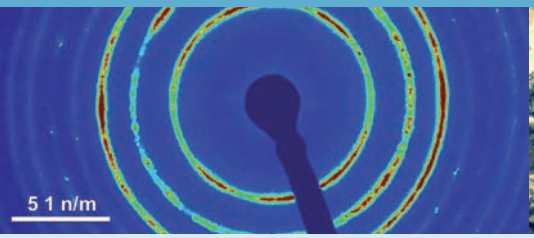
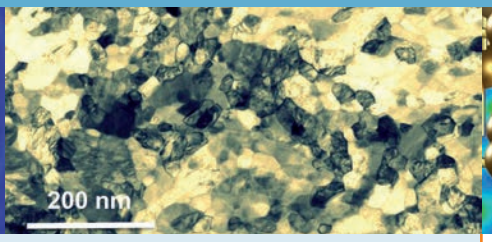
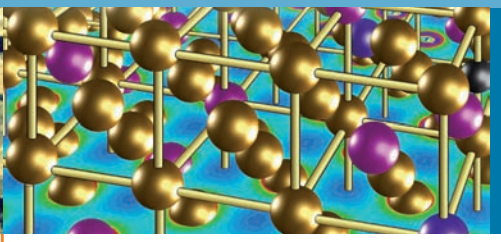
Max-Planck-Institut für Eisenforschung GmbH







Structure and Nano-/Micromechanics of Materials

Plasticity, fatigue and fracture of materials are usually caused by local deformation processes. The improvement of the mechanical performance and lifetime of materials is the aim of the new department "Structure and Nano-/Micromechanics of Materials" headed by Prof Gerhard Dehm.

Yasmin A. Salem (S): What is the mission of the new department?

Prof Dr Gerhard Dehm (D): We have several aims. First of all we want to develop experimental methods to perform quantitative nano-/micromechanical and tribological tests for complex and miniaturized materials. Additionally, we aim at understanding the underlying deformation mechanisms and by that establish material laws for the local and global mechanical behaviour. The development of these laws will allow us to generate new nanostructured materials and high temperature intermetallics with superior mechanical properties.

S: So the focus will be on nano sized materials. Why this?

D: Materials show a totally different behaviour at the micro and nano scale compared to their bulk counterparts. The analysed dimensions are that small that defects in the materials correspond directly with the size of the sample. This results in exceptional material properties which then can be transferred to bulk materials.

S: Which materials will you analyse?

D: For small scale materials I am especially interested in thin film systems such as metastable metallic films or brittle films on flexible substrates. For bulk materials, high temperature materials and complex steels will play a central role. Also the assembly of ceramics and polymers with different kinds of metals will be of research interest.

S: And what about the characterisation methods?

D: A cornerstone of my work is the combination of advanced characterisation and mechanical testing in form of in situ nano-/micromechanical experiments which permit to simultaneously observe the microstructural changes while measuring the mechanical response. Therefore, atomic resolved high-resolution transmission electron microscopy (TEM), analytical and conventional TEM, scanning TEM and scanning electron microscopy with electron backscattered diffraction (SEM/EBSD), focussed ion beam microscopy (FIB), X-ray diffraction and synchrotron radiation techniques will be used. The synthesis of miniaturized nanostructured materials will be done by physical vapour deposition

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EDITORIAL

Dear Reader,

Currently, the MPIE experiences some exiting changes: A new department focussing on nanomechanics was established and new initiatives such as a group on „Functional Materials and Interaction Forces" were formed.

Here we inform you on these recent developments and on important projects such as the newly established possibility to conduct rapid alloy prototyping with methods that drastically shorten alloy maturation studies to a few hours.

Enjoy reading and all the best from the Max-Planck team,

Prof. Dr. Dierk Raabe
(Chief Executive, MPIE)

Awards and Achievements

Fady Archie, Egyptian master student at the RWTH Aachen and currently doing his research at the MPIE, won the 1st prize in the Science Slam Competition "FameLab NRW".

Dr Serhiy Cherevko received the Electrochimica Acta Travel Award for Young Electrochemists, in recognition of the quality of his scientific research and contribution to the International Society of Electrochemistry Annual Meeting 2013 in Santiago de Querétaro, Mexico.

