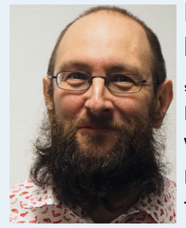
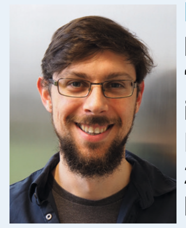
Scientists at the MPIE



Dr. Baptiste Gault, head of the group „Atom Probe Tomography", was honoured with the highest German research award, the Gottfried Wilhelm Leibniz Prize. The prize is endowed with 2.5 million euros and is awarded by the German Research Foundation.
Gault's research is focused on the analysis of materials down to the atomic scale to better understand how these influence the material's properties. Key applications are for instance in structural and functional materials like steel, aluminium or nickel alloys found in cars or planes, but also relevant for magnets in electrical vehicles and windmills. Other projects are relevant to materials for energy conversion, for instance, solar cells, thermoelectrics and catalysts for water splitting. In a recent project, funded by the European Research Council, Gault and his team are studying the distribution of hydrogen atoms in complex alloys to find ways to prevent hydrogen embrittlement. Another topic combines field ion microscopy, atom probe tomography and big data techniques to reach an even higher atomic precision enabling Gault to tailor new alloys. However, Gault does not only analyse metallic alloys, he adjusts the atom probe to analyse biological materials as well. Recently, he studied protein fibrils that are relevant to Alzheimer, to be able to understand how these fibrils cluster with metals found in the human body and effect the brain.
Over the course of his career, Baptiste Gault worked in France, Australia, the UK and Canada, before joining the MPIE in 2016. He also holds a part-time position as *Reader in Materials* at the Imperial College London.

Selected Publications:

1. S. Katnagallu et al.: *Imaging individual solute atoms at crystalline imperfections in metals.* New J Phys 21 (2019).
2. T. Li et al.: *Atomic-scale insights into surface species of electrocatalysts in three dimensions.* Nat Catal 1 (2018).



Dr. Liam Huber is head of the group "Thermodynamics and Kinetics of Defects" since mid-2019. Before that, he was postdoctoral researcher in the department Computational Materials Design, where his current group is also located. Huber did his doctoral thesis about quantum simulations of the interaction between solutes and spatial defects in metals, at the University of British Columbia in Vancouver, Canada. He was supported by the Natural Sciences and Engineering Research Council of Canada, which granted him a Alexander Graham Bell Canada Graduate scholarship.
Huber focusses on the interplay and co-evolution of chemical and structural defects in metals to better understand and predict their role on the material's properties. Using both *ab initio* and classical atomistic methods, he is trying to bridge the gap between calculated point defects at thermodynamic equilibrium and materials in real environments containing a variety of defects, often influencing each other. The motivation here is to understand the relation between the behaviour of structural defects like dislocations and grain boundaries and chemical defects, which are introduced intentionally through alloying or unintentionally through exposure to the surrounding environment. Therefore, Huber combines physical models, multi-scale methodology and machine learning techniques.

Selected Publications:

1. L. Huber, R. Hadian, B. Grabowski, J. Neugebauer: *A machine learning approach to model solute grain boundary interaction.* Npj Comput Mater 4 (2018).
2. L. Huber, B. Grabowski, M. Militzer, J. Neugebauer, J. Rottler: *Ab initio modelling of solute segregation energies to a general grain boundary.* Acta Mater 132 (2017).

Selected Publications

Computational Materials Design (CM):

H. I. Sözen, S. Ener, F. Maccari, K. P. Skokov, O. Gutfleisch, F. Körmann, J. Neugebauer, T. Hickel: *Ab initio phase stabilities of Ce-based hard magnetic materials and comparison with experimental phase diagrams.* Phys Rev Materials 3 (2019) 084407.

A. Glensk, B. Grabowski, T. Hickel, J. Neugebauer, J. Neuhaus, K. Hradil, W. Petry, M. Leitner: *Phonon lifetimes throughout the Brillouin zone at elevated temperatures from experiment and ab initio.* Phys Rev Lett 123 (2019) 235501.

Interface Chemistry and Surface Engineering (GO):

A. Merz, M. Uebel, M. Rohwerder: *The protection zone: a long-range corrosion protection mechanism around conducting polymer particles in composite coatings: Part I.* Polyaniline and Polypyrrole. J Electrochem Soc 166 (2019) C304.

