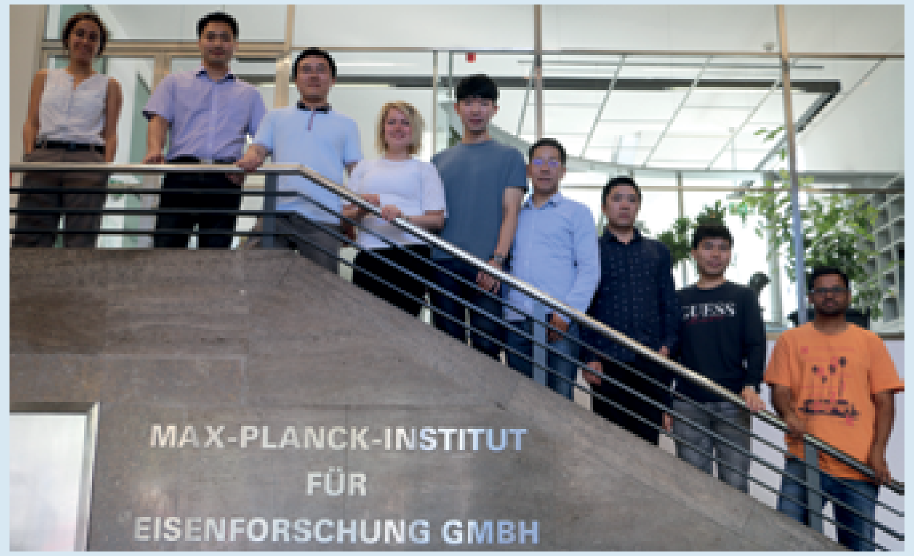
Scientists at the MPIE: The Humboldt Community



The MPIE Humboldt community (from left to right): Raheleh Hadian, Xiankang Zhong, Hong Luo, Olga Kasian, Seok Su Sohn, Xu Zhang, Sai Tang, Jianjun Li and Surendra Makineni (missing: Fengkai Yan and Xufei Fang).

The Alexander von Humboldt Society supports excellent researchers from outside Germany with an up to two years scholarship to continue their work in a German research institution of their choice. Currently, 11 Humboldt research fellows take this opportunity and are working at the MPIE. The researchers, mainly postdoctoral students and senior scientists, work in the different departments of the institute, each one following their own research project.

Asking them why they decided to come to the MPIE and continue their research here, the answer is often similar: "The MPIE is well known when it comes to materials science and the dense infrastructure provided here is difficult to find somewhere else", so Dr. Surendra Makineni, who is a postdoctoral researcher originally from India, but joining the MPIE after a research stay at the University of Michigan, USA. He is currently trained on the MPIE's atom probes, as this technique of analysing a material down to the atomic scale is just evolving in India.

"The close link between basic research on the one hand and industrial application on the other hand, is what really attracted me to choose this institute", says Dr. Olga Kasian, who is currently working in the field of electrocatalysis and originally comes from Ukraine.

"What surprised me when I started at the MPIE is the fact that people from different departments are working so closely together and discussing scientific topics even when they are not directly linked to their own research. This opens up totally new point of views and can be very beneficial. I would like to apply this way of management when I get back to China", explains Dr. Fengkai Yan.

Besides science, the Humboldt researchers also gathered many impressions of Germany and Düsseldorf: "Honestly, back in China, online payment is much more convenient and online shopping as well", admits Fengkai, "in China we just show a QR code on our mobile phones to any cashier, and this is how you pay. No credit card, no pin codes." At the same time both Fengkai and Surendra enjoy the good public transport system here in Germany and like the green sides of Düsseldorf which remind them of villages in their home countries.