Dr Martin Friak won the Best Poster Award for his poster about Ab initio studies of single-crystalline and polycrystalline elastic properties of Mg-substituted calcite crystals at the Euro BioMat 2013 in Weimar, Germany.

Dr Anna Janus received the 1st prize of the Polish Materials Society for the best doctoral thesis in 2011 at the Institute of Metallurgy and Materials Science of the Polish Academy of Sciences. She studied the morphology of hydroxyapatite of natural origin.

Dr Ioannis Katsounaros received a Marie Curie International Outgoing Fellowship. He will continue his research in the Argonne National Laboratory (USA) and at the University of Leiden (Netherlands).

techniques.

S: How is the department structured?

D: The department is structured in interlinked groups each led by one group head. The groups are:
- Nano-/micromechanics of materials
- Advanced microstructure characterisation
- Nanotribology
- Synthesis of nanostructured materials
- Intermetallic materials

Moreover, my department will closely collaborate with the other MPIE departments especially in terms of modelling the phenomena on the nano scale by crystal plasticity and DFT methods, characterisation by means of atom probe tomography and in terms of developing new coatings for applied materials.

S: Are there already external collaborations?

D: We have well established links with research institutes and universities especially in the field of advanced TEM, synchrotron radiation and micro-/nanomechanical testing. However we also collaborate with industry on basic research topics. Just in April we started a research project on small scale mechanics within an EU project driven by industry developing reliable materials for the next generation of power semiconductor devices.

S: What are the main challenges in your research?

D: There are several challenges. Firstly, we have to develop mechanical testing techniques which permit to obtain quantitative data of materials with micron and submicron dimensions. While some commercial solutions exist, new developments have to be made to permit tests at variable temperatures or in different chemical environments. As the tested material volume is small, interpretation of the mechanical data needs new testing protocols and complementary simulations to extract meaningful data. To link the mechanical results to mechanisms we have to implement the testing techniques as in situ methods into the SEM, TEM, and X-ray/synchrotron facilities. What we want to learn are how material dimensions, internal interfaces and surfaces control the material properties from the atomistic level up to the micron scale with a focus on mechanical issues such as dislocation plasticity, fatigue, and fracture. Small scale mechanics will also help to explore the mechanical limits and reliability of materials independent whether they are used as structural or functional components.

S: Where do you see the main application possibilities?

D: The department's research is especially interesting for applications in the nano- and microelectronics e.g. for automotive electronics, in power engineering and for flexible electronics. Other application possibilities are found in the field of corrosion protection and the processing of surfaces as the assembly of ceramics and polymers with metals will be a research question.

Short CV:

Prof Gerhard Dehm did his doctorate 1995 in material sciences at the Max Planck Institute for Metals Research in Stuttgart (Germany). Before joining the University of Leoben (Austria) in 2005 as a professor for Materials Physics, he continued his research as a post doc and later as a group leader in Stuttgart and had a research stay at the Technion in Haifa (Israel). In Leoben, Dehm was head of the Department of Materials Physics at the University of Leoben and director of the Erich Schmid Institute of Material Science of the Austrian Academy of Sciences. He joined the MPIE in October 2012.

Combinatorial Metallurgy and Processing: Rapid Alloy Prototyping

The conventional approach for the experimentally guided development of metallic structural materials typically consists of a number of iterative loops of bulk casting, hot and/or cold deformation, heat treatment, machining of tensile specimens and mechanical testing. However, this approach is often too time consuming. A more efficient investigation for the maturation of complex alloy systems is a method called Rapid Alloy Prototyping developed at the MPIE.

The idea of the group "Combinatorial Metallurgy and Processing" is to develop and deploy innovative methods for the accelerated synthesis, processing and testing of bulk metallic structural materials. The goal is to address the associated basic metallurgical questions and corresponding engineering issues more rapidly and efficiently and thus with a higher throughput than with conventional methods and step-by-step iterations of these parameters. One of the challenges is to produce not only reliable data with a limited amount of method-specific artifacts, but also enable to perform controlled thermo mechanical variations as they greatly influence the microstructure and mechanical properties of structural materials.