S. K. Song, A. Samad, S. Wippermann, H. W. Yeom: *Dynamical metal to charge-density-wave junctions in an atomic wire array.* Nano Letters 19 (2019) 5769.

Microstructure Physics and Alloy Design (MA):

D. Raabe, C. Tasan, E. A. Olivetti: *Strategies for improving the sustainability of structural metals.* Nature 575 (2019) 64.

E.P. George, D. Raabe, R.O. Ritchie: *High entropy alloys.* Nat Rev Mater 4 (2019) 515.

Structure and Nano-/Micromechanics of Materials (SN):

M. Palm, F. Stein, G. Dehm: *Iron aluminides.* Annu Rev Mater Res (2019) 49.

A.K. Saxena, A. Kumar, M. Herbig, S. Brinckmann, G. Dehm, C. Kirchlechner: *Micro fracture investigations of white etching layers.* Mater Design 180 (2019) 107892.

Selected Talks

Computational Materials Design (CM):

J. Neugebauer: *Ab initio descriptors to design materials with superior mechanical properties.* Materials Day 2019 "Materials Modeling: Across Scales, Across Materials", ETH Zürich, Switzerland, 20 Nov 2019.

J. Neugebauer: *Machine learning in materials screening and discovery.* GRC Physical Metallurgy "Coupling Computation, Data Science and Experiments in Physical Metallurgy", Southern New Hampshire University, Manchester, USA, 7-12 July 2019.

Interface Chemistry and Surface Engineering (GO):

S. Wippermann: *Electrically triggered reactions at interfaces: a first principles perspective.* Workshop AGEF and CRC/TRR247 "Interfacial Solvent", University Duisburg-Essen, Germany, 5 Dec 2019.

M. Rohwerder: *Intelligent coatings for corrosion protection: on the need for new coating concepts.* International Conference on Corrosion Protection and Application (ICCPA 2019), Chongqing, China, 10-12 Oct 2019.

Microstructure Physics and Alloy Design (MA):

D. Raabe: *Chemistry at lattice defects probed at atomic scale.* 20th International Union of Materials Research Societies International Conference in Asia IUMRS, Perth, Australia, 22-26 Sep 2019.

D. Raabe: *The chemical nature of defects probed at atomic scale.* The 53rd Annual Meeting of the Israel Society for Microscopy, Tel Aviv, Israel, 29 May 2019.

Structure and Nano-/Micromechanics of Materials (SN):

G. Dehm: *Micro- and nanomechanical testing of materials - from materials physics to materials design.* Convegno Nazionale INSTM XII, Ischia Porto, Italy, 21-24 July 2019.

G. Dehm, N. Peter, T. Meiners, C. Liebscher: *Resolving grain boundary phase transformations by advanced STEM for fcc metals and multinary alloys.* 6th International Symposium on Metastable, Amorphous and Nanostructured Materials (ISMANAM-2019), Anna Salai, India, 8-12 July, 2019.

Selected Upcoming Events

4 - 6 Feb 2020: Nanobrücken 2020 - A Nanomechanical Testing Conference
The conference will focus on new trends in nanomechanical and nanotribological research. Participants can take part in practical workshops and exchange research ideas in discussions and poster competitions. The conference takes place at the MPIE.
https://www.bruker.com/events/users-meetings/surface-analysis/nanobruecken-2020/overview.html

06 Feb 2020: KopfSalat – Mobility of the Future: The Change from Manual to Autonomous Driving
Lecture by Prof. Torsten Bertram, Technische Universität Dortmund (in German). The automation of driving functions, the networking of road users and the individualization of traffic systems will shape the mobility of the future. There will be a shift from manual to fully automatic driving to driverless vehicles. Our future promises not only more safety on the roads, but also more comfort. The lecture presents the current technology of automated driving and discusses current and future issues. The talk will be held at the MPIE.
https://www.mpie.de/events/19305/3225857

16 - 20 Feb 2020: 4th MSIT Winter School on Materials Chemistry
The MSIT Winter School aims to provide subjects closely related to the study of phase equilibria in materials science, such as crystallography and computational thermodynamics. Each module includes lectures, demonstrations and problem classes given mainly by members of the MSIT who are experts in their respective fields. The conference takes place at the Ringberg Castle, Bavaria.
http://www.msiport.com/msit-school/next-msit-school/

