Scientists at the MPIE

Dr. Paraskevas Kontis works as a postdoctoral researcher in the group "Atom Probe Tomography" since 2016. He focuses on hydrogen embrittlement in engineering alloys, damage and crack initiation mechanisms in superalloys and the relationship between grain boundaries and mechanical performance at elevated temperatures in superalloys. Thereby he uses atom probe tomography as a tool to understand deformation mechanisms at high performance materials, which allows to design strategies for the development of materials exhibiting enhanced performance.

Before joining the MPIE, Kontis worked as a postdoctoral researcher at the University of Oxford, where he also did his PhD in 2016 about grain boundary elements on polycrystalline superalloys. His thesis was supported by a scholarship of Siemens. Kontis did his master thesis project at the RWTH Aachen University with a main focus on the determination of the Nb content in nickel-based superalloys.

Selected Publications:

P. Kontis, D.M. Collins, A.J. Wilkinson, R.C. Reed, D. Raabe, B. Gault: *Microstructural degradation of polycrystalline superalloys from oxidized carbides and implications on crack initiation*. Scripta Mater, 147, 59-63 (2018)

P. Kontis, Z. Li, D.M. Collins, J. Cormier, D. Raabe, B. Gault: *The Effect of Chromium and Cobalt Segregation at Dislocations on Nickel-based Superalloys*. Scripta Mater, 145, 76-80 (2018)

E. Chauvet, P. Kontis, E.A. Jägle, B. Gault, D. Raabe, C. Tassin, J.-J. Blandin, R. Dendievel, B. Vayre, S. Abed, G. Martin: *Hot Cracking Mechanism Affecting a Non-weldable Ni-based Superalloy Produced by Selective Electron Beam Melting*. Acta Mat, 142, 82-94 (2018)

Dr. Dirk Ponge is head of the group "Alloy Design and Thermomechanical Processing". His group's mission is the optimization of properties of novel complex engineering steels through a detailed characterization and interpretation of materials' microstructures and through advanced ways of thermomechanical processing. Coupling alloy design strategies with processing enables to influence bulk phase transformations, precipitates and grain refinement mechanisms. Application fields are for example medium and high manganese and dual phase steels for lightweight automotive design. The group is also investigating mechanisms of hydrogen embrittlement in high strength alloys. The mission here is to create tailored microstructures providing high strength but with a low sensitivity against hydrogen embrittlement.

Before joining the MPIE in 2001, Ponge did his PhD at the RWTH Aachen in the field of dynamic recrystallization of Ni_3Al. After that he was head of the materials testing department at the Schweißtechnische Lehr- und Versuchsanstalt Nord in Hamburg where he also was involved in training of welding engineers.

Selected Publications:

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(1), 1137, (2018)

Z. Tarzimoghadam, D. Ponge, J. Klöwer, D. Raabe: *Hydrogen-assisted failure in Ni-based superalloy 718 studied under in situ hydrogen charging: The role of localized deformation in crack propagation*. Acta Mat, 128, 365-374 (2017)

M.-M. Wang, C.C. Tasan, D. Ponge, D. Raabe: *Spectral TRIP enables ductile 1.1 GPa martensite*. Acta Mat, 111, 262-272 (2016)

Selected Publications

Computational Materials Design:

Y. Ikeda, F. Körmann, B. Dutta, A. Carreras, A. Seko, J. Neugebauer, I. Tanaka: *Temperature-dependent phonon spectra of magnetic random solid solutions*. npj Comput Mater, 4, 7 (2018)

S. Yoo, M. Todorova, J. Neugebauer: *Selective solvent-induced stabilization of polar oxide surfaces in an electrochemical environment*. Phys Rev Lett, 120 (6) (2018)

Interface Chemistry and Surface Engineering:

W. Krieger, S. V. Merzlikin, A. Bashir, A. Szczepaniak, H. Springer, M. Rohwerder: *Spatially resolved localization and characterization of trapped hydrogen in zero to three dimensional defects inside ferritic steel*. Acta Mat, 144, 235-244 (2018)