Rapid Alloy Prototyping

The group of Hauke Springer successfully developed a method termed Rapid Alloy Prototyping (RAP) which is based on semi-continuous high-throughput bulk casting, rolling, heat treatment and sample preparation techniques and currently allows for the evaluation of the mechanical (tensile and hardness testing) and basic microstructural (optical microscopy, x-ray diffraction) properties of up to 50 material conditions (i.e. 5 different alloy compositions with 10 different thermo-mechanical treatments each) within about 5 days. This quasi simultaneous evaluation enables that critical material parameters can be reliably pre-selected, simulations verified and transient kinetic states readily investigated.
The time between a design idea and the final evaluation of the materials´ mechanical and microstructural properties is reduced from several weeks or even months down to hours.

Synthesis and processing of innovative iron based materials

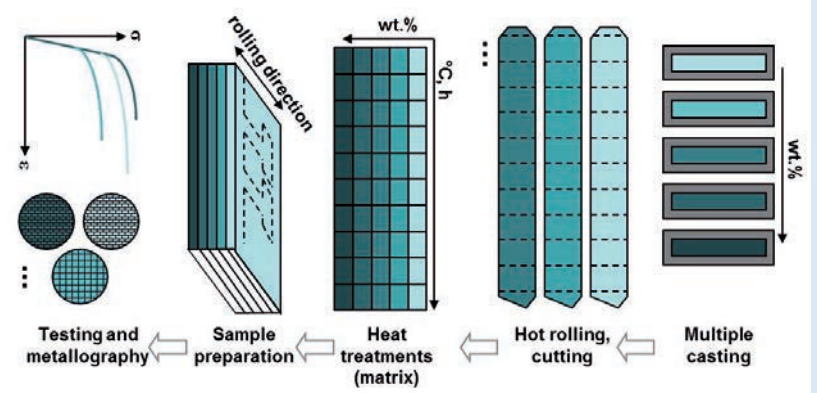
Currently, the focus of the alloy design performed within the group lies on high strength steels with inherent weldability, the generation of local microstructures by targeted creation of local chemical gradients and ultra-high strength pearlitic steel wires.
The design of such novel steels often goes hand in hand with the adaption and development of the synthesis and processing techniques. Furthermore, the early integration of key engineering properties such as weldability can greatly increase the overall scientific efficiency of the alloy design process. Examples for such developments are the installation of a new high power laser facility and an injection system for metallic or ceramic powders in a strip casting machine.

Maximum flexibility for a multitude of possible experimental conditions

The available instrumentation of the „Combinatorial Metallurgy and Processing" group ensures maximum flexibility for a multitude of possible experimental conditions, in order to perform highly controlled scientific experiments as well as material production close to industrial processing. The available equipment for material synthesis covers a range from small charge, high purity levitation and arc melting setups up to induction melting of about 70 kg of steel. Special experimental conditions comprise e.g. rapid solidification techniques, single crystal growth or electron beam remelting. Heat treatments can be performed under greatly varying conditions regarding atmosphere, heating media, heating- and cooling rates and sample size. Thermo mechanical processing of materials is done by rolling, forging, swaging or wire drawing.

Lightweight metallic systems, intermetallic materials and bulk metallic glasses

The spectrum of materials ranges from novel lightweight metallic systems such as titanium or magnesium-based alloys with additions of rare-earth elements, intermetallic materials such as Laves phases, to amorphous alloys such as bulk metallic glasses.



Rapid Alloy Prototyping: The mechanical and basic microstructural properties of up to 50 material conditions (i.e. 5 different alloy compositions with 10 different thermo-mechanical treatments each) can currently be evaluated within about 5 days.

Adhesion Reloaded
Interaction Forces and Functional Materials

A large variety of glues, adhesion promoting substances and functional coatings, with enhanced performances in wet or humid environments, are currently used in industrial applications. However, a fundamental understanding of their structure-property relationships in terms of the molecular interfacial details is very limited.

