering. Singapore. 2018-09-21).

Scheu, C.: *Insights in the structure and functionality of doped and undoped $Nb_3O_7(OH)$ nanoarrays*. (nanoGe Fall Meeting 2018. Torremolinos, Spain. 2018-10-22 to 2018-10-26).

Scheu, C.: *Interface characterization of applied materials at ultimate resolution*. (Seminar, Beijing Institute of Technology, Beijing, China. 2018-09-24).

Scheu, C.: *Degradation analysis of electrocatalyst using identical location STEM measurements*. (3rd Sino-German Symposium on Advanced Electron Microscopy of Interface Structures and Properties of Materials. Tsinghua University, Beijing, China. 2018-09-24 to 2018-09-27).

Sohn, S. S.; Jo, Y. H.; Choi, W.-M.; Kim, D. G.; Kim, H. S.; Lee B. J.; Lee S.: *Transformation-induced plasticity in HEA: FCC to BCC transformation*. (Thermec 2018. Paris, France. 2018-07-08 to 2018-07-13).

Todorova, M.; Surendralal, S.; Yoo, S.; Neugebauer, J.: *Atomistic insights into surface stability and reactivity at solid/liquid interfaces from first principles calculations.* (Technical University Vienna, Austria. 2018-04-10).

Todorova, M.; Surendralal, S.; Yoo, S.; Neugebauer, J.: *Insights into corrosion mechanisms from ab initio calculations.* (BASF "Corrosion Forum", Ludwigshafen, Germany. 2018-04-24).

Todorova, M.; Neugebauer, J.: *Insights into electrochemical problems from the perspective of semiconductor defect chemistry.* (Tutorial Lecture, International Workshop on Computational Electrochemistry (IWCE). Aalto University, Helsinki, Finland, 2018-07-09).

Todorova, M.; Yoo, S.; Surendralal, S.; Neugebauer, J.: *Stability and reactivity of solid/liquid interfaces from ab initio calculations.* (International Workshop on Computational Electrochemistry (IWCE), Aalto University, Helsinki, Finland. 2018-07-10 to 2018-07-12).

Todorova, M.; Yoo, S.; Surendralal, S.; Neugebauer, J.: *Ab initio modelling of solid/liquid interfaces: Challenges and insights.* (FS Seminar, DESY, Hamburg, Germany. 2018-10-30).

Todorova, M.; Vatti, A.K.; Yoo, S.; Surendralal, S.; Neugebauer, J.: *From semiconductor defect chemistry to electrochemistry: Challenges and insights.* (Keynote talk, AMaSiS 2018 Workshop. Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany. 2018-10-08 to 2018-10-10).

Soler, R.; Gleich, S.; Fager, H.; Achenbach, J.O.; Kirchlechner, C.; Schneider, J.M.; Scheu, C.; Dehm, G.: *$Mo_2BC$ thin films - a material system combining hardness and ductility?* (Keynote Lecture, 5th European Conference in Nanofilms ECNF2018. Cranfield University, Cranfield, UK. 2018-03-20 to 2018-03-22).

Stein, F.: *Microstructure Design from Liquidus Surfaces - The Value of Phase Diagrams for Materials Development*. (64th Metal Research Colloquium, Department for Metal Research and Materials Testing of the Montanuniversität Leoben. Lech am Arlberg, Austria. 2018-04-09 to 2018-04-11).

Stein, F.; Takaja, S.; Vogel, S. C.: *On the Structure and Stability of the γ Brass-type High-temperature Phase in Al-rich Fe–Al(–Mo) Alloys.* (TOFA 2018, Discussion Meeting on Thermodynamics of Alloys. Seoul, South Korea. 2018-10-01 to 2018-10-05).

Uebel, M.: *Redox-responsive coatings for smart corrosion protection: how to design highly responsive coatings?* (AMI's Self-Healing Polymers 2018. London, UK. 2018-10-08 to 2018-10-09).

Valtiner, M.: *Interfacial Structuring of Ionic Liquids in the Presence of Water: From Neat Liquids to Aqueous Solutions.* (Gordon Conference Aqueous Solutions and Electrolytes. Holderness, NH, USA. 2018-07-23 to 2018-07-28).

Waseda, O.: *Machine-Learning assisted Heisenberg model for systems with ill-defined magnetic interactions.* (Thermec 2018 Conference, Paris, France. 2018-07-08 to 2018-07-13).

Wippermann, S.: *Modeling electrochemical solid/liquid interfaces from first principles*. (Materialforschungstag Mittelhessen. Marburg, Germany. 2018-05)

Wippermann, S.: *Modeling electrochemical solid/liquid interfaces from first principles*. (IEEE Nano. Cork, Ireland. 2018-07)

Wippermann, S.: *Ab initio molecular dynamics simulations at constant electrode potential*. (Colloquium KIT. Karlsruhe, Germany. 2018-11)

Zavašnik, J.: *Beyond beautiful pictures: nanowires, nanotubes and nanoparticles in Transmission Electron Microscope*. (Talk at Zentrum für molekulare Spektroskopie und Simulation solvensgesteuerter Prozesse (ZEMOS), Fakultät für Chemie und Biochemie, Ruhr-Universität Bochum, Germany. 2018-08-02).

Zaefferer, S., Shan Y., Madivala M.: *Combination of nano-indentation and electron channeling contrast imaging (ECCI) to understand the interaction of hydrogen and dislocations in a high-Mn TWIP steel.* (Nanobrücken 2018. Erlangen, Germany. 2018-02-20 to 2018-02-22).

Zaefferer, S.: *Understanding the correlation of crystallographic character and corrosion behaviour of grain boundaries in a stainless steel using large-area 3D EBSD.* (RMS-EBSD conference. Plymouth, UK. 2018-04-10 to 2018-04-11).

Zaefferer, S., Abdellaoui, L., Rogowitz, A.: *Controlled electron channelling contrast imaging, cECCI, for quantitative and in-situ characterization of lattice defects in bulk samples of metals and minerals.* (19th International Microscopy Conference. Sydney, Australia. 2018.09-09 to 2018-09-14).

