regular and up-to-date basis. Industry should not wait for the spread of publications, but instead be engaged in a direct and permanent exchange with researchers. Thirdly, industry should not hope for outsourcing effects. Research institutes cannot provide ready-made innovations. Innovations have to be generated by industry itself to guarantee long-term success. Moreover, science and industry must be open for new developments. There is a guideline which says 'form follows function': new materials will be hybrid, with complex structures and combining different elements. The same is true for the processing technique and the development of new materials. All these developments need to be perfectly handled by intelligent computer systems. This adaptation potential can only be achieved if appropriate research structures are in place. Finally: industry and research institutions have to foster joint research projects and share the responsibility. "One of my main objectives for my time as President of the Max Planck Society is to pool resources in Germany and build up an ideal research infrastructure with top institutions that are able to attract the best scientists from all over the world to study and do their research here", concludes Stratmann.

Stratmann was elected as President for the Max Planck Society during the general assembly in June 2013. Since June 2014, he is head of the Society for a six-year-term. At the same time, his department 'Interface Chemistry and Surface Engineering' at the MPIE will continue under the temporary leadership of Prof. Jörg Neugebauer, director of the department 'Computational Materials Design' at the MPIE.
(Photo: Frank Vinken)

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Scientists at the MPIE

Dr. Michael Rohwerder is head of the research group "Molecular Structure and Surface Modification" within the department "Interface Chemistry and Surface Engineering" and leads the Christian Doppler Laboratory "Diffusion and segregation mechanisms during production of high strength steel sheet" at the MPIE. Amongst other topics, he is currently analyzing novel applications of Kelvin probe techniques, self-healing mechanisms and grain boundary oxidation. Dr. Rohwerder has successfully issued patents for the process of coating fine particles with conductive polymers and of coating metallic surfaces with an anti-corrosive coating. Current projects include novel corrosion protection systems for hot stamping and guidelines for the use of welded stainless steel in corrosive environments. Besides his research, Rohwerder is also teaching at the Ruhr-University Bochum, Germany.

PD Dr. Stefan Zaefferer is head of the research group "Microscopy and Diffraction" within the department "Microstructure Physics and Alloy Design". During his PhD and postdoctoral studies he developed algorithms for electron diffraction analysis in TEM and SEM and studied deformation mechanisms of Titanium alloys and recrystallization mechanisms in cubic face centred metals. Zaefferer passed his habilitation treatise in 2009 at the University of Aachen, Germany, where he lectures since then a master course in materials technology. His research group at the MPIE examines mechanisms of microstructure and texture formation in metals and intermetallic materials mainly by electron microscopy. One of the current main research interests is the development of electron diffraction tools for scanning electron microscopes (EBSD & ECCI).

Selected Publications

Computational Materials Design:
R. Nazarov, T. Hickel, J. Neugebauer: *Ab initio study of H-vacancy interactions in fcc metals: Implications for the formation of superabundant vacancies*. Phys. Rev. B89, 14, 144108 (2014)

M. Todorova, J. Neugebauer: *Extending the concept of defect chemistry from semiconductor physics to electrochemistry*. Phys. Rev. Applied, 1, 014001 (2014)

Interface Chemistry and Surface Engineering:
S. Wippermann, M. Vörös, A. Gali, F. Gygi, G. Zimanyi, G. Galli: *Solar Nanocomposites with Comtemplementary Charge Extraction Pathways for Electrons and Holes: Si Embedded in ZnS*. PhysRevLett. 112, 106801 (2014)

I. Katsounaros, S. Cherevko, A.R. Zeradjanin, K.J.J. Mayrhofer: *Oxygen Electrochemistry as a Cornerstone for Sustainable Energy Conversion*. Angew. Chem. Int. Ed. 2014, 53, 102-121

Microstructure Physics and Alloy Design:
J. Duarte, J. Klemm, S. Klemm, K. Mayrhofer, M. Stratmann, S. Borodin, A. Romero, M. Madinehei, D. Crespo, J. Serrano, S. Gerstl, P. Choi, D. Raabe, F. Renner: *II. Element-Resolved Corrosion Analysis of Stainless-Type Glass-Forming Steels*. Science 2013; 341: 372-376

M. Herbig, D. Raabe, Y. Li, P. Choi, S. Zaefferer, S. Goto: A*tomic-Scale Quantification of Grain Boundary Segregation in Nanocrystalline Material*. PhysRevLett. 112 126103 (2014)