Selected Publications

Computational Materials Design:

L. Huber, B. Grabowski, M. Militzer, J. Neugebauer, J. Rottler: *Ab initio modelling of solute segregation energies to a general grain boundary*. Acta Mat, 132, 138-148 (2017)

Z. Pei, X. Zhang, T. Hickel, M. Friák, S. Sandlöbes, B. Dutta, J. Neugebauer: *Atomic structures of twin boundaries in hexagonal close-packed metallic crystals with particular focus on Mg*. npj Comput Mater, 3 (1), 6, (2017)

Interface Chemistry and Surface Engineering:

T. Frigge, B. Hafke, T. Witte, B. Krenzer, C. Streubühr, A. Samad Syed, V. Miksic Trontl, I. Avigo, P. Zhou, M. Ligges, D. von der Linde, U. Bovensiepen, M. Horn von Hoegen, S. Wippermann, A. Lücke, S. Sanna, U. Gerstmann, W. G. Schmidt: *Optically excited structural transition in atomic wires on surfaces at the quantum limit*. Nature, 544, 207-211 (2017)

C. Toparli, A. Sarfraz, A. D. Wieck, M. Rohwerder, A. Erbe: *In situ and operando observation of surface oxides during oxygen evolution reaction on copper*. Electrochim Acta, 236, 104-115 (2017)

Microstructure Physics and Alloy Design:

S. Jiang, H. Wang, Y. Wu, X. Liu, H. Chen, M. Yao, B. Gault, D. Ponge, D. Raabe, A. Hirata, M. Chen, Y. Wang, Z. Lu: *Ultrastrong steel via minimal lattice misfit and high-density nanoprecipitation*. Nature, 544, 460-464 (2017)

M. Koyama, Z. Zhang, M. Wang, D. Ponge, D. Raabe, K. Tsuzaki, H. Noguchi, C.C. Tasan: *Bone-like crack resistance in hierarchical metastable nanolaminate steels*. Science, 355 (6329), 1055-1057 (2017)

Structure and Nano-/Micromechanics of Materials:

S.W. Hieke, B. Breitbach, G. Dehm, C. Scheu: *Microstructural evolution and solid state dewetting of epitaxial Al thin films on sapphire (alpha-Al2O3)*. Acta Mat, 133, 356-366 (2017)

M. J. Duarte, A. Kostka, D. Crespo, J.A. Jimenez, A-C Dippel, F. U. Renner, G. Dehm: *Kinetics and crystallization path of a Fe-based metallic glass alloy*. Acta Mat, 127, 341-350 (2017)

Selected Talks

Computational Materials Design:

J. Neugebauer: *How to achieve interoperability - a modeler's perspective*. 1st EMMC International Workshop, Vienna, Austria, 5 – 7 Apr 2017

M. Todorova: *Ab-initio description of oxides in an electrochemical environment*. TMS Meeting, San Diego, USA, 26 Feb – 2 Mar 2017

Interface Chemistry and Surface Engineering:

S. Wippermann: *Exotic forms of silicon for photovoltaic applications*. E-MRS Spring Meeting, Strasbourg, France, 22 – 26 May 2017

M. Rohwerder: *Novel approaches for characterizing the delamination resistance of organic coatings*. 10th International Workshop on Application of Electrochemical Techniques to Organic Coatings – AETOC, Billerbeck, Germany, 25 – 28 Apr 2017

Microstructure Physics and Alloy Design:

D. Raabe, B. Gault, A. Breen, Y. Chang, M. Yao, D. Ponge, M. Herbig, C. Liebscher, G. Dehm, C. Scheu, A. Stoffers, J. Neugebauer: *Advanced atom probe tomography*. 25th Annual Meeting of the German Crystallographic Society, Karlsruhe, Germany, 27 – 30 Mar 2017

D. Raabe, B. Gault, A. Breen, Y. Chang, M. Yao, D. Ponge, M. Herbig, C. Liebscher, G. Dehm, C. Scheu, A. Stoffers, J. Neugebauer: *Atomic scale characterization of complex materials*. Physikalisches Kolloquium, Freiburg, Germany, 6 Feb 2017

Structure and Nano-/Micromechanics of Materials:

C. Kirchlechner, N. Malyar, G. Dehm: *Using nano- and micromechanics to understand interface plasticity*. Hysitron Nanobrücken 2017, Manchester, UK, 4 – 6 Apr 2017