# Publications

## 2015 (not included in the Scientific Report 2013 - 2015)

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Zaefferer, S.; Wright, S. I.; and Konijnenberg, P. J.: *3D EBSD*. In François, B. (ed.), EBSD: Analyse par diffraction des électrons rétrodiffusés. GN-MEBA, Paris, France (2015) 159, ISBN-13: 978-2759819126

### Publications in Scientific Journals

Bashir, A.; Iqbal, D.; Jain, S. M.; Barbe, K.; Abu-Husein, T.; Rohwerder, M.; Terfort, A.; and Zharniko, M.: *Promoting Effect of Protecting Group on the Structure and Morphology of Self-Assembled Mono layers: Terphenylylethanethioactate on Au(111)*. J. Phys. Chem. C 119 (2015) 25352

Berezkin, A. V. and Kudryavtsev, Y. V.: *Effect of Cross-Linking on the Structure and Growth of Polymer Films Prepared by Interfacial Polymerization*. Langmuir 31 (2015) 12279

Cairney, J. M.; Rajan, K. K.; Haley, D.; Gault, B.; Bagot, P. A. J.; Choi, P.-P.; Felfer, P. J.; Ringer, S. P.; Marceau, R. K. W.; and Moody, M. P.: *Mining information from atom probe data*. Ultramicroscopy 159 (2015) 324

Chen, Z.; Liu, Y.; Wu, H.; Zhang, W.; Guo, W.; Tang, H.; and Liu, N.: *Microstructures and wear properties of surface treated Ti-36Nb–2Ta–3Zr–0.35O alloy by electron beam melting (EBM)*. Appl. Surf. Sci. 357 (2015) 2347

Choi, C. H.; Baldizzone, C.; Grote, J.-P.; Schuppert, A. K.; Jaouen, F.; and Mayrhofer, K. J. J.: *Stability of Fe–N–C Catalysts in Acidic Medium Studied by Operando Spectroscopy*. Angew. Chem. Int. Ed. 54 (2015) 12753

Choi, W. S.; De Cooman, B. C.; Sandlöbes, S.; and Raabe, D.: *Size and orientation effects in partial dislocation-mediated deformation of twinning-induced plasticity steel micro-pillars*. Acta Mater. 98 (2015) 391

Duff, A.; Davey, T.; Korbmacher, D.; Glensk, A.; Grabowski, B.; Neugebauer, J.; and Finnis, M.*: Improved method of calculating ab initio high-temperature thermodynamic properties with application to ZrC*. Phys. Rev. B. 91(2015) 214311

Erbe, A.; Schneider, P.; Gadiyar, C.; and Renner, F. U.: *Electrochemically triggered nucleation and growth of zinc phosphate on aluminium-silicon-coated steel*. Electrochim. Acta 182 (2015) 1132

Feckl, J. M.; Dunn, H. K.; Zehetmaier, P. M.; Müller, A.; Pendlebury, S. R.; Zeller, P.; Fominykh, K.; Kondofersky, I.; Döblinger, M.; Durrant, J. R.; Scheu, C.; Peter, L. M.; Fattakhova-Rohlfing, D.; and Bein, T.: *Ultrasmall $Co_3O_4$ Nanocrystals Strongly Enhance Solar Water Splitting on Mesoporous Hematite*. Adv. Mater. Interfaces 2 (2015) 1500358

Friák, M.; Tytko, D.; Holec, D.; Choi, P. P.; Eisenlohr, P.; Raabe, D.; and Neugebauer, J.: *Synergy of atom-probe structural data and quantum-mechanical calculations in a theory-guided design of extreme-stiffness superlattices containing metastable phases*. New J. Phys. 17 (2015) 093004

Gao, G.; Zhang, H.; Gui, X.; Tan, Z.; Bai, B.; and Weng, Y.: *Enhanced strain hardening capacity in a lean alloy steel treated by a "disturbed" bainitic austempering process*. Acta Mater. 101 (2015) 31

Geiger, S.; Cherevko, S.; and Mayrhofer, K. J. J.: *Dissolution of Platinum in Presence of Chloride Traces*. Electrochim. Acta 179 (2015) 24

Goerler, J. V.; Brinckmann, S.; Shchyglo, O.; and Steinbach, I.: *Gamma-channel stabilization mechanism in Ni-base superalloys*. Philos. Mag. Lett. 95 (2015) 519

Greczynski, G.; Patscheider, J.; Lu, J.; Alling, B.; Ektarawong, A.; Jensen, J. M.; Petrov, I. G.; Greene, J. E.; and Hultman, L.: *Control of $Ti_{1-x}Si_xN$ nanostructure via tunable metal-ion momentum transfer during HIPIMS/DCMS co-deposition*. Surf. Coat. Tech. 280 (2015) 174

Haley, D.; Choi, P.-P.; and Raabe, D.: *Guided mass spectrum labelling in atom probe tomography*. Ultramicroscopy 159 (2015) 338

Huang, L. F.; Grabowski, B.; McEniry, E.; Trinkle, D. R.; and Neugebauer, J.: *Importance of coordination number and bond length in titanium revealed by electronic structure investigations*. Phys. Status Solidi 252 (2015) 1907

Ko, W.-S.; Grabowski, B.; and Neugebauer, J.: *Development and application of a Ni-Ti interatomic potential with high predictive accuracy of the martensitic phase transition*. Phys. Rev. B 92 (2015) 134107

Koßmann, J.; Zenk, C. H.; Lopez-Galilea, I.; Neumeier, S.; Kostka, A.; Huth, S.; Theisen, W.; Göken, M.; Drautz, R.; and Hammerschmidt, T.: *Microsegregation and precipitates of an as-cast Co-based superalloy-microstructural characterization and phase stability modelling*. J. Mater. Sci. - Mater. El. 50 (2015) 6329

Körmann, F.; Hickel, T.; and Neugebauer, J.: *Influence of magnetic excitations on the phase stability of metals and steels*. Curr. Opin. Solid State Mater. Sci. 20 (2015) 77

Körmann, F.; Ma, D.; Belyea, D. D.; Lucas, M. S.; Miller, C. W.; Grabowski, B.; and Sluiter, M. H. F.: *"Treasure maps" for magnetic high-entropy-alloys from theory and experiment*. Appl. Phys. Lett. 107 (2015) 142404

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Li, Y.; Ponge, D.; Choi, P.-P.; and Raabe, D.: *Atomic scale investigation of non-equilibrium segregation of boron in a quenched Mo-free martensitic steel*. Ultramicroscopy 159 (2015) 240

Li, Z.; Sun, Y.; Lavernia, E. J.; and Shan, A.: *Mechanical Behavior of Ultrafine-Grained Ti–6Al–4V Alloy Produced by Severe Warm Rolling: The Influence of Starting Microstructure and Reduction Ratio*. Metall. Mater. Trans. A-Phys. Metall. Mater. Sci. 46 (2015) 5047

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Pašti, I. A.; Gavrilov, N. M.; Dobrota, A. S.; Momčilović, M. Z.; Stojmenović, M. D.; Topalov, A. A.; Stanković, D. M.; Babić, B. M.; Ćirić-Marjanović, G. N.; and Mentus, S. V.: *The Effects of a Low-Level Boron, Phosphorus, and Nitrogen Doping on the Oxygen Reduction Activity of Ordered Mesoporous Carbons*. Electrocatalysis 6 (2015) 498