Structure and Nano-/Micromechanics of Materials:
A. Wimmer, A. Leitner, T. Detzel, W. Robl, W. Heinz, R. Pippan, G. Dehm: *Damage evolution during cyclic tension–tension loading of micron-sized Cu lines*. Acta Materialia 67 (2014) 297–307

B. Rashkova, M. Faller, R. Pippan, G. Dehm: *Growth mechanism of Al2Cu precipitates during in situ TEM heating of a HPT deformed Al–3wt.%Cu alloy*. Journal of Alloys and Compounds 600 (2014): 43-50

Selected Talks

Computational Materials Design:
J. Neugebauer: *Ab initio thermodynamics: A novel route to understand and design structural materials*. NIMS Workshop, Tsukuba, Japan, 13-15 Jan 2014

T. Hickel: *Hydrogen-carbide interactions in steels: Ab-initio calculations combined with experiment*. Steely Hydrogen Second International Conference on Metals & Hydrogen, Gent, Belgium, 5-7 May 2014

Interface Chemistry and Surface Engineering:
A. Erbe et al: *Probing interfacial properties at metal/electrolyte interfaces of reactive materials: examples from zinc and copper*. 8th Workshop Ellipsometry initiated by Arbeitskreis Ellipsometry (AKE) - Paul Drude e. V., Dresden, Germany, 10 Mar 2014

S. Wippermann: *In/Si(111)-(4x1)/(8x2): A fascinating model system for one-dimensional conductors*. DPG-Frühjahrstagung der Sektion Kondensierte Materie, Dresden, Germany, 30 Mar-04 April 2014

Microstructure Physics and Alloy Design:
D. Raabe et al: *Atomic-Scale Mechanisms of Strengthening in Wire Drawn Pearlite*. MRS Fall Meeting, Boston, USA, 1-6 Dec 2013

D. Raabe et al: *Nanostructure Manipulation by Segregation Engineering*. 2nd ESISM International Workshop on Fundamental Issues of Structural Materials, Kyoto, Japan, 11-12 Mar 2014

Structure and Nano-/Micromechanics of Materials:
C. Kirchlechner et al: *A Novel View on Fatigue Damage at the Micron Scale by In Situ X-ray µLaue Diffraction*. TMS San Diego, USA, 16-20 Feb 2014

G. Dehm et al: *In Situ Electron Microscopy and Micro-Laue Study of Plasticity in Miniaturized Cu Bicrystals*. CAMTEC III Meeting, Cambridge, UK, 7-8 April 2014

News and Events

Past Events

Communicating Science
The MPIE organized and participated at two big science fairs in 2013. The first one was the Open Day "Fascination of Steel" in July 2013 that was organized by the MPIE and the Steel Institute VDEh with over 40 attractions for more than 2500 visitors. The second big science fair was the first Researchers' Night in Düsseldorf in September 2013. It was organized by the University and the University of Applied Science in Düsseldorf. The MPIE took part with three attractions showing fuel cells, computer simulations and ways of corrosion protection.

23rd January 2014: Workshop on Hydrogen Embrittlement
The MPIE organized a workshop on Hydrogen Embrittlement on January 23rd, 2014. The workshop was part of a series of topical one-day meetings at the institute with the intention to bring together leading experts from academia and industry. A broad variety of topics concerning hydrogen embrittlement in steels was presented; covering topics from fracture criterion to new techniques for hydrogen detection.

18 – 19 July 2013: MECANO General Meeting
MECANO is an internationally funded CNRS research network with a focus on the mechanics of nano-objects and brings together physicists, mechanical engineers and chemists. A General Meeting was organized on July 18-19th at the MPIE. It focused on the simulation of mechanical properties, on micro- and nano-diffraction and on phase transformations.

Upcoming Events

7 – 11 July 2014: Workshop on the Description of Charged Systems and Solid/Liquid Interfaces
The MPIE organizes a workshop at the International Center for Materials Research at UC Santa Barbara (California, USA) focussing on the *ab initio* description of charged systems and solid/liquid interfaces for semiconductors and electrochemistry.
http://www.icmr.ucsb.edu/index.html

14 - 15 July: International Symposium: Computational Mechanics of Polycrystals
The MPIE organizes the 4th International Symposium on Computational Mechanics of Polycrystals. The symposium will provide an up-to-date overview on the multi-scale modelling and simulation of polycrystal plasticity of metals. Special attention will be given to industrially relevant multi-phase materials and materials showing mechanical twinning and phase transformations.
http://cmcn2014.mpie.de/