S. Brinckmann, C. Fink, G. Dehm: *Severe microscale deformation of pearlite cementite*. 2017 MRS Spring Meeting, Phoenix, USA, 17 – 21 Apr 2017

News and Events

Selected Upcoming Events

29 Aug 2017: Symposium on 3D Materials Characterization

This symposium introduces some major experimental and theoretical tools for 3-dimensional materials characterization and discusses their potentials, applications and limits. Moreover, a number of results emphasizing the combination of theoretical and experimental characterization in 3D will be presented, as well as ways how the iron and steel industry can use 3D characterization. The symposium takes place at the MPIE.
http://www.mpie.de/3646655/symposium-3d-materials-characterization-at-all-length-scales-and-its-applications-to-iron-and-steel

11 – 12 Sep 2017: Symposium on Alloys for Additive Manufacturing

The focus lies on experimental and theoretical research on powder making, in-process materials behaviour, post-processing and the resulting materials properties. All materials scientific issues pertaining to the additive manufacturing of metals, alloys and composites including a metallic phase, will be discussed. The symposium takes place at the Empa Academy in Dübendorf, Switzerland. It is followed by a conference on Additive Manufacturing in Products and Applications, which takes place at the ETH Zürich.
http://www.mpie.de/aams2017

11 – 15 Sep 2017: Summer School on Experimental Nano- and Micromechanics

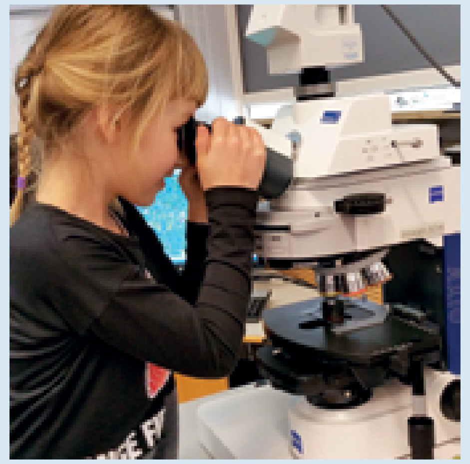
The summer school aims at providing a comprehensive overview on experimental nano- and micromechanical testing methods. In the focus are material properties which can be reliably extracted from *in situ* micromechanical experiments. The school will deal with nanoindentation and methods to explore the plastic and fracture properties of materials and interfaces, frequently used characterization techniques with *in situ* capabilities and simulation techniques. The school will take places at the MPIE.
http://www.mpie.de/3583669/summer-school-on-experimental-nano-and-micromechanics

Selected Past Events

26 Jan – 12 Jul: 100 years MPIE - various events

This year is marked by the milestone anniversary of the MPIE. The highlight of the celebrations will be the ceremonial act on 6th October. Nevertheless the institute organized various successful events since January 2017. Kopf-Salat, a series of talks for the broad public, took place every two months covering the topics neurology, material science, experimental physics and conflict research and reaching over 640 people. Moreover the institute organized two kids' universities for 70 children who experienced in small experiments the fundamentals of materials research. The MPIE also engaged at the Girls' Day, a nation wide day where girls are encouraged to participate at male dominated jobs. Thereby the MPIE opened its material testing, nano science and additive manufacturing laboratories.

If you want to be informed about upcoming events, please write an e-mail to: pr@mpie.de



During the kids' university the children had the chance to learn basics about metals and to do small experiments themselves.