Pei, Z.; Friák, M.; Sandlöbes, S.; Nazarov, R.; Svendsen, B.; Raabe, D.; and Neugebauer, J.: *Rapid theory-guided prototyping of ductile Mg alloys: from binary to multi-component materials*. New J. Phys. 17 (2015) 093009

Pierce, D. T.; Jiménez, J. A.; Bentley, J.; Raabe, D.; and Wittig, J. E.: *The influence of stacking fault energy on the microstructural and strainhardening evolution of Fe–Mn–Al–Si steels during tensile deformation*. Acta Mater. 100 (2015) 178

Pradeep, K. G.; Herzer, G.; and Raabe, D.: *Atomic scale study of CU clustering and pseudo-homogeneous Fe-Si nanocrystallization in soft magnetic FeSiNbB(CU) alloys*. Ultramicroscopy 159 (2015) 285

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Tholander, C.; Tasnádi, F.; Abrikosov, I. A.; Hultman, L.; Birch, J.; and Alling, B.: *Large piezoelectric response of quaternary wurtzite nitride alloys and its physical origin from first principles*. Phys. Rev. B 92 (2015) 174119

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Utzig, T.; Stock, P.; Raman, S.; and Valtiner, M.: *Targeted Tuning of Interactive Forces by Engineering of Molecular Bonds in Series and Parallel Using Peptide-Based Adhesives*. Langmuir 31 (2015) 11051

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Wheeler, J. M.; Niederberger, C.; Raghavan, R.; Thompson, G. B.; Weaver, M. L.; and Michler, J.: *Elevated Temperature, In Situ Micromechanical Characterization of a High Temperature Ternary Shape Memory Alloy*. JOM-J. Miner. Met. Mater. Soc. 67 (2015) 2908

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Dusthakar, D. K.; Menzel, A.; and Svendsen, B.: *A laminate-based modelling approach for rate-dependent switching in ferroelectric materials*, Proc. Appl. Math. Mech. (Special Issue). 15 (2015) 3

Soni, P. U.; Cojocaru-Mirédin, O.; and Raabe, D.: *Interface engineering and nanoscale characterization of Zn(S,O) alternative buffer layer for CIGS thin film solar cells*, 2015 IEEE, 42nd Photovoltaic Specialist Conf., PVSC 2015. (2015) 7355889

## 2016

### Books, Book Chapters and Editorial Work

Ebin, B. and Isik, M. I.: *Pyrometallurgical Processes for the Recovery of Metals from WEEE*. In WEEE Recycling: Research, Development, and Policies. Elsevier, New York, NY, USA (2016) 107, ISBN-13: 9780128033647

Erbe, A.; Sarfraz, A.; Toparli, C.; Schwenzfeier, K.; and Niu, F.: *Optical absorption spectroscopy at interfaces*. In Lang, P. R. and Y. Liu (eds.), Soft Matter at Aqueous Interfaces (Lecture Notes in Physics), Chapter 14. Springer International Publishing, Switzerland (2016) 459, ISBN-13: 978-3-319-24500-3

Fernández Solis, C. D.; Vimalanandan, A.; Altin, A.; Mondragon Ochoa, J. S.; Kreth, K.; Keil, P.; and Erbe, A.: *Fundamentals of Electrochemistry, Corrosion and Corrosion Protection*. In Lang, P. R. and Y. Liu (eds.), Soft Matter at Aqueous Interfaces (Lecture Notes in Physics), Chapter 2. Springer International Publishing, Switzerland (2016) 29, ISBN-13: 978-3-319-24500-3

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### Publications in Scientific Journals

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Lehmhus, D.; Busse, M.; von Hehl, A.; and Jägle, E. A.: *State of the Art and Emerging Trends in Additive Manufacturing: From Multi-Material processes to 3D printed Electronics*, MATEC Web Conf. 188 (2018) 03013

Schemmann, L.; Stallybrass, C.; Schröder, J.; Liessem, A.; and Zaefferer, S.: *Formation in Charpy tests of the heat-affected zone of large-diameter linepipe material*, Proceedings of the 12th International Pipeline Conference (2018)

Shalan, K. M.; AbdelMeguid, M. E.; Hatem, T. M.; Hegazi, H. A.; and Bahei-El-Din, Y. A.: *Model-based damage detection in piezoelectric fiber based composites*, Minerals, Metals and Materials Series 210809 (2018) 119

# Habilitation, Doctoral, Diploma, Master and Bachelor Theses

## Habilitation Theses

### 2016

*PD Dr. rer. nat. M. Rohwerder:* Wasserstoff in Metallen: neue Messverfahren zum Nachweis mit hoher räumlicher Auflösung (Ruhr-Universität Bochum)

### 2018

*Dr. rer. mont. C. Kirchlechner:* Dislocation Slip Transfer Mechanisms: Quantitative Insights from *in situ* Micromechanical Testing (Montanuniversität Leoben)

*PD Dr.-Ing. H. Springer:* Integrated Alloy and Processing Design of High Modulus Steels (RWTH Aachen)

## Doctoral Theses

### 2015 (not included in the Scientific Report 2013 - 2015)

*Dr.-Ing. C. Begau:* Characterization of crystal defects during molecular dynamics simulations of mechanical deformation (Ruhr-University Bochum)

*Dr. rer. nat. S. Betzler:* 3D Hierarchical $Nb_3O_7(OH)$ Superstructures: Synthesis, Structural Characterization and Photophysical Properties (LMU München), **with distinction "summa cum laude"**

*Dr. rer. nat. A. Müller:* Transmission Electron Microscopic Investigation of Several Nanostructured Photoelectrodes for Photoelectrochemical Water Splitting (LMU München)

*Dr.-Ing. J. Nellessen:* Effects of strain amplitude, cycle number and orientation on low cycle fatigue microstructures in austenitic stainless steel and aluminum (RWTH Aachen)

*Dr.-Ing. V. Schnabel:* Stiff and damage-tolerant metallic glasses (RWTH Aachen), **with distinction "summa cum laude"**

*Dr.-Ing. M. Wang:* Nanolaminate TRIP-TWIP martensite matrix steels: Design and Characterization (RWTH Aachen)

*Dr.-Ing. D. Yan:* Micromechanically guided design of graded ultrafine-grained dual-phase steel (Ruhr-Universität Bochum)

### 2016

*Dr. rer. nat. M. von Avenarius:* Mechanical properties in metallic glasses and their deformation mechanisms (RWTH Aachen)

*Dr. rer. nat. U. Aydin:* Interstitial solution enthalpies derived from first-principles: Knowledge Discovery using High-Throughput Databases (Universität Paderborn)

*Dr.-Ing. V. S. P. K. Bhogireddy:* Liquid metal induced grain boundary embrittlement: A multi-scale study (Ruhr-Universität Bochum)

