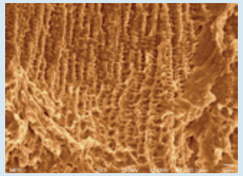
Scientists at the MPIE

Dr. Eric Jägle is head of the newly established research group “Alloys for Additive Manufacturing” in the department “Microstructure Physics and Alloy Design”.

The main funding of the group comes from a joint project of the MPIE and the Fraunhofer Institute for Laser Technology. The group’s key purpose is to understand the impact of additive manufacturing (AM) on the micro- and nanostructures of the employed alloys. This understanding is necessary to, on the one hand, develop metallic materials suitable for additive manufacturing (alloys for AM) and, on the other hand, exploit the AM processes in novel material synthesis routes (alloys by AM).

Jägle did his PhD at the Max-Planck-Institut für Metallforschung in Stuttgart (Germany) about the mesoscopic simulation of microstructures during solid-solid phase transformations and continued his studies as a postdoctoral researcher at the MPIE since 2011, focusing on the analysis of phase transformations by Atom Probe Tomography, before becoming group head in 2015.



Fracture surface of a Ni-base superalloy produced by selective laser melting showing the dendritic structure of process-induced hot cracks as well as ductile fracture of the surrounding matrix.

Dr. Christian Liebscher is head of the newly established group “Advanced Transmission Electron Microscopy” in the department “Structure and Nano-/Micromechanics of Materials”.

The group’s main target is to analyse the atomic structures of materials and their relationship to the materials’ properties by using advanced transmission electron microscopy (TEM) techniques.

Before being group head at the MPIE, Liebscher worked as a staff scientist at the Interdisciplinary Center for Analytics on the Nanoscale of the University Duisburg-Essen (Germany). He did his postdoctoral studies at the University of California, Berkeley and the National Center for Electron Microscopy at the Lawrence Berkeley National Laboratory (both USA) where he remained for three years. Liebscher pursued his PhD studies at the University of Bayreuth (Germany) about “High resolution phase and dislocation analysis in Pt- and Ni-based superalloys”.

One of Liebscher’s current research projects deals with S in Cu and its location in the lattice and segregation to the grain boundaries. Having investigated this topic, the results can easily be transferred to steel and related alloys. The impact of grain boundary segregations in Cu will also be investigated by in situ nanomechanical testing in the TEM. Another research topic revolves around the nanostructural design of precipitation strengthened ferritic alloys with hierarchical microstructure for high temperature applications.

Selected Publications

Computational Materials Design:

A. Glensk, B. Grabowski, T. Hickel, J. Neugebauer: Understanding anharmonicity in fcc materials: From its origin to ab initio strategies beyond the quasiharmonic approximation. Phys. Rev. Lett., 114, 195901 (2015)

K.D. Bauer, M. Todorova, K. Hingerl, J. Neugebauer: A first principles investigation of zinc induced embrittlement at grain boundaries in bcc iron. Acta Mat 90, 69-76 (2015)

Interface Chemistry and Surface Engineering:

T.H. Tran, A. Vimalanandan, G.Genchev, J. Fickert, K. Landfester, D. Crespy, M.Rohwerder: Regenerative Nano-Hybrid Coating Tailored for Autonomous Corrosion Protection. Adv Mater, 27, 3825-3830 (2015)

L. Rossrucker, A. Samaniego, J.-P. Grote, A. M. Mingers, C. A. Laska, N. Birbilis, G. S. Frankel, K. J. J. Mayrhofer: The pH Dependence of Magnesium Dissolution and Hydrogen Evolution during Anodic Polarization. JES, 162 (7), C333-C339 (2015)

Microstructure Physics and Alloy Design:

A. Prakash, J. Guénolé, J. Wang, J. Müller, E. Spiecker, M.J. Mills, I. Povstugar, P. Choi, D. Raabe, E. Bitzek: Atom probe informed simulations of dislocation-precipitate interactions reveal the importance of local interface curvature. Acta Mat, 92, 33-45 (2015)