Imprint

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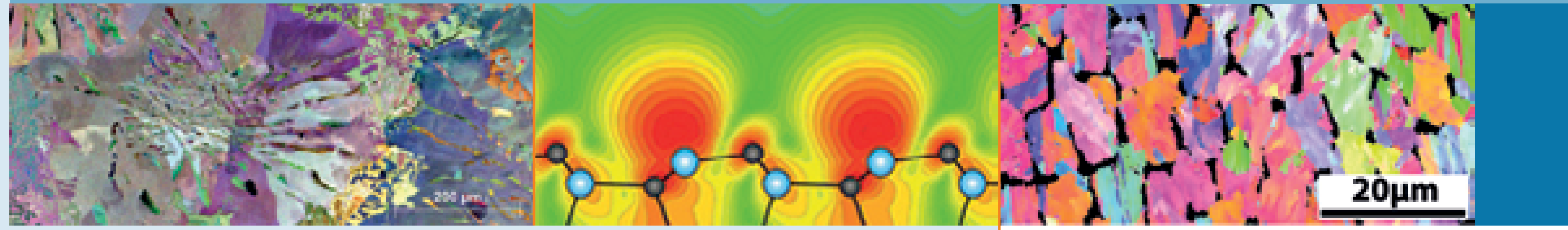

The Complex Interplay of Grain Boundary Structure and Mechanics

The significant impact of grain boundaries on the mechanical response of crystalline materials had been recognized ever since the concept of dislocations as carrier of plasticity in metals had been established. Nevertheless, a comprehensive and quantitative understanding of plasticity at grain boundaries, the impact of slip geometry, atomic structure and chemistry is still lacking. Today´s advanced characterization tools with outstanding *in situ* capabilities permit unprecedented insights into dislocation slip transfer – being a central topic of the Structure and Nano-/ Micromechanics department of the MPIE.

Grain and phase boundaries are omnipresent in materials. It is commonly known that increasing the boundary density (i.e. decreasing the crystallite size) results in pronounced hardening, empirically described via the Hall-Petch relation. However, the impact of the local slip geometry, the atomistic grain boundary structure and chemistry on the breakthrough stress of dislocations is quantitatively unknown.

To unravel the fundamental question of the underlying slip transfer mechanism and establish general material models a research strategy comprising small scale *in situ* deformation in the scanning electron microscope (SEM) and at Laue microdiffraction (µLaue) synchrotron beamlines together with advanced microstructure characterization in the transmission electron microscope (TEM), is currently applied. Testing the mechanical response of single and bi-crystalline submicron sized samples permits to study the mechanical impact of one individual grain boundary without being blurred by the surrounding bulk (see Fig. 1 a, b). But the testing protocol allows for more than just being a mechanical microscope. Due to the *in situ* capabilities of µLaue and SEM based techniques, the number and type of stored and transmitted dislocations can be measured while monitoring the required stresses for deformation – giving a comprehensive picture of the collective transmission properties of a grain boundary. The additional use of TEM based techniques does not only give insights on the interaction of one individual dislocation with a grain boundary, but can also be used to establish the atomic structure and chemistry of the grain boundary before and eventually after deformation.

First results show that the dislocation transmission stress through coherent copper twin boundaries can be as low as 17 MPa, which is currently supported by atomistic modelling made by

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EDITORIAL

Dear Colleagues and Friends of the MPIE,

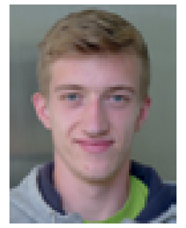
Grain boundaries, their structure, mechanics and migration, are in the spotlight of this newsletter edition. Better understanding of grain boundaries enables improvement of the mechanical, electronic and chemical behaviour of materials. Here we present the work of three groups which focus on different aspects of this topic.

Please also have a look at our upcoming workshops focussing on additive manufacturing and nanomechanics. More research activities and events are listed on our website.

Enjoy reading and best regards,

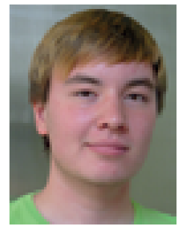
Prof. Dr. Dierk Raabe, Chief Executive, MPIE

Awards and Achievements



Heidi Bögershausen, **Luca Bender** (**photo**) and **Christian Broß**, materials testers, won the second and third place for their posters at the "MikPräp 2017", a conference for microscopy and preparation.