*Dr. rer. nat. C. D. Fernández Solis:* Application of biopolymer-organosiloxane hybrid films as protective barrier on metallic surfaces (Ruhr-Universität Bochum)

*Dr. rer. nat. J.-P. Grote:* Design of a Novel Electrochemical Activity and Selectivity Analysis Instrument (Ruhr-Universität Bochum)

*Dr.-Ing. T. P. Harzer:* Nanostructure, thermal stability and mechanical properties of vapor phase deposited supersaturated Cu–Cr thin film alloys (Ruhr-Universität Bochum)

*Dr.-Ing. M. Lai:* Experimental-theoretical study of the interplay between deformation mechanisms and secondary phases in metastable β titanium alloys (RWTH Aachen)

*Dr. rer. nat. M. M. Lange:* The microstructural impact on high temperature corrosion in DMV 617 mod under coal-fired conditions (RWTH Aachen)

*Dr.-Ing. X. Li:* Al-rich Fe–Al based alloys: Phase equilibria, microstructures, coarsening kinetics and mechanical behavior (Ruhr-Universität Bochum)

*Dr.-Ing. V. M. Marx:* The mechanical behavior of thin metallic films on flexible polymer substrate (Ruhr-Universität Bochum)

*Dr.-Ing. P. Neddermann:* Martensitic Stainless Steel: Evolution of Austenite during Low Temperature Annealing and Design of Press Hardening Alloys (RWTH Aachen)

*Dr.-Ing. B. Philippi:* Micromechanical characterization of lead-free solder and its individual microstructure elements (Ruhr-Universität Bochum)

*Dr.-Ing. F. Ram:* The Kikuchi bandlet method for the intensity analysis of the Electron Backscatter Kikuchi Diffraction Patterns (RWTH Aachen), **with distinction „summa cum laude“**

*Dr.-Ing. A. Szczepaniak:* Investigation of intermetallic layer formation in dependence of process parameters during the thermal joining of aluminium with steel (RWTH Aachen)

*Dr.-Ing. Y. Toji:* Transformation Phenomena during Quenching and Partitioning Heat Treatment (RWTH Aachen)

*Dr.-Ing. T. Utzig:* A contribution to understanding interfacial adhesion based on molecular level knowledge (Ruhr-Universität Bochum), **with distinction ”summa cum laude”**

*Dr.-Ing. A. K. Vatti:* An ab initio study of muscovite mica and formation energy of ions in liquid water (Ruhr-Universität Bochum)

*Dr.-Ing. E. D. Welsch:* On the strain hardening mechanisms of a high-Mn lightweight steel (RWTH Aachen)

*Dr.-Ing. X. Wu:* Elementary deformation processes during low temperature and high stress creep of Ni-base single crystal superalloys (Ruhr-Universität Bochum)

*Dr.-Ing. J. Zhang:* Microstructure design via site-specific control of recrystallization and nano-precipitation (RWTH Aachen)

## 2017

*Dr. rer. nat. A. Altin:* Cyclodextrin for Zinc Corrosion Protection (Ruhr-Universität Bochum)

*Dr.-Ing. C. Baron:* On the design of alloys and synthesis for composite steels (RWTH Aachen)

*Dr. Eng. D. J. Bowden:* Assessment of Co-free hardfacing stainless steel alloys for nuclear applications (Manchester University, UK)

*Dr. rer. nat. H.-W. Cheng:* Probing the Solid/Liquid Interfacial Structure of Ionic Liquids and Battery Fluids by Surface Force Measurements: Influence of water, ions and surface chemistry in interfacial structuring (Ruhr-Universität Bochum), **with distinction ”summa cum laude”**

*Dr.-Ing. V. Dandapani:* Hydrogen Permeation based Potentiometry as a New Quantification Tool for Electrochemical Reactivity at Buried Interfaces and under Nanoscopic Electrolyte Layers (Ruhr-Universität Bochum)

*Dr.-Ing. N. N. Elhami:* Influence of strain path changes during cup drawing on the twinning activity in TWIP steels investigated by ECCI (RWTH Aachen)

*Dr. rer. nat. A. Folger:* The Influence of Post-Growth Heat Treatments and Etching on the Nanostructure and Properties of Rutile $TiO_2$ Nanowires (RWTH Aachen), **with distinction “summa cum laude”**

*Dr. rer. nat. S. Geiger:* Stability investigations of iridium-based catalysts towards acidic water splitting (Ruhr-Universität Bochum), **with distinction ”summa cum laude”**

*Dr. rer. nat. S. Gleich:* Investigation of Sputtered $Mo_2BC$ Hard Coatings: Correlation of Nanostructure and Mechanical Properties (RWTH Aachen)

*Dr. rer. nat. K. A. Hengge:* Investigation of alternative catalyst and support materials and their effect on degradation in high-temperature polymer-electrolyte-membrane fuel cells (RWTH Aachen), **with distinction "summa cum laude"**

*Dr. rer. nat. S. W. Hieke:* Solid state dewetting phenomena of aluminum thin films on single crystalline sapphire (RWTH Aachen)

*Dr. rer. nat. A. Koprek:* Element redistribution and defect formation at the CdS/CIGS interface (RWTH Aachen)

*Dr.-Ing. N. V. Malyar:* Dislocation transmission through copper grain boundaries at the micron scale (Ruhr-Universität Bochum)

*Dr.-Ing. K. D. Molodov:* Investigation of deformation mechanisms in magnesium crystals (RWTH Aachen)

*Dr.-Ing. L. Morsdorf:* Fundamentals of ferrous low-carbon lath martensite: from the as-quenched, to tempered and deformed states (RWTH Aachen)

*Dr.-Ing. E. Pizzutilo:* Towards On-Site Production of Hydrogen Peroxide with Gold-Palladium catalysts in Electrocatalysis and Heterogeneous Catalysis (Ruhr-Universität Bochum), **with distinction "summa cum laude"**

*Dr.-Ing. G. Polymeros:* Performance of catalysts in electrode structure – bridging the gap between fundamental catalyst properties and behavior in real applications (Ruhr-Universität Bochum)

*Dr.-Ing. G. Stechmann:* A Study on the Microstructure Formation Mechanisms and Functional Properties of CdTe Thin Film Solar Cells Using Correlative Electron Microscopy and Atomistic Simulations (RWTH Aachen)

*Dr. rer. nat. A. Stoffers:* Grain boundary segregation in multicrystalline Silicon studied by correlative microscopy (RWTH Aachen)

*Dr.-Ing. M. Stricker:* Die Übertragung von mikrostrukturellen Eigenschaften aus der diskreten Versetzungsdynamik in Kontinuumsbeschreibungen (KIT, Karlsruhe)

*Dr.-Ing. Z. Tarzimoghadam:* An investigation of hydrogen/microstructure interaction in complex nickel-based alloys: Multi-scale detection and embrittlement mechanisms (RWTH Aachen)