M. Ledendecker, J. S. Mondschein, O. Kasian, S. Geiger, D. Göhl, M. Schalenbach, A. Zeradjanin, S. Cherevko, R. E. Schaak, K. Mayrhofer: *Stability and activity of non-noble-metal-based catalysts toward the hydrogen evolution reaction*. Angew Chem Int Ed, 56, 9767-9771 (2017)

Microstructure Physics and Alloy Design:

Y. Yu, S. Zhang, A. Mio, B. Gault, A. Sheskin, C. Scheu, D. Raabe, F. Zu, M. Wuttig, Y. Amouyal, O. Cojocaru-Miredin: *Ag-segregation to dislocations in PbTe-based thermoelectric materials*. ACS Appl Mater Interfaces, 10 (4), 3609–3615 (2018)

J. Han, S.-H. Kang, S.-J. Lee, M. Kawasaki, H.-J. Lee, D. Ponge, D. Raabe, Y.-K. Lee: *Superplasticity in a lean Fe-Mn-Al steel*. Nat Commun, 8, 751 (2017)

Structure and Nano-/Micromechanics of Materials:

J. Guo, G. Haberfehlner, J. Rosalie, L. Li, M. 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 Commun, 9 (1), 946 (2018)

C. H. Liebscher, M. Yao, P. Dey, M. Lipińska-Chwalek, B. Berkels, B. Gault, T. Hickel, M. Herbig, J. Mayer, J. Neugebauer, D. Raabe, G. Dehm, C. Scheu: T*etragonal fcc-Fe induced by κ-carbide precipitates: Atomic scale insights from correlative electron microscopy, atom probe tomography, and density functional theory*. Phys Rev Materials, 2 (2) (2018)

Selected Talks

Computational Materials Design:

J. Neugebauer, J. Janssen, et al: *Exploration of Large Ab Initio Data Spaces to Design Structural Materials with Superior Mechanical Properties*. TMS 2018, Phoenix, USA, 11 – 15 Mar 2018

J. Neugebauer, S. Surendralal, et al: *A first principles approach to model electrochemical reactions in an electrolytic cell*. Workshop - The Electrode Potential in Electrochemistry - A Challenge for Electronic Structure Theory Calculations. Reisensburg, Germany, 26 – 29 Nov 2017

Interface Chemistry and Surface Engineering:

M. Rohwerder, T. H. Tran: *Novel zinc-nanocontainer composite coatings for intelligent corrosion protection*. 11th International Conference on Zinc and Zinc Alloy Coated Steel Sheet - GALVATECH 2017, Tokyo, Japan, 12 – 16 Nov 2017

M. Rohwerder: *Organic coatings for corrosion protection: self-healing at the delaminated interface*. 232th Meeting of the Electrochemical Society, National Harbor, USA, 1 – 6 Oct 2017

Microstructure Physics and Alloy Design:

D. Raabe, B. Gault, et al: *Textures studied at near atomic-scale*. 18th International Conference on Textures of Materials - ICOTOM-18, St George Utah, USA, 6 Nov 2017

D. Ponge, C. Tasan, et al: *1 billion tons of nanostructure - metastability alloy design and segregation engineering*. 38th Risø International Symposium on Materials Science - Advanced Metallic Materials by Microstructural Design, Roskilde, Denmark, 4 Sep 2017

Structure and Nano-/Micromechanics of Materials:

R. Soler, S. Gleich, et al: *Mo_2BC thin films - a material system combining hardness and ductility*? 5th European Conference in Nanofilms - ECNF2018, Cranfield, UK, 20 – 22 Mar 2018

C. Kirchlechner, N. Malyar, et al: Mechanism based description of dislocation grain-boundary interactions. DPG-Frühjahrstagung der Sektion Kondensierte Materie gemeinsam mit der EPS, Berlin, Germany, 11 – 16 Mar 2018