31 August – 4 September 2014: International Conference: High Manganese Steel
The MPIE and the RWTH Aachen University organize an International Conference on High-Manganese Steels on 31st August - 4th September 2014 at the RWTH Aachen University. The focus lies on austenitic high manganese steels as well as on medium manganese steels with ferritic and martensitic microstructures.
www.hmns2014.de

5 - 8 October 2014: Summer School: Theory and Practice of Modern Powder Diffraction
The summer school is intended for students and young scientists active in solid state research, geo-sciences, crystallography, and materials science. The aim is to give an overview on the capabilities of powder diffraction methods on polycrystalline matter, and on the characterization of atomic structures and microstructures.
http://www.kofo.mpg.de/iycr/

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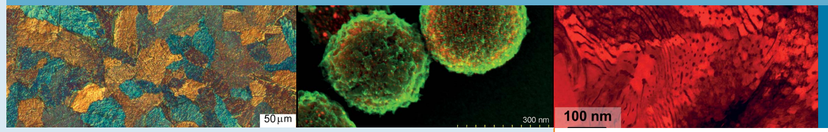

Development of ab initio simulation techniques to investigate surfaces under realistic environmental conditions

Electrochemical processes of practical importance are complex phenomena that involve different length and time scales. They are at the basis of important phenomena like corrosion, water electrolysis and batteries, photo catalytic water splitting or electro catalysis and take place at the interface between a solid (electrode) and a liquid phase (electrolyte). They depend on the materials composition, the environment and the pre-treatment. At present our understanding of key steps of electrochemical processes, let alone their interplay, is incomplete, which impedes rational design and the advancement of targeted functionalities. Ab initio based simulation techniques, as developed and applied in the Computational Materials Design Department at the MPIE, will allow determining critical reaction steps taking place at a solid-liquid interface and thus provide new insights into the mechanisms governing above mentioned phenomena.

Let us take the example of corrosion – while it is known that, at the fundamental scale, a metal reacts with species from the environment and transforms into an oxidised form, the reactive intermediates in the occurring multi-step electrochemical reaction and their exact place within the reaction chain continues to be a subject of heavy debate. Gaining insight into the microscopic processes occurring at a solid/liquid interface presents a challenge to both experimental measurements and theoretical modelling. This is due to the involvement of different classes of material systems on the solid side of the interface (metals or semiconductors), which may impose different requirements on investigational approaches. Electrolytes are, on the other hand, probably most challenging regarding their dynamics, configurational diversity and tendency of aqueous electrolytes to form H-bonding networks. The electric fields evolving at the interface couple to and influence the relevant surface processes, while the involved time and length scales present a challenge to any form of theoretical modelling based on quantum mechanical methods.

The posed questions can be systematically addressed by determining the thermodynamics and kinetics of the surface, as well as of the ions in solution and in the oxidised layer. In this context, ab initio electro-

EDITORIAL

Dear Colleagues and friends of MPIE,

here we share with you some recent developments at MPIE. One of the most important structural changes is the departure of Prof. Stratmann who left the institute for becoming the next president of the Max-Planck-Society. His view about the relationship between research and industry is one important topic in this newsletter. Other items relate to the development of computational simulations for investigating surfaces under realistic environmental conditions and the microstructural evolution in single crystal Ni-base superalloys. Also please have a look at the upcoming workshops.

Enjoy reading and all the best from the MPIE-team,

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

Awards and Achievements

Dr. Theodoros Baimpos from the University of Patras, Greece, received a stipend of the Alexander von Humboldt Foundation and works on gas sensors for metal-organic thin films.

Jennifer Baseler received the Azubipreis of the Max Planck Society as one of the best trainees in material testing in 2013. And she was honoured by the IHK Düsseldorf.

Angelika Bobrowski and **Heidi Bögershausen** received the Metallography Award 2013 from the Deutsche Gesellschaft für Materialkunde for their achievements and efforts in the ‚Gesellschaft für Materialografie Rhein-Ruhr' that was founded 2000 by them.

Dr. Björn Lange was awarded the Otto Hahn Medal for his dissertation about p-doping limitations of gallium nitride at the University Paderborn, Germany.

Dr. Gerard Leyson, Philippine grantee of a scholarship from the Alexander von Humboldt Foundation, works on computational design of hydrogen embrittlement.

nic structure calculations can offer a complementary view to experimental investigations, in analogy to what is common and very successful practice in the realm of surface science. There, a key to success are surface phase diagrams, which identify the thermodynamically preferred surface termination as a function of chemical potentials. Such diagrams rely on an accurate determination of free energies at finite temperatures and are constructed by coupling density-functional theory calculations to thermodynamic considerations, which opens a route to explore and understand the impact the environment has on a system while retaining the predictive power of the first-principles method.