*Dr.-Ing. C. Toparli:* Passivity and passivity breakdown on copper: In situ and operando observation of surface oxides (Ruhr-Universität Bochum)

*Dr.-Ing. T. H. Tran:* Regenerative Nanocomposite-Coatings tailored for Smart Corrosion Protection (Ruhr-Universität Bochum)

*Dr.-Ing. Z. Wang:* Investigation of crystallographic character and molten-salt-corrosion properties of grain boundaries in a stainless steel using EBSD and ab-initio calculations (Ruhr-Universität Bochum)

*Dr.-Ing. M. Yao:* κ-carbide in a high-Mn light-weight steel: precipitation, off-stoichiometry and deformation (RWTH Aachen)

## 2018

*Dr.-Ing. F. Archie:* Microstructural influence on micro-damage initiation in ferritic-martensitic DP-steels (RWTH Aachen)

*Dr. rer. nat. Y.-H. Chen:* A comprehensive in situ spectroscopic study of 2-mercaptobenzothiazole as a corrosion inhibitor for copper (Ruhr-Universität Bochum)

*Dr.-Ing. W. S. Choi:* Deformation mechanisms and the role of interfaces in face-centered cubic Fe-Mn-C micro-pillars (RWTH Aachen)

*Dr. rer. nat. A. Frank:* Synthesis and in-depth electron microscopic characterization of solvothermally grown copper indium sulfide thin films (RWTH Aachen)

*Dr.-Ing. Q. Hu:* A Contribution to Elucidate Interfacial Electric Double Layer Structures and Their Effects on Tribological Phenomena Using Force Microscopy (Ruhr-Universität Bochum)

*Dr.-Ing. S. S. Katnagallu:* On chemically sensitive atomic scale imaging (Ruhr-Universität Bochum), **with distinction "summa cum laude"**

*Dr.-Ing. W. Krieger:* Charakterisierung von Wasserstofffallen und deren Einfluss auf die Wasserstoffversprödung in ferritischen Stählen (Ruhr-Universität Bochum)

*Dr.-Ing. A. Kwiatkowski da Silva:* Phase nucleation through confined spinodal fluctuations at crystal defects in Fe–Mn alloys (RWTH, Aachen), **with distinction "summa cum laude"**

*Dr. rer. nat. F. Niu:* Investigation of interfacial water structure at Ge(100)/electrolyte interfaces by attenuated total reflection infrared spectroscopy (Ruhr-Universität Bochum)

*Dr. rer. nat. J. S. Mondragón Ochoa:* Preparation of Polyacrylic Thin Films on Iron by Controlled Radical Polymerization and their Delamination Behaviour (Ruhr-Universität Bochum)

*Dr.-Ing. Z. Peng:* Nano-scale investigation of the degradation mechanism of multilayer protective coating for precision glass molding (RWTH Aachen)

*Dr. rer. nat. J. Rechmann:* Modification of metal surface electronic properties by phenothiazine based SAMs (Ruhr-Universität Bochum)

*Dr.-Ing. M. Schwan:* Synthese und Eigenschaften flexibler Resorcin-Formaldehyd- und Kohlenstoffaerogele (RWTH Aachen)

## Master Theses

## 2015 (not included in the Scientific Report 2013 - 2015)

*Grabowski, M.:* Implementation of atomic spin constraints in the density-functional theory package S/PHI/nX (Heinrich-Heine-Universität, Düsseldorf)

*Lennartz, F.:* Entwicklung eines automatisierten Profiling-Systems zur Dokumentation von Laufzeit und Speicherverbrauch für die Kristallplastizitätssoftware DAMASK (Fachhochschule Aachen)

*Lu, L.:* Characterization of the crack formation mechanism in Ni-based superalloy Inconel 738LC produced by Selective Laser Melting (SLM) (RWTH Aachen)

## 2016

*Ksiazkiewicz, A.:* Investigation of the surface chemistry of gelatine films on zinc (Ruhr-Universität Bochum)

*Li, X.:* Investigation of grain boundary fracture resistance in DP steel (RWTH Aachen)

*Pander, M.:* Depth-dependent vibrational spectroscopy at a water/electrode interface (Ruhr-Universität Bochum)

*Qin, S.:* Measurement of solidification characteristics of steel during Selective Laser Melting using high-speed pyrometry (RWTH Aachen)

*Rashevski, D.:* Development of an Interface to Couple the Düsseldorf Advanced Material Simulation Kit (DAMASK) with the Open Source Finite Element Library deal.II (RWTH Aachen)

*Surendralal, S.:* Automated Calculations for Charged Point Defects in Magnesium Oxide and Iron Oxides (Ruhr-Universität Bochum)

*Wu, L.:* Characterization of the microstructure and impurities of Al–Mg–Sc alloy produced by Laser Additive Manufacturing (RWTH Aachen)

## 2017

*Ackers, M.:* Recommissioning of a metal powder atomisation system and investigation of its suitability to produce powders for additive Manufacturing processes (Ruhr-Universität Bochum)

*Mishra, A.:* First principles calculations on field evaporation from metal surfaces (Ruhr-Universität Bochum)

*Nastola, J.:* Multi-scale modeling of hydrogen transport (Heinrich-Heine Universität, Düsseldorf)

*Parra Moran, C.:* Atomic scale analysis of grain boundary segregation in pearlitic steel (Escuela Superior Politécnica del Litoral, Guayaquil, Ecuador)

*Qin, Y.:* Effect of post-heat treatment on the microstructure and mechanical properties of SLM-produced IN738LC (RWTH Aachen)

## 2018

*Baumgartner, L.-M.:* Adsorption of coiled-coil peptides on substrates for ATR-IR spectroscopy (Heinrich-Heine-Universität, Düsseldorf)

*Böckmann, M.:* High-throughput thermodynamic modelling of precipitate formation employing empirical potentials (Heinrich-Heine-Universität, Düsseldorf)

*Changizi, R.:* Cathodoluminescence study of lanthanide-doped oxides (Heinrich Heine Universität, Düsseldorf)

*Gänsler, T.:* Synthesis approaches to $Nb_3O_7(OH)$ nanostructures and new studies on their growth mechanism (LMU München)

*Qin, S:* Measurement of solidification characteristics of steel during Selective Laser Melting using high-speed pyrometry (RWTH Aachen)

*Shan, Y.:* Investigation on the Influence of Hydrogen on Dislocation Formation during Nanoindentation in TWIP Steels (RWTH Aachen)

*Shayanfar, N.:* Ab-initio Thermodynamics of Interfaces of Metal-Heusler Composites (Ruhr-Universität Bochum)

*Yang, Y.:* 3-dimensional investigation of the crystallographic prior-austenite grain boundary characters in martensitic steels (RWTH Aachen)