Dr. Martin Diehl, postdoctoral researcher in the group "Theory and Simulation" received the Dr. Klaus-Körper Award of the International Association of Applied Mathematics and Mechanics (GAMM) and the Borchers-Plakette by the RWTH Aachen University for his doctoral thesis on "High-Resolution Crystal Plasticity Simulations".



Till Freieck, materials tester, gave an excellent talk at the "MikPräp 2017" and won the Apprentice Prize 2017 of the Max Planck Society.

Shyam Katnagallu, doctoral student in the group "Atom probe Tomography", was awarded by the International Field Emission Society (IFES) for his outstanding paper contributed to the Microscopy and Microanalysis meeting 2017.

Dr. Christoph Kirchlechner, head of the group "Nano-/ Micromechanics of Materials" received the Heinz Maier-Leibnitz Prize of the Deutsche Forschungsgemeinschaft, one of the most important German awards for young scientists.

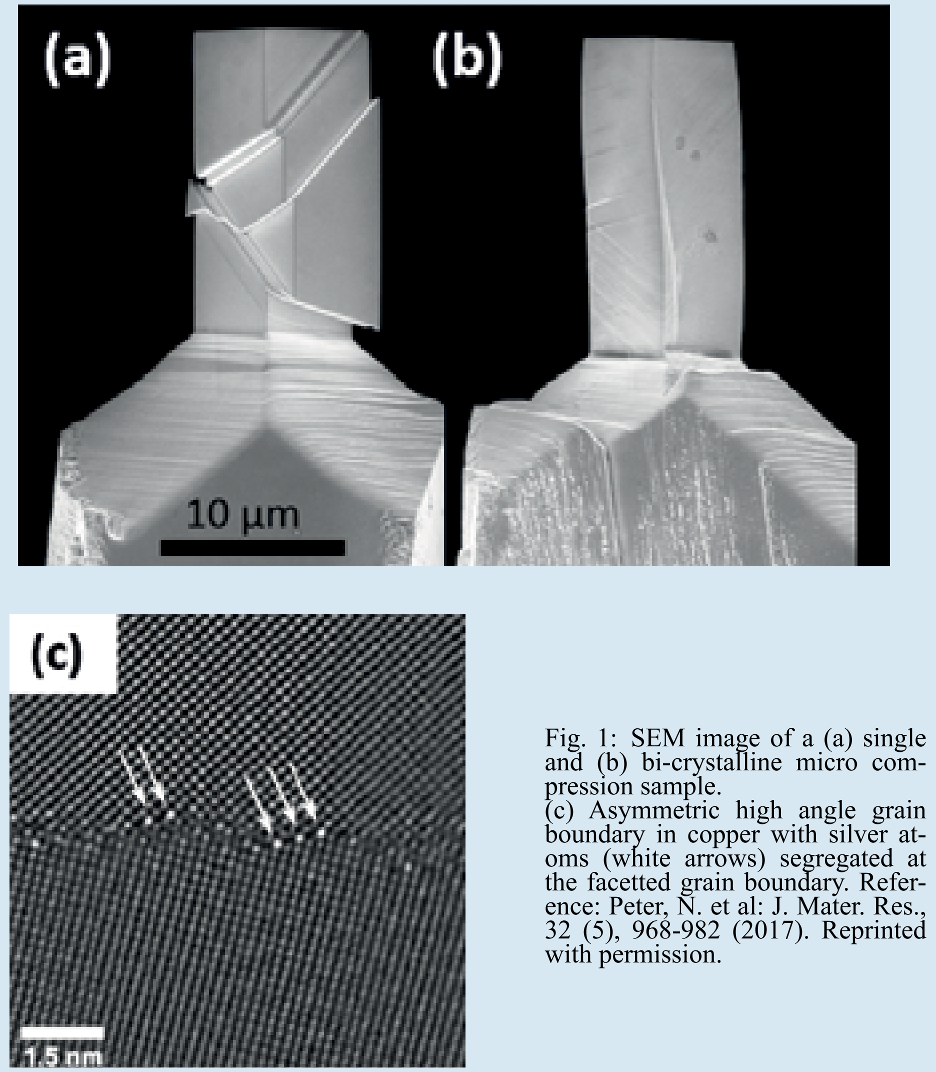


Fig. 1: SEM image of a (a) single and (b) bi-crystalline micro compression sample.
(c) Asymmetric high angle grain boundary in copper with silver atoms (white arrows) segregated at the facetted grain boundary. Reference: Peter, N. et al: J. Mater. Res., 32 (5), 968-982 (2017). Reprinted with permission.

