Scientists at the MPIE

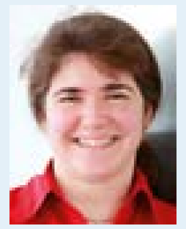
Dr. Steffen Brinckmann is head of the group "Nanotribology" in the department "Structure and Nano-/ Micromechanics of Materials" since 2014. Before that he was a senior researcher in the same department, which he joined in 2013. Brinckmann had several research stays as postdoctoral fellow after doing his PhD in applied physics at the University of Groningen (The Netherlands) about the role of dislocations in fatigue crack initiation, in 2005. Before joining the MPIE, Brinckmann was a postdoctoral research associate at the Purdue University (USA) and at the California Institute of Technology (USA) from 2005-2008. After that he worked at the Interdisciplinary Centre for Advanced Materials Simulations (ICAMS) of the Ruhr University Bochum leading the group "Discrete Micromechanics and Fracture" from 2009-2012 and leading the project group "Microstructure – Property – Relationships" from 2010-2012.

His research focus lies on tribology experiments where he investigates microstructure evolution during friction and wear. His projects investigate the tribology using micrometer asperities that mimic a single asperity on macroscale components with the aim to fundamentally understand the irreversible mechanisms that result in the energy and structural loss. Additionally, Brinckmann investigates the brittle and ductile numerical fracture mechanics at the microscale.

Selected Publications:

S. Brinckmann, K. Matoy, C. Kirchlechner, G. Dehm: *On the influence of microcantilever pre-crack geometries on the apparent fracture toughness of brittle materials.* Acta Mat 136, 281-287 (2017)

S. Brinckmann, G. Dehm: Nanotribology in austenite: *Plastic plowing and crack formation*. Wear 338-339, 436-440 (2015)



Dr. Mira Todorova is head of the group "Electrochemistry and Corrosion" in the department "Computational Materials Design" since 2015. Before joining the MPIE at the end of 2006 as a project group leader in the same department, she spend two years as a postdoctoral researcher at the University of Sydney in Sydney, Australia. In 2004, Todorova received a PhD from the Technical University Berlin for her PhD work on the oxidation of palladium surfaces, which she carried out at the Fritz Haber Institute of the Max Planck Society in Berlin. Since 2005, she had several research stays at the University of California, Los Angeles, as a fellow of the Institute for Pure and Applied Mathematics (IPAM).
Her research aims at the development and application of *ab initio* based multi-scale simulation techniques to tackle problems in electrochemistry, with a strong focus on corrosion and related topics. Her group and she perform calculations for a variety of systems, such as metallic alloys, semiconductors or water, investigating both bulk and surface properties by means of density-functional theory calculations, thermodynamic integration, molecular dynamics or Monte Carlo simulations.

Selected Publications:

S. Surendralal, M. Todorova, M. Finnis, J. Neugebauer: *First-Principles Approach to Model Electrochemical Reactions: Understanding the Fundamental Mechanisms behind Mg Corrosion*. Phys. Rev. Lett. 120, 246801 (2018).

M. Todorova, J. Neugebauer: *Identification of bulk oxide defects in an electrochemical environment*. Faraday Discuss. 180, 97 (2015).

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

Selected Publications

Computational Materials Design:

C. Freysoldt, J. Neugebauer: *First-principles calculations for charged defects at surfaces, interfaces, and two-dimensional materials in the presence of electric fields*. Phys Rev B, 97 (20), 205425 (2018)

R. Hadian, B. Grabowski, M.W. Finnis, J. Neugebauer: *Migration mechanisms of a faceted grain boundary*. Phys Rev Mat, 2 (4), 043601 (2018)

Interface Chemistry and Surface Engineering:

E. Scalise, V. Srivastava, E. Janke, D. Talapin, G. Galli, S. Wippermann: *Surface chemistry and buried interfaces in all-inorganic nanocrystalline solids*. Nat Nanotech, 7 (2018)