*Yilmaz, C.:* Microstructural Investigations of Heavily Rolled Ni-9at.%W Sheets Designed as Substrate for Superconducting Layers (RWTH Aachen)

## Bachelor Thesis

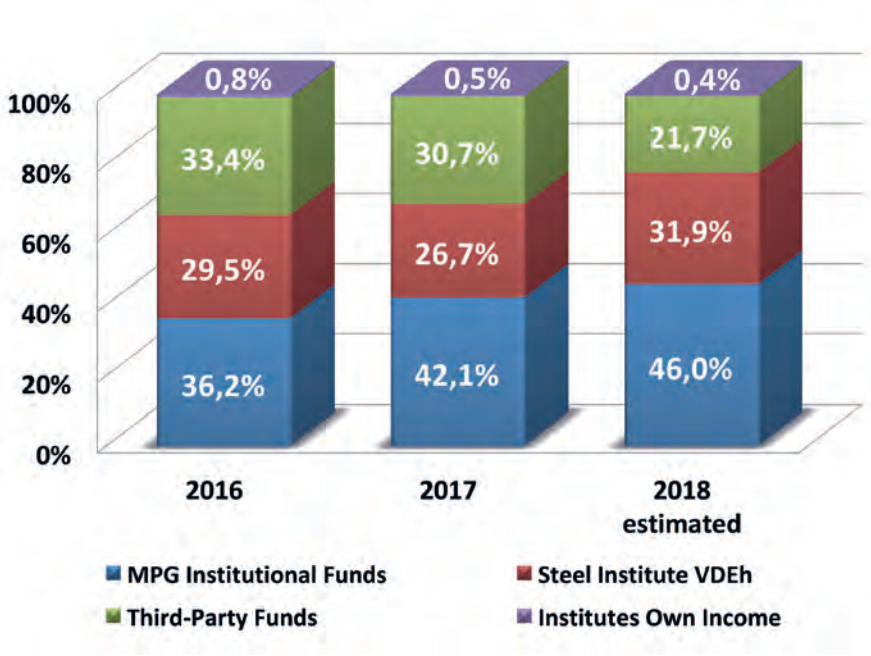
## 2018

*Bueno Villoro, R.:* Effect of the processing route on the microstructure of $Ag_{18}Sb_{29}Te_{53}$ (AST) based thermo-electrics (Universitat Autonoma de Barcelona, Spain)

# Budget of the Institute

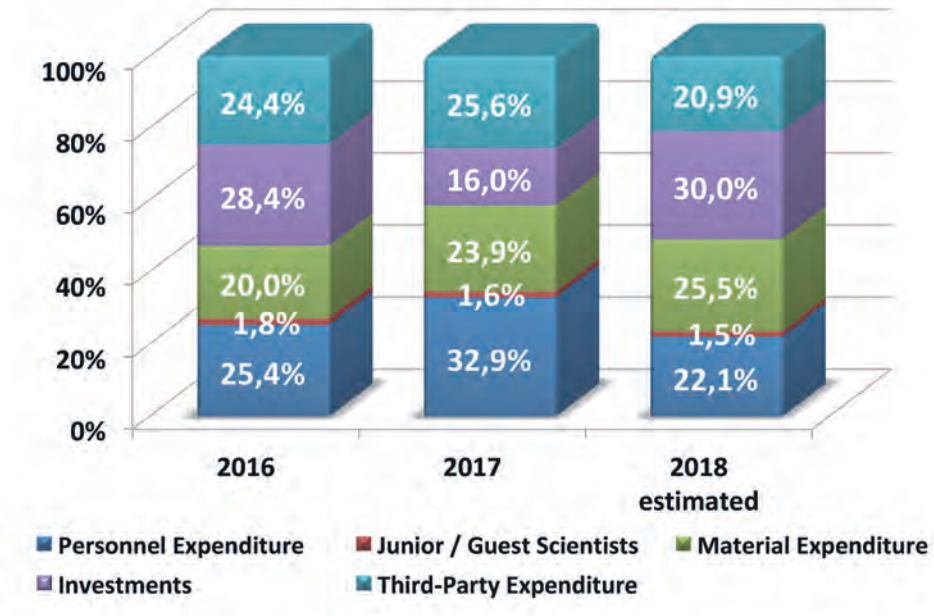
## Revenue

(Percentual contributions to total revenue without appointment-related investment funds and general reconstruction of the buildings; year 2018 data estimated)



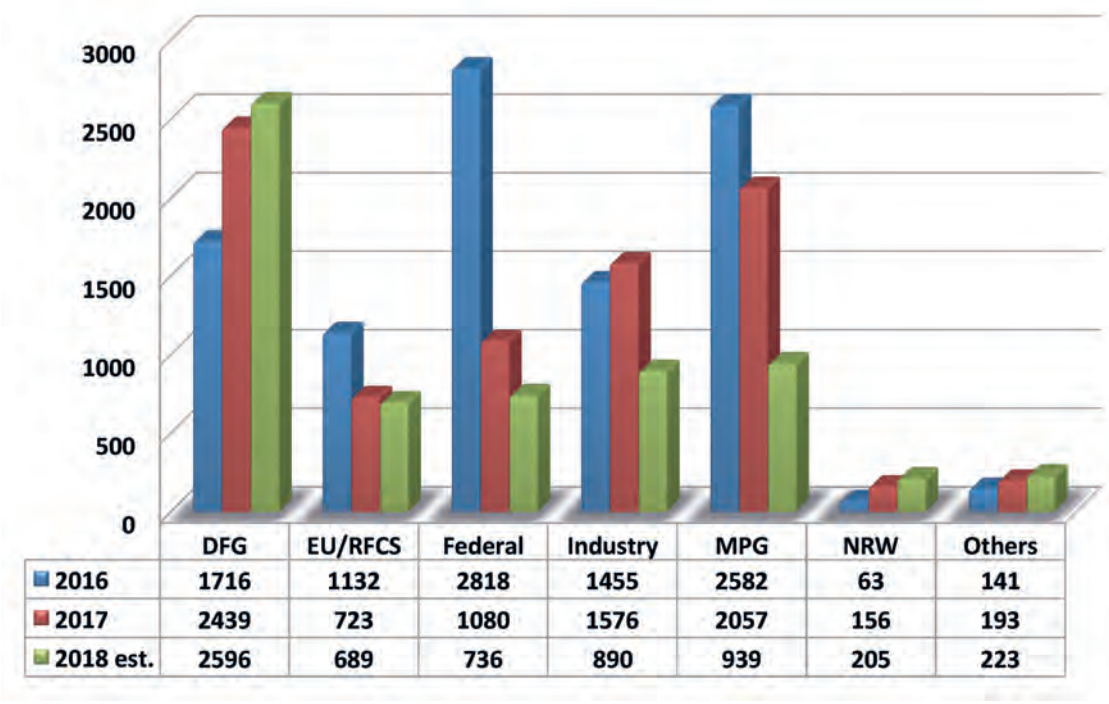

## Expenditure

(Percentual distribution of total expenditure; investments include large-scale apparatus, electronic data processing, appointment-related investments, separate investment for basic equipment; year 2018 data estimated)