20 - 22 April 2020: BiGmax Workshop 2020 on Big-Data-Driven Materials Science
This workshop is an interdisciplinary discussion forum that connects materials scientists with experts from physics, machine learning, computer and data science. The aim is to discuss state-of-the-art examples of machine learning methods to characterize the structure and plasticity of materials, quantify microstructured material properties, and perform data diagnostics in imaging. The workshop takes place at the MPIE.
https://www.mpie.de/4171441/bigmax-workshop-2020-on-big-data-driven-materials-science.html

How will self-driving cars change our future mobility? And which steps need to be done for a safe traffic? Join our next KopfSalat-talk on 6th February.

Imprint

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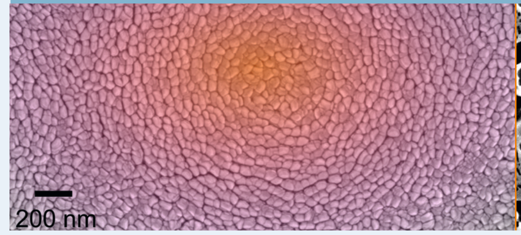
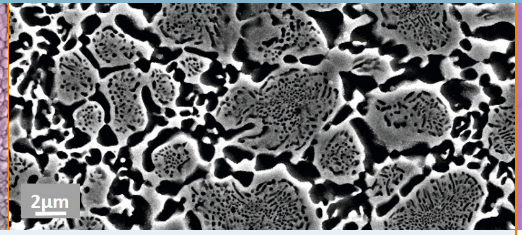
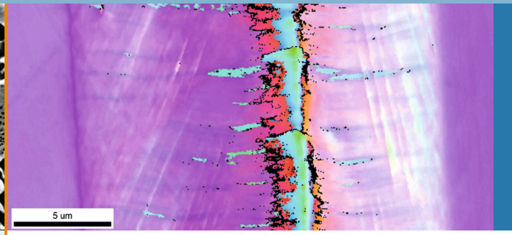
NEWSLETTER 2/2019

Max-Planck-Institut für Eisenforschung GmbH







New High Strength Steels with Reduced Hydrogen Embrittlement Sensitivity

Experience indicates a high sensitivity of high strength materials against hydrogen embrittlement (HE). Steels with a yield strength exceeding 1000 MPa are usually not employed for applications where a critical hydrogen (H) uptake during processing or service might take place. But especially in transportation, steels with higher strength would allow increased weight reductions. Our approach is to understand the mechanisms of HE, which not only depend on H concentration and stress level, but also on the microstructure of the steel itself. Exposing weak microstructural features enables to design modified thermomechanical processing routes to avoid them. With taylored modifications of the microstructure, we were able to increase the yield strength plus reduce the HE sensitivity of the steel.

We investigated a medium Mn steel with the chemical composition 0.2C-10.2Mn-2.8Al-1Si (in wt.%). Medium Mn steels combine high strength and ductility and are candidates for future automotive applications. But not much is known about HE sensitivity and embrittlement mechanisms in these multiphase steels. A method to quantify the sensitivity against HE is the slow strain rate tensile test. Curve 1 in Fig. 1 shows the stress-strain curve for this steel after conven-

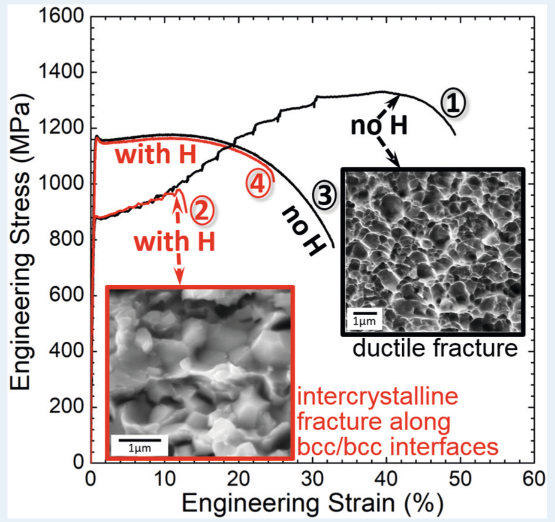
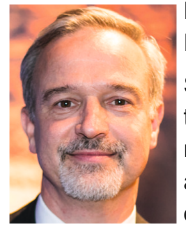