S. Geiger, O. Kasian, M. Ledendecker, E. Pizzutilo, A. M. Mingers, W. T. Fu, O. Diaz-Morales, Z. Li, T. Oellers, L. Fruchter, A. Ludwig, K. J. J. Mayrhofer, M. T. M. Koper, S. Cherevko: *The stability number as a metric for electrocatalyst stability benchmarking*. Nat Catal, 1, 508–515 (2018)

Microstructure Physics and Alloy Design:

A. Kwiatkowski da Silva, D. Ponge, Z. Peng, G. Inden, Y. Lu, A. Breen, B. Gault, D. Raabe: *Phase nucleation through confined spinodal fluctuations at crystal defects evidenced in Fe-Mn alloys*. Nat Commun, 9 (2018)

S. Basu, Z. Li, K.G. Pradeep, D. Raabe: *Strain rate sensitivity of a TRIP-assisted dual-phase high-entropy alloy*. Front Mater, 5 (30), 1-10 (2018)

Structure and Nano-/Micromechanics of Materials:

J. Guo, G. Haberfehlner, J. Rosalie, L. Li, J. Duarte, G. Kothleitner, G. Dehm, Y. He, R. Pippan, Z. Zhang: *In-situ atomic-scale observation of oxidation and decomposition processes in nanocrystalline alloys*. Nat Comm, 9, 946 (2018)

C. H. Liebscher, A. Stoffers, M. Alam, L. Lymperakis, O. Cojocaru-Mirédin, B. Gault, J. Neugebauer, G. Dehm, C. Scheu, D. Raabe: *Strain-Induced Asymmetric Line Segregation at Faceted Si Grain Boundaries*. Phys Rev Lett, 121 (1) (2018)

Selected Talks

Computational Materials Design:

J. Neugebauer: *Fundamental compositional limitations in the thin film growth of metastable alloys*. 3rd Conference on Advanced Functional Materials (AFM2018), Vildmarkshotellet Kolmården, Norrköping, Sweden, 21 – 23 Aug 2018

L. Huber: *High-throughput calculations and modelling of solute-GB segregation*. International Conference on PROCESSING & MANUFACTURING OF ADVANCED MATERIALS (Thermec'2018), Paris, France, 8 – 13 Jul 2018

Interface Chemistry and Surface Engineering:

S. Wippermann: *Modeling Electrochemical Solid/Liquid Interfaces from first principles*. IEEE NANO 2018, Cork, Ireland, 23 – 26 Jul 2018

M. Valtiner: *Water in Ionic Liquids: Form Neat Ionic Liquids to aqueous solutions*. Gordon Conference for Water and Aqueous Solutions, Holderness, USA, 21 – 26 Jul 2018

Microstructure Physics and Alloy Design:

D. Raabe, D. Ponge, et al: *Advancing Alloys by Segregation Engineering*. 18th International Conference on the Strength of Materials (ICSMA18), Columbus, USA, 15 – 19 Jul 2018

D. Raabe, D. Ponge, et al: *From Seeing Atoms Towards Understanding Atoms: Methods, Results and Challenges of Advanced Atom Probe Tomography*. Hausdorff Lecture 2018, Bonn, Germany, 8 Jun 2018

Structure and Nano-/Micromechanics of Materials:

C. Kirchlechner, N. Malyar, et al: *Quantifying dislocation slip transmission by in situ micromechanics*. 18th International Conference on the Strength of Materials (ICSMA18), Columbus, USA, 15 – 19 Jul 2018

G. Dehm, N. J. Peter, et al: *Ag Induced Phase Transformation of a Sigma 5 Grain Boundary in Copper*. International Conference on PROCESSING & MANUFACTURING OF ADVANCED MATERIALS (Thermec'2018), Paris, France, 8 – 13 Jul 2018

News and Events

Selected Upcoming Events

23 Oct 2018: Workshop "Mechanisms of White Etching Matter (WEM) Formation"
The workshop focuses on the fundamental materials processes behind this phenomenon. Topics will range from WEM formation mechanisms in bearings and rails, over WEM generation by heat, surface machining and high pressure torsion, and the role of hydrogen and electric current, to the remarkable resistance of high nitrogen steels to WEC failure. The workshop takes place at the MPIE. Participants must register via wem-workshop@mpie.de till September 30th.