# Third-Party Funds

(Contributions in 1,000 € to total revenue including personnel, material and investements, year 2018 data estimated)

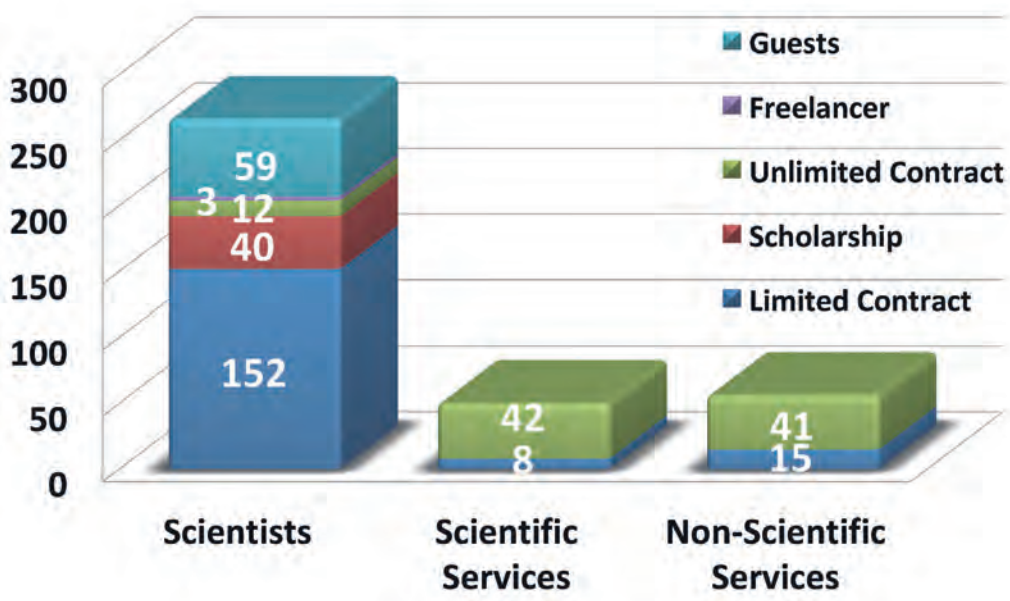



| | DFG | EU/RFCS | Federal | Industry | MPG | NRW | Others |
|---|---|---|---|---|---|---|---|
| 2016 | 1716 | 1132 | 2818 | 1455 | 2582 | 63 | 141 |
| 2017 | 2439 | 723 | 1080 | 1576 | 2057 | 156 | 193 |
| 2018 est. | 2596 | 689 | 736 | 890 | 939 | 205 | 223 |

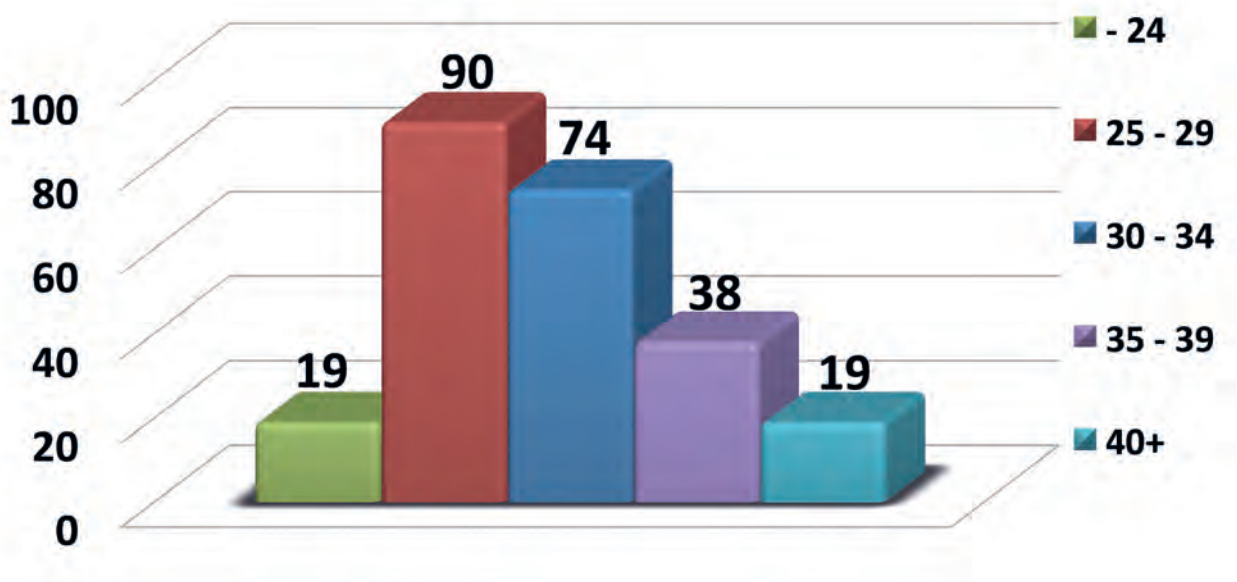
DFG: German Science Foundation
EU: European Union
RFCS: Research Fund for Coal and Steel
Federal: BMBF & BMWi
BMBF: Federal Ministry of Science and Education
BMWi: Federal Ministry of Economics and Technology
Industry incl. Christian Doppler Society and MaxNet
MPG: Max Planck Society
NRW: State of North Rhine-Westphalia
Others: Diverse expenditure on material costs (e.g. Humboldt Foundation, Merkle Foundation)