the MPIE's Computational Materials Design department. Nevertheless, for pure general high angle grain boundaries the definition of a break-through stress might not be a suitable strategy to describe the slip transfer properties of a grain boundary, as in this case the slip transfer behaviour is highly strain rate dependent. These characteristics can be vastly different in the case of alloyed materials, where segregation induced changes in grain boundary chemistry occur: An indication of faceting, either caused or stabilized by solutes was recently observed by high resolution scanning TEM in Ag alloyed Cu samples (see Fig. 1c). These changes in atomic structure and chemistry can result in local stress concentrations and / or a hindered, non-conservative motion of dislocations in the grain boundary plane. The connection of both, the atomic structure of individual grain boundaries and their interaction behaviour with dislocations is focus of our current investigations.

Authors: C. Kirchlechner, N.V. Malyar, N. Peter, C. Liebscher, G. Dehm

Grain Boundary Migration in Metals

The migration of grain boundaries plays a pivotal role in the evolution of materials' microstructures, strongly impacting the mechanical, chemical, or electronic response of a material. For designing optimized materials with tailored microstructures, a detailed understanding of grain boundary kinetics and of the underlying atomistic mechanisms is therefore crucial. Identifying these fundamental mechanisms and understanding their impact on grain boundary migration has been a key topic both from an experimental as well as a theoretical perspective for several decades.

In a recent work [1] we, the group "Adaptive Structural Materials" in the department "Computational Materials Design", studied the kinetics of general grain boundary migration using classical Molecular Dynamics (MD) simulations. Because the time scale of MD simulations is orders of magnitude smaller than in the relevant experiments on migration, we used a multi-scale approach to predict grain boundary migration at experimentally relevant time scales. Having identified the atomistic mechanisms of motion, we developed mesoscale models and extrapolated the migration energy barrier to small, experimentally applied forces. The asymptotic behaviour of these models in the zero driving force limit can now be compared to experimental results. Note that theoretically flat (symmetric) grain boundaries are immobile at low driving forces. The studied non-symmetric and general grain boundaries have energy barriers that are a few factors up to an order of magnitude smaller than the experimental ones derived from our collaborators at the RWTH Aachen

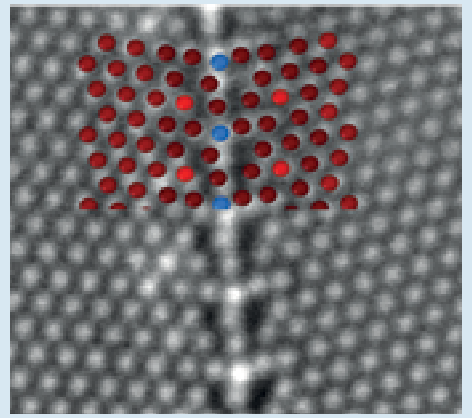


Fig. 1: A TEM observation of the Σ7 Al grain boundary studied in the grain boundary migration experiments. The overlapping simulation results show that the binding energy of copper atoms to the Al grain boundary is strong at the blue sites in perfect agreement with the experimentally observed segregation.