20 Nov 2018: Workshop "Towards an Atomistic Understanding of Reactions at Surfaces and Interfaces"
The joint workshop of the doctoral programmes SurMat and Recharge deals with highly selective and controlled reactions at interfaces, which play an important role in newest technologies. Its main aim is to discuss opportunities, recent developments, methods and tools to identify reaction mechanisms and elemental steps at the atomistic scale in catalysis, electrochemistry and corrosion. It will take place at the MPIE.

14 – 15 Jan 2018: Workshop "Laves Phases"
The workshop focuses on Laves phases, the largest class of intermetallic phases. Topics will include their synthesis and characterisation, kinetics, defects and properties. The workshop is devoted to summarise the state of the art and identify future research topics. It will take place at the MPIE.

31 Mar – 3 Apr 2019: 4th International Conference on Medium and High Manganese Steels
The conference covers all scientific and technical aspects of medium and high Mn steels. Mn will be addressed to cover the ongoing scientific and industrial developments in the design and processing of Mn-rich high-strength steels. The event will take place at the RWTH Aachen University and addresses participants from both research and industry.
https://www.hmns2019.de/

Selected Past Events

6 Mar 2018: Career Talk by Dillinger
Dillinger gave a presentation on career possibilities for scientists and on the transition from research to industry on the invitation of the PhD representatives and the MPIE's board of executives. The MPIE scientists had the chance to ask about application strategies and potential work fields. Furthermore, a group of scientists from the MPIE visited the production sites in Dillingen in June 2018.

A group of MPIE scientists visited Dillinger on 8th June 2018 after a career talk by Dillinger at the MPIE in March.

14 Sep: Max Planck Day
The Max Planck Society organized a nation wide Max Planck Day to show the variety of basic research. The Max-Planck-Institut für Eisenforschung (MPIE) offered two events in Düsseldorf: a kids' lab for children with numerous interactive experiments. And a KopfSalat-talk by Dr. Christoph Freysoldt about "Big Data, simulations and artificial intelligence in materials science" which was visited by 180 guests. At the same time a group of MPIE-scientists went to a science marketplace in Munich to present their research about 3D-printing of metals and to take part at a science slam where scientists of different Max Planck Institutes competed with short, entertaining research presentations.

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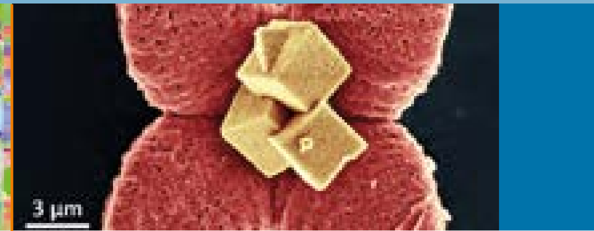


Hotter, safer and greener aero-engines

Aviation has a very high impact on greenhouse gas emissions. In order to tackle CO_2 emissions, it has become necessary to increase the operational temperature of aircraft engines, which will result in a higher efficiency and reduced CO_2 emissions. However, the higher the operation temperature, the more likely is a catastrophic failure of safety-critical components. Thus, new, advanced high-performance materials for aero-engines are required which can withstand harsher service conditions and maintain structural integrity.