Fig. 1: *Stress-strain curves for the steel from slow strain rate tensile tests. Conventionally processed sample without H (curve 1): ductile fracture and high total elongation. Charging with H (curve 2): intercrystalline fracture and high loss of total elongation. Modified processing (curve 3 and 4) increases yield strength and lower loss of total elongation by H.*

EDITORIAL



Dear Colleagues and Friends of the MPIE,

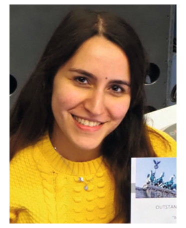
Shaping our future in terms of sustainable technologies, new materials and industrial processes is one of the most important topics of our generation and we are in need of scientific and engineering answers. How can we avoid the use of carbon as energy and reductant carrier in the entire field of materials science and engineering? How can we make better and rare-earth free permanent magnets for electrical vehicles? How can we render alloys sustainable and improve recycling rates? Which are the novel materials that can withstand embrittlement caused by hydrogen? And what is the potential of new thermoelectric and solar cell absorber materials for green power generation? We have devoted our efforts to provide answers to these pressing questions, showing you here some of our current research in the field of sustainability. Please contact us if you like to know more.

Enjoy reading,

Prof. Dr. Dierk Raabe, managing director

Awards and Achievements

Priyanshu Bajaj, PhD student in the group "Alloys for Additive Manufacturing" won the Second Poster Prize at the Alloys for Additive Manufacturing Symposium 2019 in Gothenburg, Sweden.



Rasa Changizi, PhD student in the group "Nanoanalytics and Interfaces", won the first prize in the image competition at the Microscopy Conference 2019 in Berlin, Germany.

Dr. Aniruddha Dutta, postdoctoral researcher in the group "Mechanism-based Alloy Design", won the European Science Slam Championship 2019/20 in Vienna, Austria.

Leonie Gomell, PhD student in the group "Atom Probe Tomography", received a PhD scholarship of the Studienstiftung des Deutschen Volkes.

Dr. Avinash Hariharan, postdoctoral researcher in the group "Alloys for Additive Manufacturing" won the Best Poster Prize at the Alloys for Additive Manufacturing Symposium 2019 in Gothenburg, Sweden.

Nicolas Peter and **Dr. Alisson Kwiatkowski da Silva**, researchers at the MPIE, joined the 69th Nobel Laureate Meeting in Lindau, Germany.

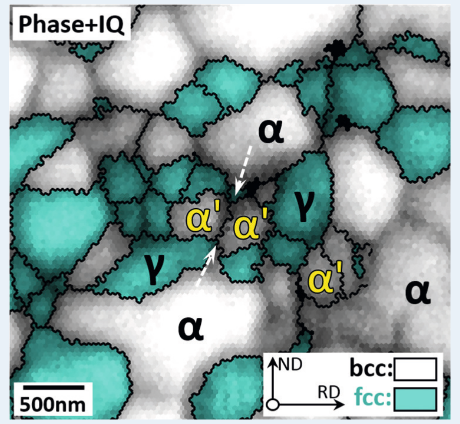


Fig. 2: *Initial microstructure: austenite (γ) with fcc structure and ferrite (α) with bcc structure. During plastic deformation austenite transforms to martensite (α').*

tional processing and no H charging. The yield strength is 890 MPa and the total elongation 51 %. When the steel is charged with H (curve 2), the total elongation is significantly reduced to 13 %. The difference between the total elongations of uncharged and H charged samples allows to quantify the HE sensitivity. Here, this loss in total elongation is high (38 %) and indicates a high HE sensitivity. The appearance of the fracture surfaces after tensile testing (Fig. 1) provides information about the failure mechanisms: Dimples on the fracture surface of the sample without H (curve 1) reveal a ductile fracture. This changes for the sample with H (curve 2), which shows a more brittle failure along interfaces. A detailed characterization reveals the mechanisms leading to HE: The microstructure of the medium Mn steels shows two phases: face centered cubic (fcc) austenite (γ) with a volume fraction of 60 % and body centered cubic (bcc) ferrite (α). In the bcc lattice H diffusion is much faster, but H solubility is much lower than in austenite. When charging with H, finally austenite contains much more H than ferrite. During deformation metastable austenite transforms partially into martensite (α`) (Fig. 2). This martensitic transformation is very fast. Therefore, martensite inherits all the H from austenite. This leads to