Y. Deng, C.C. Tasan, K.G. Pradeep, H. Springer, A. Kostka, D. Raabe: Design of a twinning-induced plasticity high entropy alloy. Acta Mat, 94, 124-133 (2015)

Structure and Nano-/Micromechanics of Materials:

B. N. Jaya, C. Kirchlechner,G. Dehm: Can micro-scale fracture tests provide reliable fracture toughness values? A case study in silicon. JMR, 30, 686-698 (2015)

V.M. Marx, F. Toth, A. Wiesinger, J. Berger, C Kirchlechner, M. J. Cordill, F. D. Fischer, F. G. Rammerstorfer, G. Dehm: The influence of a brittle Cr interlayer on the deformation behavior of thin Cu films on flexible substrates: Experiment and model. Acta Mat 89, 278-289 (2015)

Selected Talks

Computational Materials Design:

J. Neugebauer: Understanding the fundamental mechanisms behind H embrittlement: An ab initio guided multiscale approach. International Workshop MoD-P-MI, Marseille, France, 25 - 27 May 2015

J. Neugebauer: Ab initio description of finite temperature phase stabilities and transformations. PTM Conference, Whistler, Canada, 28 Jun - 3 Jul 2015

Interface Chemistry and Surface Engineering:

M. Rohwerder: Understanding the origins of hydrogen embrittlement: a novel method for detecting hydrogen in metals at high local resolution and ultra-high sensitivity. EDSA 2015, IIT Madras, Chennai, India, 27 Feb – 2 Mar 2015

K. Mayrhofer: State-of-the-Art Tutorial on Diagnostics in Low-Temperature Fuel Cells. 227th annual meeting of the Electrochemical Society, Chicago, USA, 24 – 28 May 2015

Microstructure Physics and Alloy Design:

D. Raabe, J. Neugebauer, C. Tasan, F. Roters, D. Ma, S. Sandlöbes, M. Diehl: Materials Simulation: Mechanisms and Processes. BMBF Wing Conference, Dresden, Germany, 28 Apr 2015

R. Kuzmina, P. Choi, D. Ma, T. Hickel, J. Neugebauer, M. Friak, M. Herbig, D. Ponge, C. Tasan, S. Sandlöbes, D. Raabe: Scale hoping simulations and real atoms. ICAMS Workshop ‘From Atoms to Continuum’, Ruhr University Bochum, Germany, 16 Jun 2015

Structure and Nano-/Micromechanics of Materials:

G. Dehm: Probing deformation mechanisms of Cu structures relevant for electronic applications. Electronic Materials and Applications, Orlando, USA, 21 – 23 Jan 2015

B. N. Jaya, R. Raghavan, C. Kirchlechner, G. Dehm: Probing deformation and fracture of materials with high spatial resolution. International Workshop on Stress Assisted Environmental Damage in Structural Materials. EDSA-2015, IIT Madras, Chennai, India, 27 Feb – 2 Mar 2015

News and Events

Past Events

11 March 2015: MPIE-POSTECH Cooperation

The MPIE and the Max Planck POSTECH/Korea Research Initiative agreed on intensifying their collaboration by signing a memorandum of understanding. The collaboration will focus on in situ transmission electron microscopy to improve the understanding of phase transformations and failure of materials. This is the first step of building up a trilateral research initiative between the MPIE, POSTECH and the University of Berkeley (California, USA). The collaboration involves the exchange of doctoral students and the usage of each other’s facilities.

27 March & 4 May 2015: Career Talk with ThyssenKrupp Steel Europe

The MPIE board of executives and the PhD representatives invited ThyssenKrupp Steel Europe (TKSE) for the first informative event at the MPIE about career perspectives in industry. TKSE presented its trainee and transfer programme. Former MPIE scientists who now work at TKSE showed their career path and provided the students and post docs of the MPIE with advice concerning application strategies and possible fields of work. Moreover, a group of MPIE doctoral students visited the production sites in Dortmund on 4th May 2015. The doctoral students were able to watch the industrial application of surface refinements at the continuous production lines for annealing and hot-galvanizing at the Dortmunder OberflächenCentrum.