Developing novel material-design strategies requires a thorough understanding of the behaviour of these metallic materials at elevated temperatures. Through systematic characterization with near-atomic resolution by atom probe tomography (APT) combined with electron microscopy, we, a team of researchers of the department Microstructure Physics and Alloy Design (MA), provide new fundamental insights into the role of crystalline imperfections on the lifetime of nickel- and cobalt-based superalloys. Both groups of alloys derive their erational conditions are enhanced at elevated temperatures by the presence of high dislocation density. As a consequence, recrystallization and directional coarsening of γ' precipitates occur leading to severely reduced fatigue and creep performance. Direct observation of solutes segregation at dislocations by APT allows us to elucidate the physical mechanism where pipe diffusion initiates the deleterious dissolution of γ' precipitates and subsequently degrades the properties of superalloys of industrial relevance [1,2].

Fig. 1: a) cECCI micrograph showing a high dislocation density in the fully rafted γ/γ' microstructure of a single-crystal nickel-based superalloy. b) Atom probe reconstruction from a rafted γ' precipitate, showing dislocations within a γ' precipitate. c) 1D concentration profile perpendicular to a dislocation revealing segregation of chromium and cobalt at partial dislocations and at the planar defect.

outstanding strength from the $L1_2$ ordered γ' precipitates. In the case of the nickel-based alloys, their dissolution kinetics under extreme op-

Similarly, in cobalt-based alloys, understanding high temperature deformation is of utmost importance. During deformation, dislo-

EDITORIAL

Dear Colleagues and Friends of MPIE,

the analysis of microstructures and phase transformations is key to tuning and predicting their properties and lifespan for different application scenarios. This applies particularly to superalloys and intermetallics used for aero engines which we have thus chosen to highlight in this newsletter edition.

Please also have a look at our upcoming workshops and selected publications.

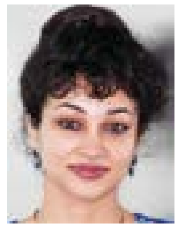
Enjoy reading,

Prof. Dr. Dierk Raabe, Chief Executive, MPIE

Awards and Achievements

Lamya Abdellaoui, doctoral student in the group "Nanoanalytics and Interfaces", won the Best Oral Communication Award at the 1st International Meeting on Alternative and Green Energies (IMAGE18).

Prof. Gerhard Dehm, director and head of the department "Structure and Nano-/Micromechanics of Materials", received an Advanced Grant of 2.5 million euros by the European Research Council for his research project on correlating grain boundary phase transformations and material properties.



Dr. Poulumi Dey, postdoctoral researcher in the group "Computational Phase Studies" won one of two Best Poster Awards at the 3rd International Conference on Metals and Hydrogen "SteelyHydrogen2018".

Prof. Dr. Haidong Fan from China, received a research fellowship from the Alexander von Humboldt Foundation and is now working in the department "Microstructure Physics and Alloy Design".

Dr. Simon Geiger, scientist in the group "Electrocatalysis", was awarded the prize of the German Chemical Society (GDCh) for his dissertation titled "Stability investigations of iridium-based catalysts towards acidic water splitting".