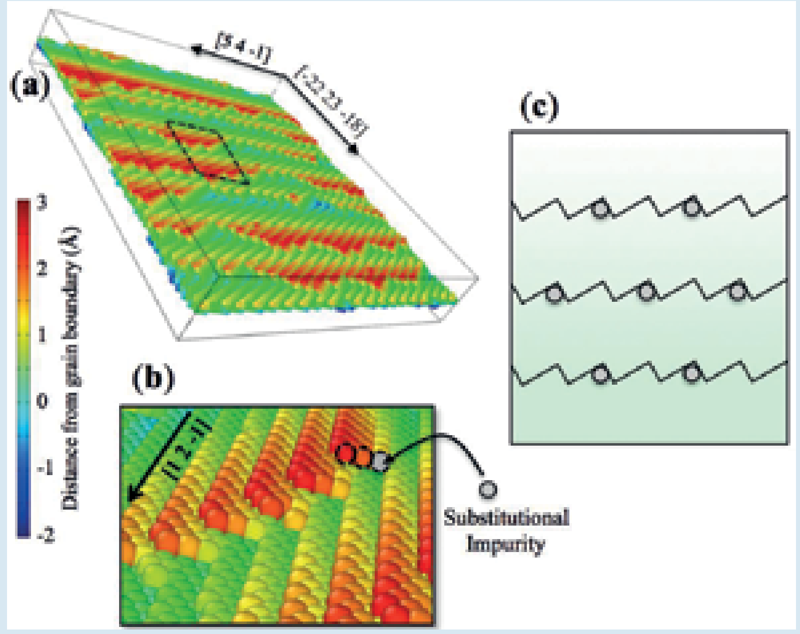


Fig. 2: This figure shows the general structure of a moving grain boundary. The kink sites serve as the positions for the substitutional impurities (a and b). A 2D kinetic Monte Carlo model as schematically shown in (c) will be used to simulate the migration in the presence of impurities at experimental time scales.

University [2]. This gap can be attributed to impurities segregating at grain boundaries.

To investigate this gap in migration barriers we produced transmission electron microscopy (TEM) samples from the experimental bi-crystals that were used to study grain boundary migration. Fig. 1 depicts the atomic structure of a Σ7 boundary captured by high resolution TEM measurements performed by the department "Structure and Nano-/Micromechanics of Materials" at the MPIE. Even though the purity of the macroscopic Al samples has been reported to be about 5 ppm, the grain boundary structure has been fully decorated with Cu atoms. We use this observation as corroborative evidence that impurities can always be existent in experimental settings, thus affecting the results.

To further investigate the role of impurities in migration, we are currently utilizing our knowledge about the kinked migration of a general grain boundary (see Fig. 2a and b) to place substitutional impurities at the kink sites (those have the highest binding energies), to run MD simulations and to design 2D kinetic Monte Carlo simulations with the geometries such as the one shown in Fig. 2c. We expect higher energy barriers due to changes in atomic shuffling mechanism at the kink sites caused by the impurity atoms.

References:
[1] Hadian, R. and Grabowski, B. and Race, C. P. and Neugebauer, J, PRB, vol 94, 2016.
[2] Molodov, Dmitri A. and Gorkaya, Tatiana and Gottstein, Günter, Scripta Mater., vol 65, 2011.

Authors: R. Hadian and B. Grabowski

Comprehensive Characterization of Grain Boundaries

Grain boundaries are important 2-dimensional microstructural elements. They strongly influence most of the properties of polycrystalline materials like mechanical, chemical, or electronic behaviour. Understanding materials properties, therefore, requires understanding the correlation of their character and their properties.

The crystallographic character of every flat grain boundary (GB) segment is determined by 8 parameters: 5 rotational parameters describing the rotational positions of the two crystals across the boundary and of the boundary plane, and 3 translational parameters describing the relative shift of the two crystal lattices at the atomic level. Additionally, on curved boundaries these parameters may change from place to place giving rise to further degrees of freedom and changing properties.

gramme (QUBE, commercialized by Bruker nano) which allows alignment of the slices and, e.g., reconstruction and display of the 3D-GBs. An example is given in Fig. 1a showing 3 grains of an FeNi martensitic microstructure and their crystallographic properties in form of inverse pole figures.