News and Events

Selected Upcoming Events

14 Sep 2018: Max Planck Day

A kids' laboratory will give young children the chance to do experiments and experience how different chemicals react and how physical phenomena function. The evening offers a Kopf-Salat-talk about big data, machine learning and computational materials design. At the same time a group of MPIE scientists will present their work on additive manufacturing and join a science slam at a science marketplace in Munich, where the headquarter of the Max Planck Society is located. All these activities take place on the occasion of the Max Planck Day, where all Max Planck institutes will offer various events to honour the founder of the Max Planck Society who celebrates in 2018 his 160th birthday and his 100th jubilee of receiving the Nobel Prize. Moreover, the Max Planck Society itself turns 70th years old.

4 – 9 Nov 2018: Workshop "*Ab initio* Description of Iron and Steel"

The 7th ADIS workshop will focus on thermodynamics, kinetics as well as structural defects, with a particular aim on the impact of magnetism on these properties. It will take place at the Ringberg Castle (Tegernsee, Germany).

5 – 6 Nov 2018: Opening of the transmission electron microscopy and atom probe tomography facilities

The colloquium is dedicated to the various research topics evolving through the advanced new facilities of atom probe tomography and transmission electron microscopy at the MPIE. These include new trends and advances in applying these techniques to interfaces, functional and structural materials and in the developing of new methodologies and correlative studies.

7 – 9 Nov 2018: European APT workshop

The workshop includes talks about current progress and problems in atom probe tomography as well as advanced training sessions for APT users. It will take place at the MPIE and is open for people from academia and industry.

Selected Past Events

23 Mar 2018: Senate of the Max Planck Society

The Senate of the Max Planck Society met at the MPIE in March. It is the central decision-making and supervisory body of the Max Planck Society and consists of representatives from different areas of society such as science, industry, politics and the media. Part of the programme was a lab tour through the institute, which showed recent work in the areas of additive manufacturing, transmission electron microscopy and corrosion science with the scanning kelvin probe.

Priyanshu Bajaj, doctoral student, explains to State Secretary and member of the senate of the Max Planck Society Cornelia Quennet-Thielen his work on alloy design for additive manufacturing.

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

Imprint

Chief Editor: Yasmin Ahmed Salem, M.A.

Publisher: Max-Planck-Institut für Eisenforschung GmbH
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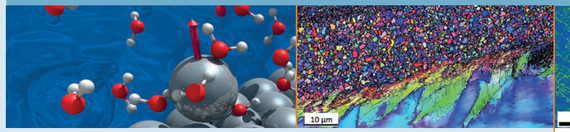

Computational high-throughput Design of ductile Magnesium Alloys

Magnesium alloys have an outstanding position in the search for the next-generation light-weight materials. However, their application is still hampered by their inherent brittleness. Based on an interdepartmental, computational high-throughput strategy, scientists at the MPIE have found a solution, which makes the material both ductile and affordable.

Thinking about light-weight structural materials, e.g., for automotive applications, Al alloys are often considered first. Although magnesium is 1.7 times lighter than Al and has a comparable price, its brittleness makes applications very rare. A few alloying strategies to improve the situation have been suggested in recent years, but are mostly expensive due to the involvement of rather expensive and environment-unfriendly rare-earth elements such as yttrium. Therefore, we have optimized the ductility of Mg alloys, by screening several thousand alloying concepts and identifying the most promising and economical solution [1].