Intermetallic Phases & Materials

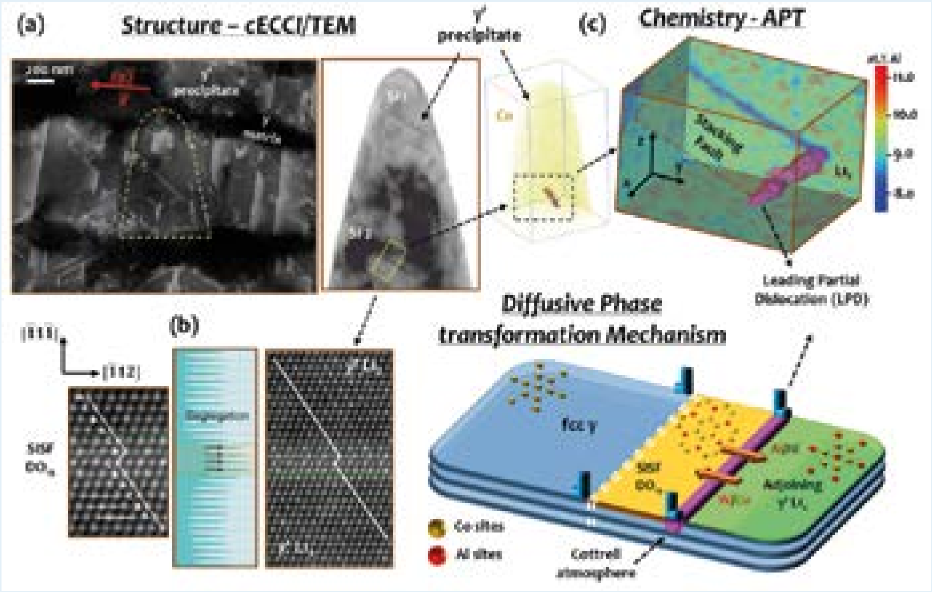


Fig. 2: a) cECCI overview image showing bright lines corresponding to stacking faults (SFs) in γ' precipitates and a BF TEM image of an APT tip showing two dark lines depicting SFs. b) HR-STEM of a SF in cubic [110] edge-on condition showing local DO_{19} ordering that is different from the surrounding $L1_2$ γ'. c) APT reconstruction showing a partial dislocation (pink colour, 5.6at.% Cr iso-compositional surface) associated to a confined Al depleted stacking fault plane and a schematic that shows the proposed solute diffusional mechanism occurring in the vicinity of the planar defect.

cations are generated in the γ matrix and their movement across γ' precipitates results in the formation of planar defects such as stacking faults (SF) (bright lines in Fig. 2a) and anti-phase boundaries. Combined high-resolution scanning transmission electron microscopy (HR-STEM) and APT of a stacking fault evidences a distinct structural-compositional contrast with respect to the surrounding lattice [3,4,5]. In Fig. 2b, the stacking fault possess different atomic structure of $D0_{19}$ order compared to the $L1_2$ order of the surrounding γ'. Additionally, the 3D compositional field in the vicinity of the planar defect enabled us to know that the diffusivity of the selective solutes to these defects and their diffusion directions are the rate limiting steps for the overall creep deformation of the superalloy.

These insights will help define strategies for alloys' additions that may help slow down creep deformation and hence enhance the lifetime of safety-critical parts at high temperatures.

References:

[1] P. Kontis, Z. Li, et al: T*he effect of chromium and cobalt segregation at dislocations on nickel-based superalloys*. Scr. Mater. 145 (2018)

[2] P. Kontis, D.M. Collins, et al: *Microstructural degradation of polycrystalline superalloys from oxidized carbides and implications on crack initiation*. Scr. Mater. 147, 59–63 (2018)

[3] S.K. Makineni, M. Lenz, et al: *Elemental segregation to anti-phase boundaries in crept CoNi-based single crystal superalloys*. Scr. Mater. (2018) accepted.

[4] S.K. Makineni, A. Kumar, et al: *On the diffusive phase transformation mechanism assisted by extended dislocations during creep of a single crystal CoNi-based superalloy*. Acta Mater. 155, 362–371 (2018)

[5] S.K. Makineni, M. Lenz, et al: *Correlative Microscopy - Novel Methods and Their Applications to Explore 3D Chemistry and Structure of Nanoscale Lattice Defects: A Case Study in Superalloys*. JOM, 1–8 (2018)

MA authors: P. Kontis, S. K. Makineni, B. Gault

Intermetallic phases – intermetallics for short – are phases which have different crystallographic structures than the elements they are composed of. Compared to conventional alloys with a solid solution matrix, additional chemical bonding in the intermetallics usually results in higher melting points, significantly increased strength, and high wear resistance, however on the expense of ductility. Because of their low density and good oxidation behaviour, aluminides are of specific interest for the development of novel materials with enhanced properties. Fundamental research for the development of intermetallic materials is a long-term topic at the MPIE.