23 April 2015: Girls‘ Day

At the nationwide Girls’ Day a group of girls had the chance to get an insight on the work of a Max Planck scientist. The pupils analysed different samples with both a light and a scanning electron microscope and learned about the structure and properties of materials. At the Girls’ Day female pupils are invited to learn about possible trainings and courses of study in fields usually dominated by men.

Upcoming Events

28 September – 2 October: Conference on Intermetallics

This conference combines contributions from industry and research on topics such as γ-TiAl, iron aluminides and silicides. There will also be a session about synergies between theory and experiment in thermodynamic assessments of intermetallics. The conference takes place in Bad Staffelstein, Germany.
http://www.intermetallics-conference.de/

20 – 21 October 2015: Workshop on Pearlite

The intention is to bring together scientists from the MPIE, the Technical University of Denmark and the Erich Schmid Institute of Materials Science in Leoben in a workshop format to enable in-depth discussions of fundamental and applied research regarding both current and preliminary research in this area. The worldwide leading experts from France and Belgium have been also invited.
http://www.mpie.de/2768772/scientific-events

25 November 2015: KopfSalat

KopfSalat is a regular public event taking place at the MPIE. In November Prof. Gerd Gigerenzer, director of the department “Adaptive Behavior and Cognition” at the Max Planck Institute for Human Development, will give an insight on how to rationally deal with decision making and risk taking.
http://kopfsalat.mpie.de

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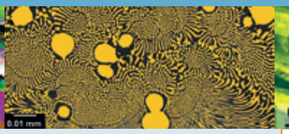
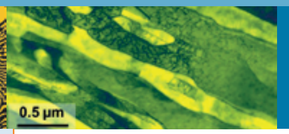




O‘Hydrogen where art thou?

Hydrogen may be by far the most abundant element in the universe, but one of the most important challenges in the materials science community today is to actually locate where it is. And not just for scientific curiosity: understanding where hydrogen atoms prefer to be located in a microstructure can help us design materials that can efficiently store it - as it might be our best bet for the cleanest source of energy -, or design materials that can efficiently avoid it - as it might be the most detrimental embrittler for high strength alloys. It is thus no surprise that the MPIE with its strong ties to various related industries (e.g. steel, automotive, energy) and its focus on achieving fundamental understanding, attacks this strategic topic with full power.

One of the experimental goals of the Adaptive Structural Materials group is to understand the hydrogen embrittlement micro-mechanisms in advanced high strength alloys (AHSA). The challenge enroute is immense, since most novel AHSA have complex micro-composite structures consisting of multiple phases of high mechanical contrast. To simultaneously deliver high strength and toughness, these phases often differ in crystal structure, mechanical-stability, defect density, active deformation or cracking mechanisms etc. With increasing deformation each phase evolves differently, essentially resulting in a different micro-composite response at different deformation levels. In presence of hydrogen the picture gets even complexer: First of all, different phases have different solubility of hydrogen. Second, hydrogen diffusion kinetics differ in different phases. Third, hydrogen may cause different embrittlement mechanisms in different phases. This complex process clearly cannot be fully understood by traditional ‚post-mortem‘ approaches.
We approach this as a multi-field mapping problem. By employing various tools and techniques the evolution of micro-structure, micro-strains, micro-stresses and micro-damage in such complex AHSA, can be mapped, in-situ, at high resolution (Fig. 1).

To map the deformation-induced evolution of microstructure, high resolution electron backscatter diffraction and electron channelling contrast imaging techniques are used. Micro-strains are tracked by microscopic digital image correlation, using in-lens SE images and fine SiO2 particles. Micro-stresses are experimentally difficult to measure, thus we rely on crystal plasticity simulations. Micro-damage incidents are characterized by in-lens SE imaging and post-mortem serial sectioning & imaging.