The availability of surface phase diagrams allows reducing the multitude of fast processes and the identification of the thermodynamically stable surface phases, as well as the sets of conditions which define the boundaries for their stability. Thus, such diagrams provide the basis for determining the critical reactions taking place at the interface and could, for example, help us to understand what impact hydrogen might have on the protective Zn layer used on steels or how a sour gas environment changes the properties of a steel surface. Extending such diagrams to electrochemical conditions, by accounting for changes in pH and potential conditions (as they determine and characterise the state of an electrochemical system) appears, therefore, highly desirable.

Recently a method which seamlessly and quite naturally links density functional theory calculations to such experimental observables as the pH-scale and the electrode potential was developed in the group of Mira Todorova at the Computational Materials Design department of the MPIE. The approach is based on the formation energies of ions in solution, which are utilised in a thermodynamic context. It is inspired by the observation that, from a formal point of view, ions in solution and charged defects in semiconductors – the fundamental building blocks of theoretical and modelling concepts in semiconductor defect chemistry and electrochemistry – are equivalent, which makes it possible to unify and "translate" concepts of these two fields. Employing this approach provides surprising new insight into apparently "old" problems such as water stability. It also opens, for example, new routes to the construction electrochemical phase (Pourbaix) diagrams, allowing also for the consideration of surface phases or nano-structures, which effectively extends the concept of surface phase diagrams to the consideration of electrochemical conditions.

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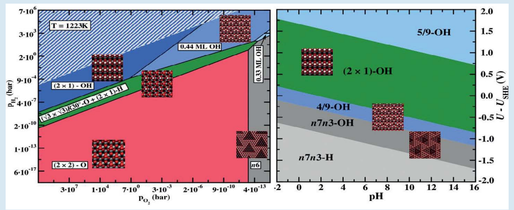

Surface phase diagram for a ZnO(0001)-Zn surface in equilibrium with a humid oxygen atmosphere at T=950ºC (left) and an electrochemical environment at T=300ºC (right). Geometries of the stable surface structures are shown as insets. Equilibrium conditions under which water would condensate on the surface are indicated by a white hashed area in the left picture.

Materials that can take the heat: Microstructural evolution in single crystal Ni-base superalloys

High temperature materials represent a fascinating research area for research in materials science and engineering. In service, they are exposed to mechanical loads at temperatures above 1000°C, where their microstructure is not stable. Therefore, a good understanding of thermodynamic stability and microstructural evolution during high temperature exposure is required.

The demand for better efficiency and performance is the driving force for research on materials for turbine blades which have to operate at very high temperatures. Single crystal Ni-base superalloys (SXs) are at the moment the best material for this purpose. They have optimum balance of mechanical and chemical properties (creep, high temperature fatigue and oxidation resistance).

Turbine blades are the critical components of modern aviation and stationary gas turbines. They are cast in a Bridgman solidification process as [001]-orientated single crystals. The cast microstructure of Ni-based SXs is governed by the growth of dendrites and the subsequent solidification of interdendritic regions. Over ten alloying elements (Cr, Mo, W, Re, Ta, Ti, or Hf - enhance the high temperature capability; Al, Cr and Co - improve oxidation resistance) are required to ensure the properties. Some of these segregate during solidification and therefore a homogenization heat treatment is required to achieve homogeneous chemical composition throughout the alloy. The final microstructure consists of 60 – 80% volume fraction of γ'-cubes (ordered L12 phase, typical cube edge length of 0.5 µm) separated by thin γ-channels (face centered cubic microstructure, typical width: 50 nm).

Understanding of correlations between chemical composition, processing parameters, microstructure and thermodynamic stability is the key to proper design of efficient high temperature turbine blades. In the last 20 years the operating temperatures of Ni-base SXs could be increased by 100°C such that blades today operate close to 1100°C. This requires an increase of refractory elements, in particularly rhenium. Re improves creep strength but also promotes the formation of brittle and harmful topologically close-packed (TCP) phases. There has also been concern that the Re price increases significantly. Therefore, alloy development and modification represent an ongoing activity in superalloy technology. Other refractory elements like tungsten and ruthenium are considered as rhenium replacements. These questions are investigated in the new collaborative research center SFB/TR 103.

The Max-Planck Fellow Research Group on High Temperature Materials (HTM) links MPIE research activities to the interdisciplinary research in the SFB/TR 103, where single crystal super alloys are in the focus of interest. By the use of latest high-resolution characterization methods (high resolution, aberration corrected transmission electron microscopy and 3D atom probe tomography) correlations between the small and large-scale microstructural heterogeneities can be analyzed and understood. This is how activities of HTM help to develop new materials and processes that overcome limitations that currently hamper advances in high temperature single crystal technology.