Limited ductility hampered a wider industrial use of intermetallic materials for long time. Breakthrough came with the application of γ-TiAl alloys for compressor blades in aero engines. Due to a fine-scaled lamellar γ-TiAl + $α_2$-Ti_3Al microstructure, they have a high specific strength. Basis for respective alloy developments is the understanding of the phase transformations leading to the formation of these microstructures and of the phase equilibria at high temperatures for the long-term stability of these microstructures during application. Investigation of phase transformations by differential thermal analysis (DTA) or high-temperature X-ray diffraction (HT-XRD) and evaluation of phase equilibria by electron probe microanalysis (EPMA) are therefore fundamental for any aimed alloy development. Such essential thermodynamic data will be determined for a number of Ti–Al–X systems within the new large-scaled, collaborative European project ADVANCE. The MPIE not only has the facilities to determine the thermodynamic data but also a variety of melting devices to produce the necessary high-purity alloys, e.g., by levitation melting. The results are used to generate an advanced ThermoCalc© data base, which is a design tool for the development of next generation γ-TiAl alloys.

Iron aluminides – an economic alternative to stainless steels

Specific interest lies on the development of iron aluminide materials based on the phases FeAl, Fe_3Al and the Heusler phase $(X)_2YA1$ (X = Fe, Ni,…; Y = Ti, V, Nb, Ta,…). These materials have an outstanding corrosion resistance in a variety of aggressive environments, high wear resistance

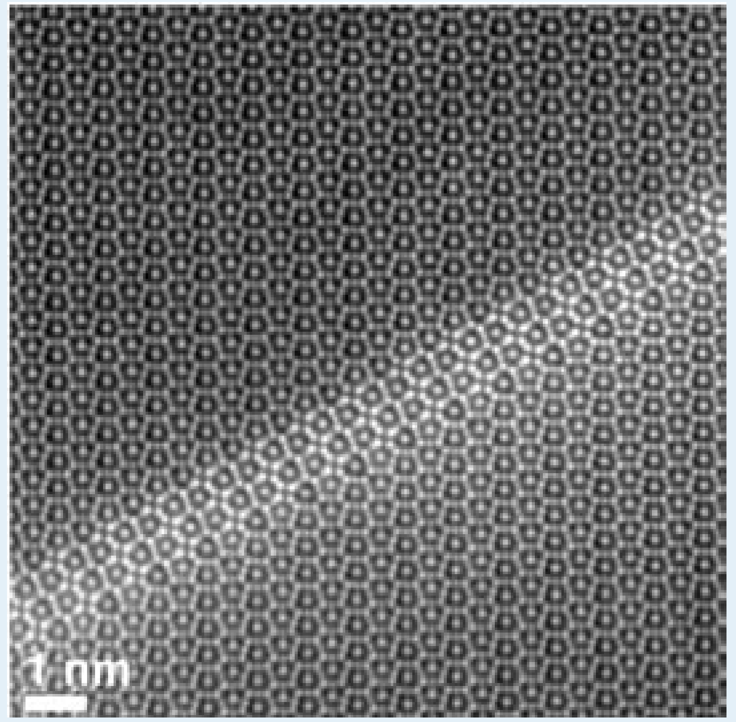


Fig. 1: High-angle annular dark-field scanning transmission electron microscopy (HAADF STEM) picture of a pyramidal fault in off-stoichiometric Nb-rich $NbFe_2$ Laves phase.

and low density and are considered as an economic alternative to stainless steels or Ni- and Co-based superalloys. However, limited strength at high temperatures inhibited any extensive application. New alloy concepts pursued at the MPIE lead to alloys which partially have much higher strength and creep resistance than advanced Cr steels. The alloy concepts include fine precipitation of borides or a film of Laves phase along grain boundaries, increasing the $D0_3$/B2 transition temperature, fine dispersion of Laves phase precipitates in the matrix, or generating coherent A2/B2/$L2_1$ microstructures. These developments have prompted new interest by industry. Casting, forging, and rolling on an industrial scale has been explored in a series of cooperations and different parts successfully passed tests under application conditions.

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 was 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. 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.