The materials science approach required in the first place a reliable yet easily accessible descriptor for optimum mechanical properties. The experimental investigation performed at the department "Microstructural Physics and Alloy Design" identified the intrinsic stacking-fault energy as such a candidate. In contrast to the dislocations processes required for the complete description of the underlying plasticity [2], this energy can be directly calculated by *ab initio* calculation employed in the department "Computational Materials Design". A direct screening of 18 transition metals as possible individual solutes did not identify better candidates than the previously identified rare-earth element yttrium [3]. Instead, it allowed us to identify, which physical properties distinguish the mechanical impact of yttrium from other solutes. Based on these insights, the yttrium similarity index (YSI, approaching 1 for yttrium-similar elements) was identified as a new figure of merit, which subsequently allowed to screen 2850 solute pairs within Mg with reasonable numerical effort (Fig. 1). Nevertheless, the evaluation of such wide-range studies requires a reliable data management system. Our recently developed software framework pyiron does not only provide such a tool for automated data generation, storage, analysis and visualization, but at the same time an integrated developing environment for new materials concepts.

As a result of this design strategy a Mg-Al-Ca system, namely, Mg-1Al-0.1Ca (wt.%) was found to show promising mechanical performance (YSI > 0.95), while still being inexpensive and non-toxic. Only afterwards, the tensile stress-strain

EDITORIAL

Dear Colleagues and Friends of the MPIE,

Big data and machine learning in materials science are still quite unexplored topics, yet, with huge potential in changing our current way of analysing and developing alloys and understanding materials-related phenomena. In this newsletter edition we present some projects on big data and machine learning methods which are currently pursued by groups in the institute.

Please also note our upcoming workshops on atom probe tomography, transmission electron microscopy and ab initio calculations. You can find a complete overview of these events on our website.

Enjoy reading !

Prof. Dr. Dierk Raabe, Chief Executive, MPIE

Awards and Achievements

Dr. Andrew Breen, postdoctoral researcher from England, was awarded a research fellowship of the Alexander von Humboldt Foundation and is now working in the group “Materials Science of Mechanical Contacts”.

Dr. Reza Darvishi Kamachali, postdoctoral researcher in the group “Theory and Simulation”, received the Heisenberg Fellowship by the German Research Foundation to pursue his research on microstructure design and the effect of chemo-mechanical coupling in heterogeneous materials.

Dr. Baptiste Gault, leader of the “Atom Probe Tomography” group was awarded with the Consolidator Grant of the European Research Council for his project about hydrogen embrittlement.

Ankit Gupta, doctoral student in the group “Computational Phase Studies”, won the Travel Award 2018 of the journal “Materials” and presented his work about first-principles investigation of thermodynamics and precipitation kinetics in Al-Sc alloys at the TMS in March in Phoenix, USA.

Dr. Michael Herbig (photo) and Prof. Dierk Raabe were awarded with the Henry Marion Howe Medal and the AIME Champion H. Mathewson Award for their research on autonomous repair of creep damage.

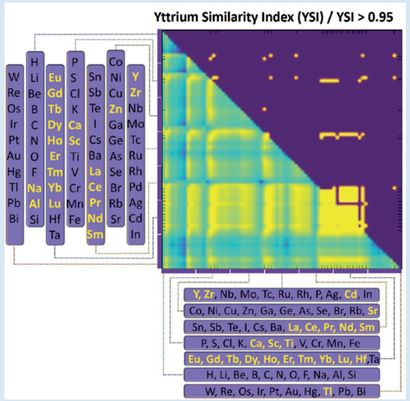

Fig. 1: Computed values of the yttrium-similarity index, YSI (Eq. 1) for the 2850 solute pairs computed in this study and visualized in the form of a symmetric matrix with yellow indicating a high similarity and blue a low one.

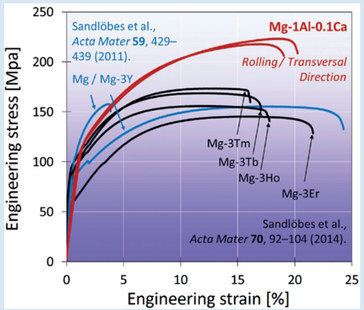

Fig. 2: Engineering stress-strain curves of the new Mg-Al-Ca alloy in comparison with not engineered (other than simple homogenization treatment) solid solution Mg-Y, Mg-RE, pure Mg and Mg-Al-0.3Ca.

behaviour of this alloy was compared with pure Mg and binary solid solution Mg-RE and Mg-Y alloys (Fig. 2). The result was outstanding: a tensile elongation of about 20% (4x more ductile than pure Mg), a well-balanced constant work hardening, and an ultimate tensile strength of about 220 MPa (40% higher than pure Mg) [1]. Such a performance makes Mg alloys highly attractive for future materials science as well as light-weight applications.