What about hydrogen? In collaboration with research partners in-

EDITORIAL

Dear Colleagues and Friends of the MPIE,

Hydrogen embrittlement has been a tough issue for materials’ research and industry ever since. In this newsletter edition we point out two of our projects on this topic, showing both an experimental and theoretical approach to first, find out where the hydrogen is exactly located in the material and second, to unravel the mechanisms of local plasticity, fracture and hydride formation. Please also have a look at the category “Scientists at the MPIE” where we present two leaders of newly established groups about additive manufacturing and advanced transmission electron microscopy.

Enjoy reading and best regards,

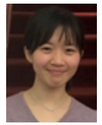
Prof. Dr. Dierk Raabe
(Chief Executive, MPIE)

Awards and Achievements

Dr. Theodoros Baimpos, postdoc in the group 'Interaction Forces and Functional Materials', has won the Best Poster Award at the '2nd International Conference of Young Researchers on Advanced Materials' (IUMRS-ICYRAM) in Haiku, China.

Dr. Pascal Beese-Vasbender, postdoc in the group 'Electrocatalysis', won the Leopoldina Prize for Young Scientists of the Leopoldina National Academy for Sciences. Moreover, he took part at this year's Lindau Nobel Laureate Meeting.

Christian Broß, apprentice in the field of materials testing, won the First Poster Award at the conference "Mikpräp 2015" at the technical vocational school in Solingen (Germany).



Su-Ting Cheng, doctoral student in the project group 'Electrochemistry and Corrosion Science', won the Best Poster Award at the 'Faraday Discussion: Corrosion Chemistry' Conference of the Royal Society of Chemistry in London, Great Britain.

Dr. Chang-Hyuck Choi, postdoc in the group 'Electrocatalysis', has received a scholarship of the Alexander von Humboldt Foundation.

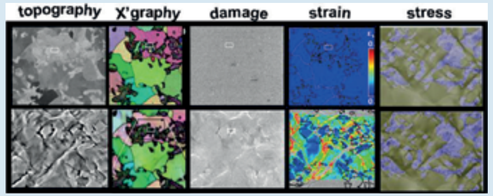


Fig. 1: Mapping of deformation induced evolution of local microstructure, strain, stress, damage fields by (from left to right) SE imaging, EBSD, Inlens SE imaging, microscopic- DIC, crystal plasticity simulations. Shown data is of a dual phase steel.

house (i.e. the group "Corrosion" of Dr. Michael Rohwerder), at the Kyushu University, and at the Luxemburg Institute of Science and Technology (LIST), various techniques are explored, each of which with different advantages and limitations. These include scanning Kelvin probe force microscopy (SKPFM), secondary ion mass spectroscopy (SIMS or Nano-SIMS), Ag decoration, all assisted by thermal desorption spectroscopy (TDS). Some examples are shown in Fig. 2.

The group "Adaptive Structural Materials" has so far applied the approach to TRIP-Maraging steels, martensitic steels, dual phase martensitic-ferritic steels, and martensitic-austenitic steels. While the incorporation of the hydrogen mapping techniques to in-situ analysis during deformation remains challenging, the overall approach still provides a unique overview of all the inter-linked micro-processes taking place during deformation. The realm of data that is produced in this manner reveals great insight on how novel alloys can be developed for better hydrogen resistance.