# Personnel Structure

## Number of Occupied Scientific / Non-Scientific Positions
(Absolute numbers, September 2018)

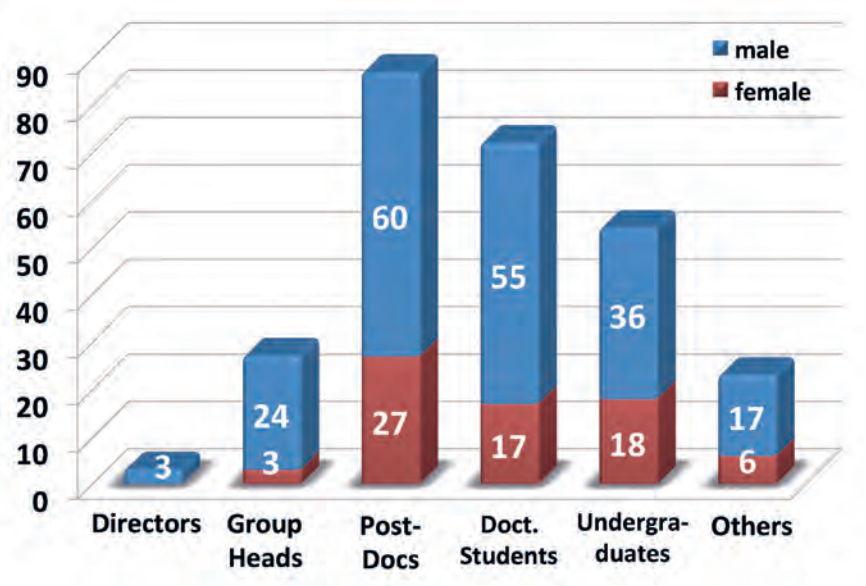



## Age Distribution of Junior Scientists
(Absolute numbers, September 2018)



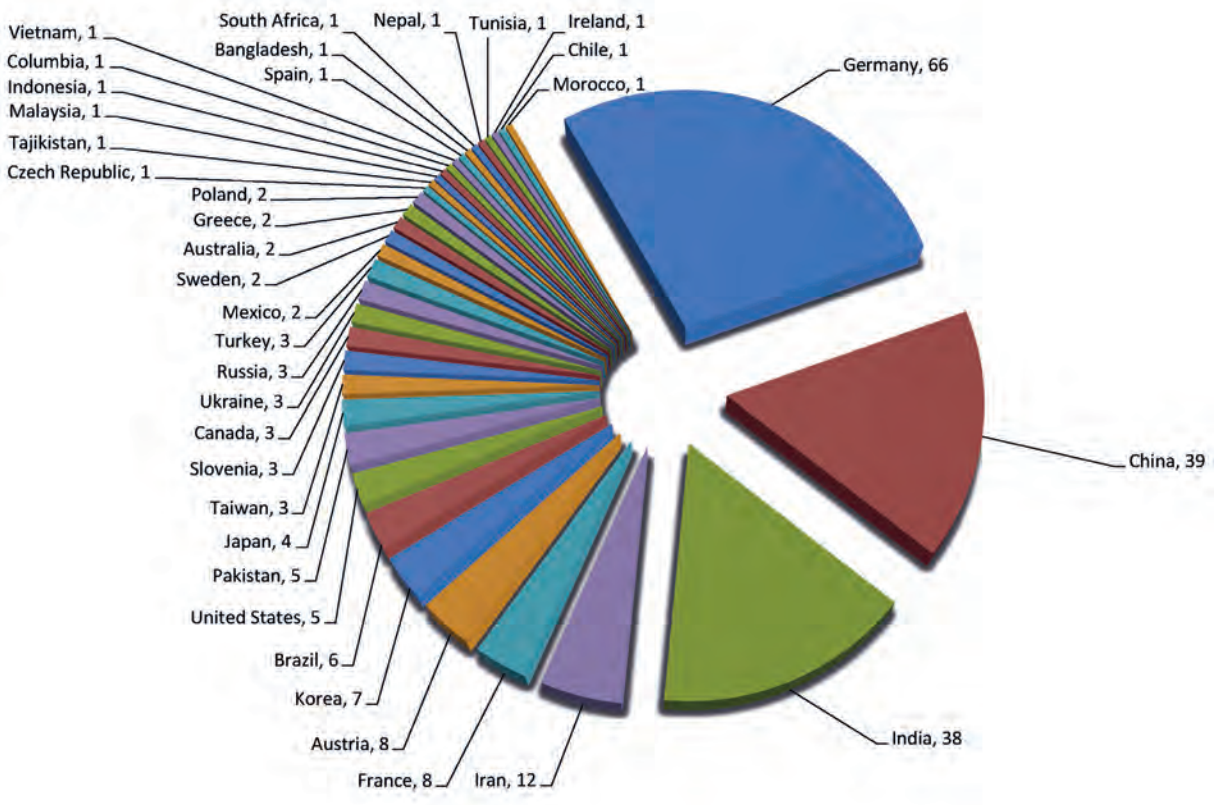
## Gender Distribution of Scientists

(Absolute numbers, September 2018)



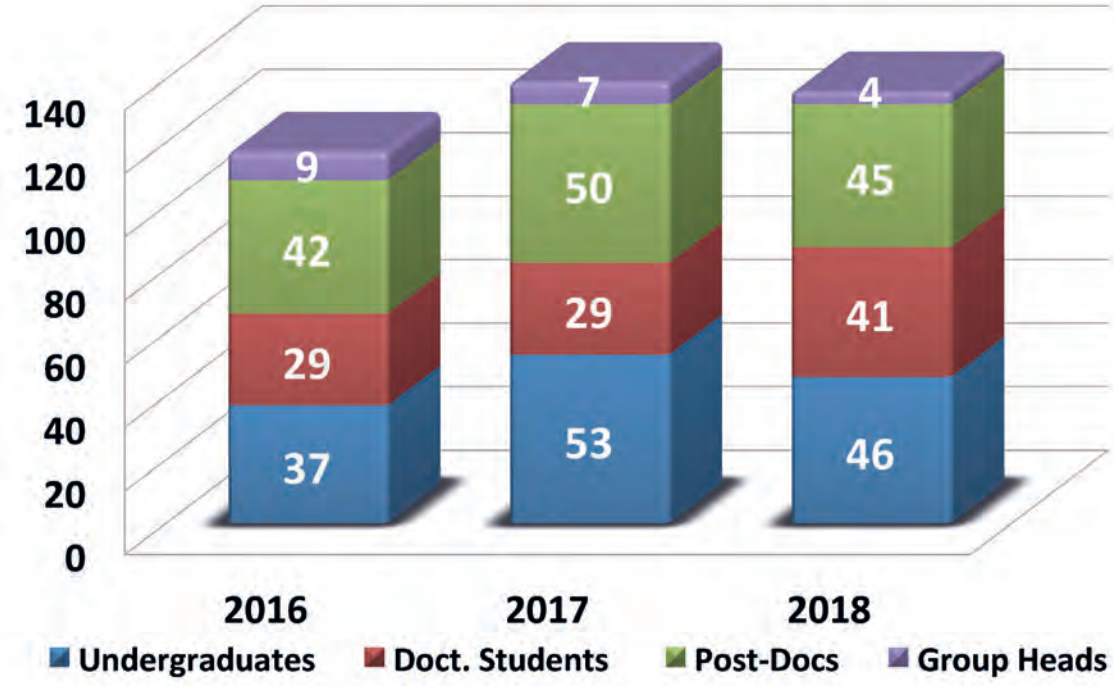

## Scientists and their Home Countries

(Absolute numbers, September 2018)



## Number of Junior Scientists (Absolute numbers, year 2018 data estimated)

### Financed via Third-Party Funds




### Not Financed via Third-Party Funds