References:
[1] S. Sandlöbes, M. Friák, S. Korte-Kerzel, Z. Pei, J. Neugebauer, D. Raabe: *A rare-earth free magnesium alloy with improved intrinsic ductility*. Sci Rep 7, 10458 (2017)
[2] Z. Wu, W.A. Curtin: *The origins of high hardening and low ductility in magnesium*. Nature 526, 62 (2014)

Authors: T. Hickel, J. Neugebauer

Artificial Intelligence in Materials Science

The amount of data produced by detectors has increased explosively. Automated tools to process and analyze the data are necessary. Artificial intelligence (AI), in particular machine learning (ML), has been exploited by an increasing number of disciplines to automate complex problem-solving tasks. Progress in ML has led to decision rules that can in some cases be automatically derived by specific algorithms. One of the successful applications of ML in materials science lies in developing fully automated algorithms for analyzing high-throughput experiments.

Field ion microscopy (FIM) is a high electric field technique, which enables the imaging of surfaces with atomic resolution. When exposing the tip not only to the minimum field strength required for ionizing the imaging gas but also for evaporating the tip atoms themselves continually, the method is rendered depth sensitive (3D-FIM). This means that the specimen can be investigated tomographically along the tip’s longitudinal axis. 3D-FIM is capable of producing large and accurate tomographic datasets containing information on sequential atomic positions, but these large datasets lead to a new tremendous challenge of how to manage the data.

Presently, there is a lack of efficient data handling algorithms to extract pertinent information from these datasets in an (a) automated; (b) fast; (c) user-independent; and (d) error quantified manner. For instance, characterization of a volume of 0.001 µm³ (a typical 3D-FIM sample size) produces in the range of 2 × 10⁵ images. Hence, there is a great need for efficient algorithms and data mining routines. To this end, we recently proposed a new method to extract atomic positions from 3D-FIM datasets, using various image processing and machine learning algorithms [1, 2].

Applying machine learning to the 3D-FIM images (> 21000 dimensions) and projecting the data to a low dimensional subspace helped us to understand the latent structure in the data. The exemplary result in Fig. 1 reveals a cyclic behaviour in the dataset, which is a consequence of the field evaporation behaviour. Field evaporation typically occurs layer-by-layer and proceeds from atoms sitting at the ledge of a terrace towards the centre. When a terrace field evaporates the atoms sitting on the ledge disappear, decreasing the number of atoms on the terrace as the evaporation proceeds. By evaporating atoms from the surface of the sample during FIM, the first terrace area decreases until it evaporates completely. The number of cycles is a measure of the number of atomic terraces evaporated during the 3D-FIM.

With the use of such advanced algorithms for data extraction, we hope not only to improve the accuracy of the data extraction from 3D-FIM but also to identify and characterize various material defects. Currently, the physics of image formation in FIM are still not completely understood, but it is our firm belief that ML can be a powerful tool in this direction.

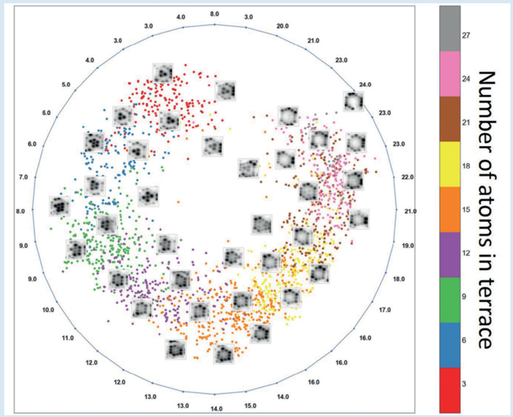

Fig. 1 : Machine learning (Isomap) on the 3D-FIM dataset. Each point represents one picture in the reduced dimensional manifold, and its colour indicates the number of atoms in the first terrace of the corresponding picture. The numbers on the outer circle represent the averages over the number of atoms in the first terrace of pictures.