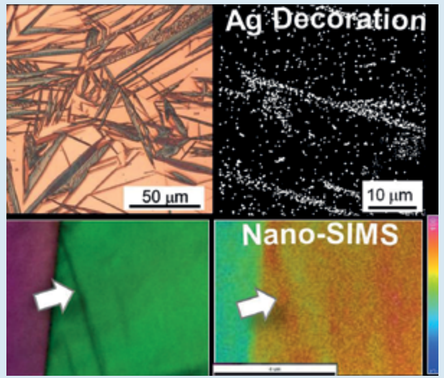


Fig. 2: Hydrogen mapping by: Ag decoration (above) in martensitic-austenitic steel (collaboration with the Kyushu University); Nano-SIMS (below) in a TWIP steel (collaboration with RWTH Aachen and LIST). In the former higher hydrogen content is observed in martensite plates, while in the latter, in deformation-induced mechanical twins.

Author: Dr. Cem Tasan

Understanding hydrogen embrittlement by scale-bridging and experimental-informed simulations

Hydrogen embrittlement is severely detrimental for steels, especially for high strength and high performance steels. Even very tiny amounts of hydrogen – in the amount of parts per million – significantly weaken the metal and lead to the loss of their originally ductile properties. The embrittlement and loss of toughness is a long-standing issue that is attributed to multiple material-scientific mechanisms: local plasticity, enhanced fracture and hydride formation.

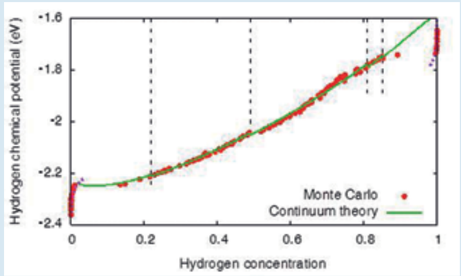
The project's aim is to unravel these mechanisms and understand the environmental influence on the embrittlement by computer simulations. Two research groups collaborate on this project. Robert Spatschek and his group from the Computational Materials Design Department use scale bridging methods from an atomistic ab-initio description up to the continuum simulations to account for different environments and geometries. Steffen Brinckmann from the Structure and Nano-/ Micromechanics of Materials Department uses experiments on the micrometre length-scale to obtain fracture and plasticity properties in hydrogen-rich environments that are supplied to continuum simulations.

Scale-bridging modelling of hydrogen embrittlement

Robert Spatschek and his group from the Computational Materials Design Department combine various computational and theoretical tools on the atomistic scale, which characterize the fundamental atomic properties. The information from these tools is carried over to larger scales, where the material failure becomes visible. The initiative is part of the DFG Collaborative Research Center 917 "Steel ab initio" as a joint programme of RWTH Aachen and MPIE Düsseldorf.

Using high manganese steels as an example, interstitial hydrogen is preferentially located in manganese rich environments, which is mainly attributed to volumetric effects at the atomistic scale. This observation already indicates that mechanical effects play a central role for the understanding of hydrogen in metals. A focus of the present activities is on the formation of brittle hydrides, which favour crack propagation because of their low fracture toughness. The requirement to link bonding information between the different elements on the atomistic level up to the description of phase separation and crack formation on much larger scales requires the development of a consistent and seamless chain of modelling tools. This tool-chain involves, apart from ab initio methods, also atomistic approaches like Monte Carlo techniques, both of which methods are limited to a restricted number of atoms. Both methods cannot account for long-range elastic effects. Therefore, the development of quantitative continuum methods is central for a successful scale bridging. Here, we have developed a description which uses the atomistic information in micrometre-scaled phase field models, which allow to efficiently describe hydride formation in mesoscopic systems under different mechanical loading conditions while maintaining the accuracy of the Monte Carlo simulations. Together with Steffen Brinckmann from the department Structure and Nano-/ Micromechanics of Materials (SN), Spatschek's group has verified the mechanical response by finite element simulations.

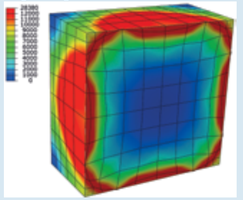
The sample geometry is of central importance. However, commonly the thermodynamics of phase separation is considered for bulk systems. Recently Spatschek found out that the behaviour of hydride formation strongly differs near surfaces and interfaces due to mechanical stress relaxation. Near free surfaces – like cracks – hydride formation occurs at significantly lower hydrogen concentrations than in the bulk. This observation implies that materials, which are usually not considered to be hydride formers under the given environmental conditions, can form these brittle phases near free surfaces.