Without knowledge of the related GB properties, the 5-parameter GB character alone is not very interesting. However, once it has been de-

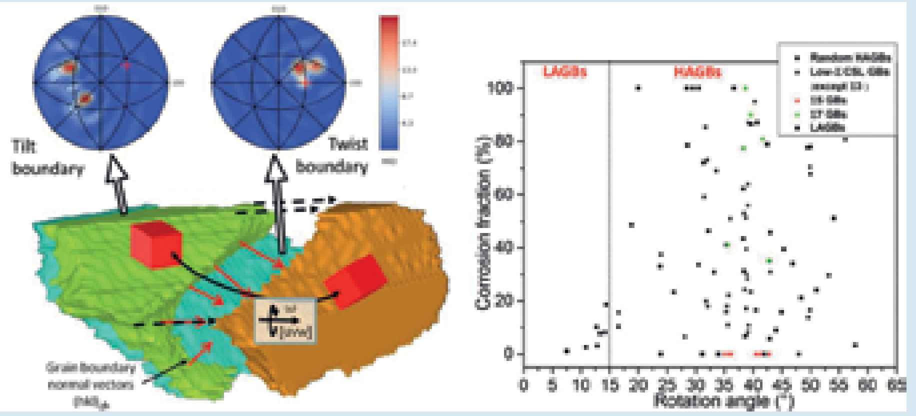


Fig. 1: (a) 3D orientation microscopy image and GB pole figures of 3 grains in a FeNi alloy. (b) Corrosion properties of GBs in a stainless steel displayed over the GB misorientation angle. For low angle GB (LAGB) corrosion increases with misorientation angle. No clear correlation is visible for high angle GB (HAGB) because GB planes are not considered in the graph.

The 3 translational parameters usually depend on the rotational ones. It is, therefore, important to determine the 5 rotational parameters and correlate them to properties. We have developed over the last years software and hardware tools to measure and analyse the 5-parameter grain boundary character and the related local properties. Hence we use 3-dimensional orientation microscopy based on a combination of orientation mapping by electron backscatter diffraction (EBSD) and serial sectioning [1].

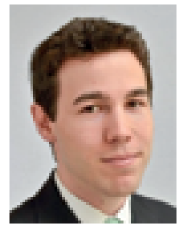
For 3D-reconstruction the successive individual slices are loaded into a self-developed computer pro-

termined it is possible to measure properties on the remaining part of the material. In this way we could measure, e.g., the cathodoluminescence activities of GBs in polycrystalline CdTe solar cells. In another example we measured the corrosion activity of different GBs in a stainless steel. It was found that both, GB planes as well as GB misorientations have strong influence on the corrosion activity (see Fig. 1b).

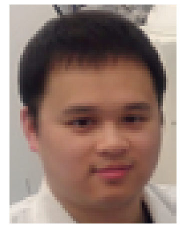
References:
[1] S. Zaefferer, S.I. Wright, (2008), in "EBSD in Materials Science", ed. A. Schwartz et al., Springer, 109-123

Authors: S. Zaefferer, P. Konijnenberg, D. An, G. Stechmann

Awards and Achievements



Philipp Kürnsteiner, doctoral student in the group "Additive Manufacturing", won the Student Scholar Award 2017 by the Microscopy Society of America and the Microanalysis Society for his paper on "In-process Precipitation During Laser Additive Manufacturing Investigated by Atom Probe Tomography".



Wei Luo, doctoral student in the group "Intermetallic Materials" won the Best Student Talk Award at the "Nanobrücken 2017" conference for his presentation on "Fracture Toughness of Hexagonal and Cubic $NbCo_2$ Laves Phases".

Prof. Dierk Raabe, chief-executive", successfully applied for a funding of 1.84 million euros by the German Federal Ministry of Education and Research to develop ultra high-strength lightweight steels.

Dr. Torsten Schwarz, senior scientist in the group "Interface Design in Solar Cells", was honoured with the Borchers-Plakette by the RWTH Aachen University for his doctoral thesis "On the Nano-scale Characterization of Kesterite Thin-films".

Ralf Selbach, head of the mechanical workshop, was awarded with the Silver Badge of Honour by the Chamber of Industry and Commerce of Düsseldorf for his longstanding work as trainer and examiner.