References:
[1] S. Katnagallu, A. Nematollahi, M. Dagan, M. Moody, B. Grabowski, B. Gault, D. Raabe, J. Neugebauer: *High fidelity reconstruction of experimental field ion microscopy data by atomic relaxation simulations*. Microsc Microanal, 23, 642 (2017)

[2] S. Katnagallu, B. Gault, B. Grabowski, J. Neugebauer, D. Raabe, A. Nematollahi: *Advanced data mining in field ion microscopy*. arXiv:1712.10245.

Authors: Gh. A. Nematollahi, B. Grabowski

Machine-learning-based extraction of crystallographic information from atom probe data

Machine learning (ML) applied to atom probe tomography (APT) will enable new high-impact materials science at the nanometre scale, including tracking orientation gradients with changes in chemistry, linking grain boundary atomic-scale structure and segregation of different atomic species. Such information is particularly valuable for understanding the mechanisms governing changes in nanostructure and the influence on displayed mechanical and functional properties of engineering materials.

APT maps the 3D position and chemical identity of up to a billion atoms in a material. The pattern formed on the single-particle detector often reveals traces of the crystallographic structure and orientation of the material. Such information enables us to elucidate structure-property relationships at the atomic scale. However, it remains largely under-utilised due to the lack of efficient and accurate extraction techniques. We have started to investigate the potential of ML to identify crystallographic patterns observed on atom probe detector maps.

Preliminary results have been very promising. Our neural network learns a set of theoretical geometric relationships, for instance the angles between different crystallographic directions, and how they relate to the maps. After image processing, the locations of the features of interest are fed into the neural network. A flow-chart outlining this process is shown in Fig. 1. For detector hitmaps obtained from pure-Al specimens, our approach correctly characterised the orientation of single crystals with 98% confidence.

A database of experimental images for training was built, but for more complex materials systems and low-symmetry crystallographic structures there is not enough labelled data yet. By full-scale, theory-driven forward calculations of such maps we can build large databases from which the machine learning algorithms will learn and refine the data analysis, as well as systematically explore the ultimate limits of APT crystallography in multi-phase multi-component samples.

Authors: Y. Wei, A. Breen, M. Ashton, M. Herbig, B. Gault, C. Freysoldt

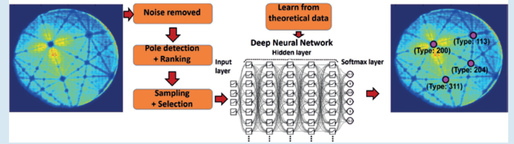

Fig. 1: Pole identification via machine-learning for atom probe crystallography (PIM-X).

Awards and Achievements

Dr. Fritz Körmann, leader of the group “Complex Concentrated Alloys”, is now supported with a funding of 800.000 euros by the Dutch Research Organisation (NWO) for systematically modeling high-entropy alloys.

Dr. Linlin Li, postdoctoral researcher from China, was awarded a research fellowship of the Alexander von Humboldt Foundation and is now working in the group “High-Entropy Alloys”.

Dr. Joohyun Lim, postdoctoral researcher from South Korea, received a research fellowship of the Alexander von Humboldt Foundation and is now working in the group “Nanoanalytics and Interfaces”.

Dr. Binhan Sun, postdoctoral researcher from Canada, was awarded a research fellowship of the Alexander von Humboldt Foundation and is now working in the group “Alloy Design and Thermomechanical Processing”.

Dr. Zhangwei Wang, postdoctoral researcher from the USA, was awarded a research fellowship of the Alexander von Humboldt Foundation and is now working in the group “High-Entropy Alloys”.