Hydrogen chemical potential in Ni at fixed volume. The red data points are calculated with molecular statics Monte Carlo simulations, the green curve segments are the predictions from the continuum theory. Depending on the hydrogen concentration different hydride precipitate shapes are found.

Experimentally-informed fracture simulations

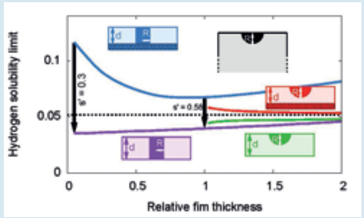
Brinckmann calculated the stress induced by hydride formation in the anisotropic metal. Conventionally, isotropic descriptions are used, which assume that the material behaves in each direction identically. However, the atomistic cubic structure found in metals results in strong variations in different directions, which is termed anisotropic behaviour. The volumetric expansion is a key in understanding hydride formation: the hydride is larger than the originating metal.



Stress distribution in MPa during hydride growth in anisotropic Ni. The hydride has an eigenstrain that results in the deformed grid highlighting the growth of the spherical inclusion in the restricted, i.e. periodic, space.

Initially in hydride growth, the hydrides are small and well separated, i.e. their stress fields do not interact. However, during growth the hydrides account for increasing amounts of material and these hydrides interact elastically.

Finally, as the space separating the hydrides becomes increasingly smaller, the volumetric expansion and the induced stresses dominate the coalescence of three dimensional hydride islands. In collaboration with Christoph Kirchlechner, also from the SN department, the material properties in hydrogen environments are determined by micromechanical experiments. Kirchlechner heads the group Nano-/ Micromechanics of Materials and focuses on fracture and plasticity experiments on small length-scales. In these experiments, a focused ion beam is used to carve geometries out of the bulk metal. Then these specimens are deformed with a nanoindenter, which measures forces and displacements, from which the material properties can be obtained. Conventionally, these experiments are executed in air or vacuum conditions. In this project, the micromechanical experiments are performed in electrolytes. Upon charging the sample, hydrogen from the electrolyte will diffuse into the metal and determine the material fracture toughness and plasticity. The material properties are then used in finite element simulations on the micrometre length-scale. These simulations take the geometry specific stresses as well as the hydrogen diffusion into account. Stresses and diffusion interact: the stresses drive the hydrogen diffusion and the hydrogen concentration results in volumetric expansion, hence additional stresses.



Hydrogen solubility limit in thin films of Nb at room temperature. The predictions stem from scale bridging simulations. For films which are attached to a rigid substrate, the solubility limit is increased in comparison to bulk samples. Detachment of a thin film leads to a drop of the solubility limit by about a factor 1/3, in agreement with experiments.

Authors:
Dr. Steffen Brinckmann
Dr. Robert Spatschek

Awards and Achievements

Dr. Blazej Grabowski, leader of the group ‚Adaptive Structural Materials' has successfully applied for a Starting Grant of the European Research Council and is financed with 1.5 million euros for five years.

Dr. Olga Kasian, postdoc in the group 'Electrocatalysis', has received a scholarship of the Alexander von Humboldt Foundation.

Dr. Sergiy Merzlikin, postdoc in the group 'Corrosion', has won the second Best Paper Award of the journal 'Metallurgical Research & Technology'.

Thomas Utzig, doctoral student in the group 'Interaction Forces and Functional Materials', has won the Best Poster Award in the section 'Surface Forces' at the Conference of the International Association of Colloid and Interface Scientists in Mainz, Germany.

Ali Zendegani, doctoral student in the group 'Computational Phase Studies', has been awarded the Larry Kaufman Scholarship to present his research at the CALPHAD XLIV conference in Loano, Italy.