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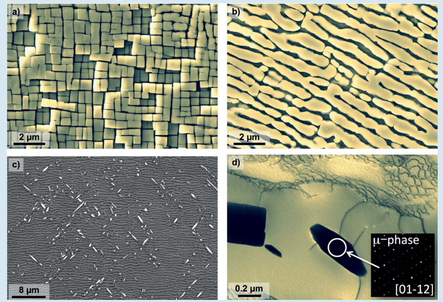
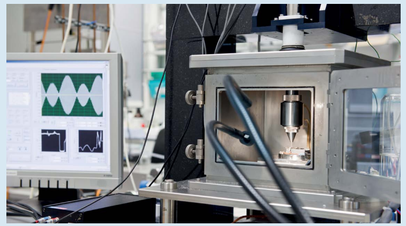


Evolution of the single crystal Ni-base superalloy during high temperature service: (a) SEM micrographs of the initial microstructure, γ' cubes in the γ matrix; (b) rafted microstructure after creep (160 MPa at 1050 °C, 1% strain) and, (c) nucleated topologically close-packed (TCP) phases in the dendritic regions. (d) TEM micrograph showing a TCP particle and its corresponding electron diffraction pattern.

We are President: The new Max Planck President is homegrown

Prof. Martin Stratmann, head of the department ‚Interface Chemistry and Surface Engineering' was elected as the Max Planck Society's new President last year and took office in June 2014.

'The Iron Man' was the headline of an article published by Süddeutsche Zeitung on June 7, 2013. The humorous title is a tribute to Martin Stratmann's scientific focus. Indeed, during his 35-year-career as an electrochemist and materials scientist, Martin Stratmann, director of the department 'Interface Chemistry and Surface Engineering' and the new President of the Max Planck Society, has mainly studied iron, steel and other related topics. He connected electrochemical, spectroscopic and interface analytical methods and was the first researcher to use the Scanning Kelvin Probe in corrosion science.



Kelvin Probe
This instrument was originally used in the semiconductor industry and adjusted for the needs of corrosion science by Martin Stratmann. The Kelvin Probe is a scanning probe method where the potential offset between a probe tip and a surface can be measured. With this method scientists are even capable of measuring corrosion under fluid or plastic surfaces. The Kelvin probe for corrosion science is now used in industry as well. (Photo: Christian Nielinger)

Alongside his research, Stratmann always kept an eye on the scientific and political landscape of Germany. In his role of Vice President of the Max Planck Society's Chemistry, Physics and Technology section and, since 2008 as Managing Director of the Minerva-Foundation, a joint German-Israeli research cooperation, one of Stratmann's priorities has been to narrow the gap between basic research and industrial application. "The Max-Planck-Institut für Eisenforschung can serve as role model for the Max Planck Society as a whole, as it highlights how a public private partnership can successfully work", states Stratmann. The institute is equally financed by the Max Planck Society and the Steel Institute VDEh. "The gap between basic research and application has started to dwindle quite some time ago. New insights are directly opening the way for innovation - not only in material sciences, but also in other disciplines."

Stratmann argues that science has rapidly become more and more interdisciplinary. To be able to follow the trend, five major obstacles must be overcome. Firstly, science needs structures that provide outstanding scientists with the greatest possible degree of freedom as it is impossible to forecast future innovations. Secondly, industry has to be eager to obtain information from science on a

Awards and Achievements

Vera Marx, doctoral student in the group 'Micromechanics', won the Best Poster Award at the ECI Conference 'Nano- and Micromechanical Testing in Materials Research and Development IV' held in October 2013 in Olhao, Portugal.

Dr. Karl Mayrhofer, leader of the group ‚Electrocatalysis', won the Science Award for Electrochemistry 2013 awarded by BASF and Volkswagen and endowed with 50 000 Euros.

Anna Schuppert, doctoral student in the group 'Electrocatalysis' took part at the 63rd Lindau Nobel Laureate Meeting as one of only 550 worldwide invited young researchers.

Dr. Mira Todorova, project leader in the department "Computational Materials Design", won the Best Poster Award at the CALPHAD XLII Conference held in May 2013 in San Sebastian, Spain.

Dr. Angel Topalov won the prize of the German Chemical Society (GDCh) for applied electrochemistry for his work on investigating dissolution pathways of platinum by the developed in-situ mass spectrometry technique and was endowed with 1000 Euros by BASF.