Laves phases - the most abundant class of intermetallics

Laves phases constitute the largest group of intermetallic phases. These very strong but brittle phases may not be usable as monolithic materials, but as strengthening phases, e.g. in iron aluminium alloys, Co-based alloys or steels. They exist with three different crystallographic structures, i.e. polymorphs, two hexagonal and a cubic. Stability of the different polymorphs in dependence on temperature and composition is another topic of basic research at the MPIE. An important aim is to understand the variation of properties in dependence of the composition, as many Laves phases do have extended homogeneity ranges and deviations from the ideal composition leading to the occurrence of different types of structural defects (e.g., see Fig. 1).

It has also been shown that novel steels and iron aluminide based alloys are substantially strengthened by micron-thick films of Laves phase on the grain boundaries. Though the Laves phases are inherently brittle, no internal cracking of the films is observed after plastic deformation, e.g. creep. Transmission electron microscopy and local strain measurements by X-ray diffraction are currently employed to understand this phenomenon.

Corrosion resistance of iron aluminides

Iron aluminides show an outstanding corrosion behaviour and many investigations have been performed to unravel the underlying mechanisms. In all cases it has been found, that the ability to form Al_2O_3 scales or Al-rich passive films is the key for the excellent corrosion resistance. In oxidizing environments, thin, dense and adhesive Al_2O_3 scales form that also withstand thermal cycling. A minimum of about 15 at.% Al is necessary for their formation. Salt spray tests, corrosion in water vapour, aqueous corrosion, and hot corrosion by molten salts yielded varying corrosion resistance. However, in all cases an improvement was seen when the Al content was high enough to form protective scales or films.

Al_2O_3 scales can also be generated by a short pre-oxidation treatment. The scales act as protecting "isolators", separating the iron aluminide from the environment. Pre-oxidation has been shown to be very effective to enhance the aqueous corrosion resistance, which otherwise is only mediocre. The anodic current density in the passive range during immersion in H_2SO_4 of pH 1.6 is significantly decreased by two orders of magnitude and also repassivation of smaller defects occurs readily. X-ray photoemission spectroscopy (XPS) revealed that the scale is comprised of an outer layer of mixed Al and Fe oxides and an inner layer of hydroxides enriched in Al, which was found to be significantly more resistant than the oxide layers formed on pure aluminium. Even long-time immersing of the scale has no effect on its beneficial performance.

Other intermetallics phases of interest for structural applications studied at the MPIE are silicides, NiAl and N_3Al, of which the latter is the strengthening gamma prime (γ´) phase in Ni-based superalloys.

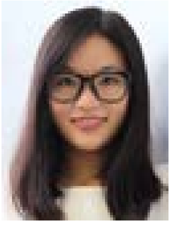
SN authors: M. Palm, F. Stein
GO authors: M. Rohwerder

YEARS 1917–2017 100

Awards and Achievements

Dr. Tilmann Hickel, head of the group "Computational Phase Studies", won the Certificate of Excellence in Reviewing by Acta Materialia and Scripta Materialia.

Dr. Christoph Kirchlechner, head of the group "Nano-/ Micromechanics of Materials", won the Certificate of Excellence in Reviewing by Acta Materialia and Scripta Materialia.



Dr. Zirong Peng, postdoctoral researcher in the group "Atom Probe Tomography", was honoured with the "2017 Chinese Government Award for Outstanding Self-financed Students Abroad".

Dr. Cigdem Toparli, formerly doctoral student in the group "Interface Spectroscopy" and now at the Massachusetts Institute for Technology, won the Young Author Prize of the Oronzio and Niccolò de Nora Foundation for her publication "*In situ* and operando observation of surface oxides during oxygen evolution reaction on copper" published in Electrochimica Acta 236, 104-115 (2017)

Dr. Fengkai Yan from China, received a research fellowship from the Alexander von Humboldt Foundation and is now working in the group "Alloy Design and Thermomechanical Processing".