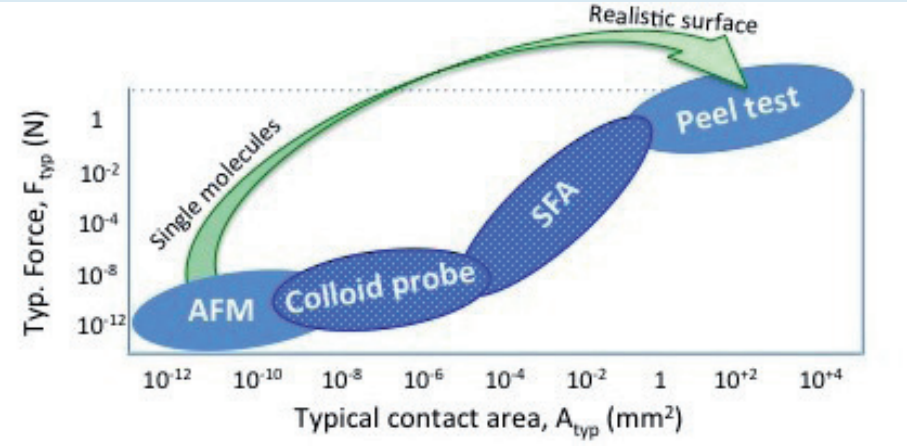
Nowadays, the replacement of toxic chromate based adhesion promoters by environmental-friendly alternatives is becoming reality in industrial applications, which use adhesives or adhesion-promoting substances e.g. for galvanically coated steel sheets or Aerospace adhesives and sealants. Beside self-assembled films, which are currently intensively investigated, bio-mimetic concepts (e.g., borrowed from musselfootproteins) are debated as environmental friendly, biodegradable green alternatives for adhesion promoters and glues[1,2].

Scaling of interactions, starting from single molecule up to multiple molecule interactions

The fundamental understanding of scaling of molecular interactions is a key-knowledge for prediction and prevention of degradation processes at composite materials interfaces, such as wet de-adhesion or electrochemically driven corrosive de-adhesion of polymers. Manipulation of single molecules, in particular measuring the mechano-chemistry of single molecules and probing their adhesive interactions have become state-of-the-art in interface science. However, a fundamental understanding and rationalization of the scaling of interactions, starting from single molecule up to multiple molecule interactions at solid-liquid interfaces remains an unexplored topic.

The novel electrochemical surface forces apparatus (EC-SFA) - Unravelling of structure/property relationships at electrified interfaces

Markus Valtiner and his group “Interaction Forces and Functional Materials” newly designed the electrochemical surface forces apparatus (EC-SFA), which is a central new experimental technique available at the MPIE. This unique set up allows for a simultaneous measurement of time dependent adhesion and friction forces, and absolute surface-surface



The new adhesion science and friction labs, which are fully operational since May 1st, allow now to test adhesion and friction at extended length and force scales, providing the means to understand macroscopic adhesion and friction phenomena based on their molecular level details. Currently, the group operates 2 AFMs (one is currently being equipped with tip enhanced Raman), one SFA-2000 and is setting up peel-test equipment.

Awards and Achievements

Dr Fritz Körmann won the Best Poster Award for his poster about Atomic forces at finite magnetic temperatures at the XLI Calphad conference in Berkeley (USA).

Andreas Leitner won the 1st prize of the Dörrenberg StudienAward for his excellent bachelor thesis about the microstructure of austenitic stainless steel $Cr_{18}Mn_{18}C0_{59}$ after total strain controlled loading at the University Duisburg-Essen.

Dr Karl Mayrhofer was awarded the Innovationspreis 2012 of North Rhine Westphalia in the category “Young Scientist“ for his research about electro catalysts.

Josef Meier received a Best Poster Award for his work on fuel cell catalyst stability as the best out of 129 contributions in the field of fuel cell research at the 63rd Annual Meeting of the International Society of Electrochemistry in Prague (Czech Republic).

Prof Dierk Raabe, chief executive, was elected as chairman of the Board of Governors of the RWTH Aachen. Moreover, he has been reappointed for a second period as a member of the German Council for Science and Humanities (Wissenschaftsrat).

separations between opposing electrified interfaces.

Correlation of molecular recognition forces and macroscopic adhesion forces

The "Interaction Forces and Functional Materials" group was established in June 2012. Future projects will focus on the direct correlation between friction forces and damage within friction traces by a combined approach of SFA (macroscale), AFM (micro- and nanoscale) and high-resolution imaging and elemental mapping techniques. Likewise, the investigation of adhesion and in particular the correlation of molecular recognition and macroscopic adhesion forces - based on design and synthesis of adhesion promoting and structure guiding molecules - will be a central focus of the group.

The technological interest of the group covers aspects from thin film coatings, surface roughness effects, electro-deposition of polymers, adhesion promoters and glues for automotive and aerospace applications to functional-bio-motivated materials for responsive coatings and sensing applications.

Selected Publications of M. Valtiner

M. Valtiner, S. H. Donaldson, M. A. Gebbie, J. N. Israelachvili:
Hydrophobic forces, electrostatic steering and acid-base bridging between atomically smooth self-assembled monolayers and end-functionalized PEGolated lipid bilayers. Journal of the American Chemical Society 134 (2012), no. 3, 1746-1753

M. Valtiner, M., K. Kristiansen, G. W. Greene, J. N. Israelachvili:
Effect of surface roughness and electrostatic surface potentials on forces between dissimilar surfaces in aqueous solution. Advanced Materials 23 (2011), 2294-2299

1 Elec. Acta 39 (8-9), 1207 (1994) & Elec. Acta 45 (15-16), 2515 (2000)

2 Science 318 (15-16), 2515 (2000) & J. of Adhesion 81 (3-4), 297 (2005)

Scientists at the MPIE

Dr Christoph Kirchlechner is head of the new group „Micro-/Nano-mechanics of Materials" since March 2013. He finished his PhD studies about plasticity at the micron scale in 2011 at the Erich Schmid Institute of the Austrian Academy of Sciences in Leoben (Austria) and worked for one year as a post doc at the University of Leoben. In 2012 he received the sub auspiciis Praesidentis rei publicae honours from the Austrian president. Since 2012 Kirchlechner works as an assistant professor at the University of Leoben. In his research at the MPIE he examines in situ micro- and nanomechanics of materials with synchrotron based characterisation techniques.

Dr Stefan Wippermann is the new head of the "Atomistic Modelling Group" in the department "Interface Chemistry and Surface Engineering". He worked as a post doc at the University of California (Davis/USA) supported by a scholarship of the Deutsche Forschungsgemeinschaft before joining the MPIE in 2013. His PhD thesis dealt with the understanding of substrate-supported atomic-scale nanowires from ab initio theory at the University of Paderborn and received the university's yearly award for an outstanding dissertation in 2011. Currently, Wippermann works on first principles electrochemistry in aqueous systems and on nano-composite materials with tailored electronic and optical properties for photovoltaics. With the latter project Wippermann successfully participated in the "NanoMatFutur" competition, organized by the German Federal Ministry of Education and Research (BMBF), and is one of seven participants now invited to submit a formal grant application to the BMBF.

Selected Publications

Computational Materials Design:
A. Nematollahi, J. v. Pezold, J. Neugebauer, D. Raabe: *Thermodynamics of carbon solubility in ferrite and vacancy formation in cementite in strained pearlite*. Acta Mat. 61, 5, 1773-1784 (2013)

J. Neugebauer, T. Hickel: *Density functional theory in materials science*. WIREs Comput Mol Sci (2013)

Interface Chemistry and Surface Engineering:
S. Nayak, P. Biedermann, M. Stratmann, A. Erbe: *A mechanistic study of the electrochemical oxygen reduction on the model semiconductor n-Ge(100) by ATR-IR and DFT.* Phys. Chem. 15 (2013), 5771-5781

S. Evers, M. Rohwerder: T*he hydrogen electrode in the "dry": A Kelvin probe approach to measuring hydrogen in metals*. Electrochemistry Communications 24 (2012) 85

Microstructure Physics and Alloy Design:
E. Marquis, P. Choi, F. Danoix, K. Kruska, S. Lozano-Perez, D. Ponge, D. Raabe, C. Williams: New insights into the atomic-scale structures and behavior of steels, Microscopy Today 20(4) 44-48 (2012)

O. Cojocaru-Miredin, P. Choi, R. Wuerz, D. Raabe: Exploring the p-n junction region in Cu (In,Ga)Se-2 thin-film solar cells at the nanometer-scale, Appl. Phys. Let. 101 (2012) 181603

Structure and Nano-/Micromechanics of Materials:
G. Dehm, J. Howe, J. Zweck: *In-situ Electron Microscopy: SEM and TEM Applications in Physics, Chemistry and Materials Science*. Wiley VCH Verlag, Weinheim, Germany 2012

Z. Zhang, H. Li, R. Daniel, C. Mitterer, G. Dehm: *Insights into the atomic and electronic structure triggered by ordered nitrogen vacancies in CrN*. Phys. Rev. B 87(2013), no. 1, 014104

Selected Talks

Computational Materials Design:

M. Todorova, J. Neugebauer: *Extending the Concept of Semiconductor Defect Chemistry to Electrochemistry.* TMS Annual Meeting and Exhibition, San Antonio, USA 3-7 Mar 2013

J. Neugebauer: *Materials Design based on Predictive Ab Initio Thermodynamics*. APS Baltimore, USA, 18-22 Mar 2013

Interface Chemistry and Surface Engineering:

M. Rohwerder: *Electrochemistry of metal surfaces under nanoscopic electrolyte layers*. 112th Bunsentagung to Karlsruhe Institute of Technology, Karlsruhe, Germany, 9-11 May 2013

K. J. J. Mayrhofer: *Stability of electrocatalysts on the nanoscale – identical-location transmission electron microscopy*. 29th One-Day-Symposium Electrochemistry Laboratory, Paul Scherrer Institut, Viligen PSI, Switzerland, 24 April 2013

Microstructure Physics and Alloy Design:

D. Raabe et al: *Nanoscale Transformations in Steels*. German-Chinese Workshop on 'Microstructure-driven Design and Performance of Advanced Metals', IMR, CAS, Shenyang, China, 12-16 April 2013

D. Raabe et al: *Scale-hoping approaches in designing complex alloys*. Royal Society International Seminar on 'Superalloys to Order' at the Kavli Royal Society International Centre, Chicheley Hall, England, 22-23 April 2013

Structure and Nano-/Micromechanics of Materials:

G. Dehm et al: *In situ micro- and nanomechanical electron microscopy studies of grain boundaries in Cu*. MRS Fall Meeting, Boston, USA, 25-30 Nov 2012

G. Dehm et al: *Plasticity and Fracture at Small Length Scales: from Single Crystals towards Interfaces. Workshop on Mechanical Behaviour of Systems - 4*. Coorg, Karnataka, India, 24-28 Feb 2013

News and Events

Past Events

Workshop: Alloy Design of Metallic High Performance Materials

On February 13th the MPIE organised a workshop on Alloy Design of Metallic High Performance Materials for leading experts from academia and industry. The programme included talks about the optimisation of dual phase steels, TRIP and TRIPLEX steels and the computational design of tool steels as well as a lab session.
This kind of workshops, with changing topics, is organised regularly and is open to experts from industry and academia. The aim is to enable in-depth discussions of fundamental and applied research.
For information on upcoming workshops, please contact:
research.coordination@mpie.de

Düsseldorf's Days of Career Planning

The MPIE took part at this year's Düsseldorf Days of Career Planning on March 20th. The aim was to present the various possibilities of doing a traineeship to pupils of different schools. The programme was organised through the Landeshauptstadt Düsseldorf, the Stiftung Pro Ausbildung and the Unternehmerschaft Düsseldorf. The MPIE presented the work of a material tester and a laboratory assistant.

Pupils doing experiments in the chemistry lab, March 20th, 2013.

Upcoming Events

Fascination of Steel: Open Day on July 12th

The MPIE, the Stahl-Zentrum and the VDEh-Betriebsforschungsinstitut open their doors for the broad public on July 12th from 2 – 10 pm. Many attractions for people of every age, such as tours through the laboratories of surface engineering and microstructure physics, will be presented. Moreover, kids will have the chance to do experiments by their own in the kids lab and during a children's lecture. Live music and an entertainment programme frame the Open Day.
The aim is to demonstrate the fascination of steel and to offer a direct contact with scientists and engineers. The entrance is free of charge.
For more information please contact:
research.coordination@mpie.de

Chemistry in everyday life: Kids Lab at the Open Day 2010.

Imprint

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