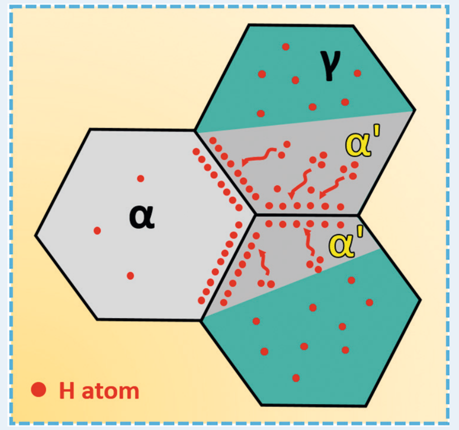


Fig. 3: *Schematically: H in oversaturated martensite (α') segregates to grain boundaries. Embrittlement of these boundaries leads to observed intercrystalline failure.*

drastic H oversaturation of martensite as martensite has a bcc lattice and hence a very low H solubility (Fig. 3). Due to the high diffusivity of H in martensite, the H can escape the oversaturated lattice by moving to interfaces like α'/ α' grain boundaries. This leads to the observed embrittlement of these interfaces.

To avoid these mechanisms, we lowered the heat treating temperature. This provides a finer grain size (higher yield strength of modified processed steel curve 3) and more Mn and C partitioning to austenite stabilizes the austenite. During deformation, less martensite is formed and the sensitivity against HE is decreased: The H charged sample (curve 4) in comparison to the uncharged sample (curve 3) shows a low loss in total elongation of 8 % and a ductile fracture mode. This indicates a much lower HE sensitivity, even with the higher yield strength of the modified processed steel of 1160 MPa.

This description is highly simplified but published in more detail elsewhere [1].

References:

1. B. Sun, W. Krieger, M. Rohwerder, D. Ponge, D. Raabe: Acta Mat 183 (2020) 313.

Authors: D. Ponge, B. Sun (MA)

Permanent Magnets – Research for Sustainability

Permanent magnets form a critical contribution to many sustainable energy technologies, such as electrical motors used in automotive applications. The hard-magnetic performance of the most promising materials is due to a substantial amount of a few rare-earth (RE) elements. However, their generation substantially harms the environment and a supply monopoly causes economical risks. To achieve technological solutions that are really sustainable, one needs to replace these permanent magnets by materials that are more abundant and accessible. Such a materials design is a key research topic at the Department of Computational Materials Design.

The RE element neodymium (Nd) is increasingly often used in high performance magnets that are employed for many applications such as electrical vehicles and wind turbines. For example, 700 kg sintered Nd magnet is needed for a wind turbine with a 1 MW power capacity. The element dysprosium (Dy) improves Nd magnets by enhancing their coercive force and resistance to demagnetization. Both elements suffer, however, from mining and processing conditions that cause a large environmental footprint. Even more severe is their supply risk (Fig. 1), since over 90 % of the RE elements worldwide are currently produced by a single country (China).

Due to the criticality for future technology, one needs to find alternative hard-magnetic materials that are based on more abundant elements. According to Fig. 1, Cerium (Ce) is a candidate with a much lower supply risk, but its potential for clean energy applications is still largely unexplored. Ce-based hard magnets are, therefore, in the focus of our research.

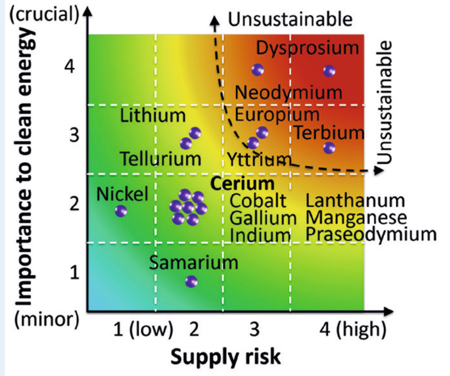


Fig. 1: *Supply risk of RE elements plotted versus their importance for clean energy applications. Adapted from [1].*

Although in particular the $CeFe_{11}Ti$ phase has – due to its excellent magnetic properties – a great potential to replace Nd-based magnets, there are

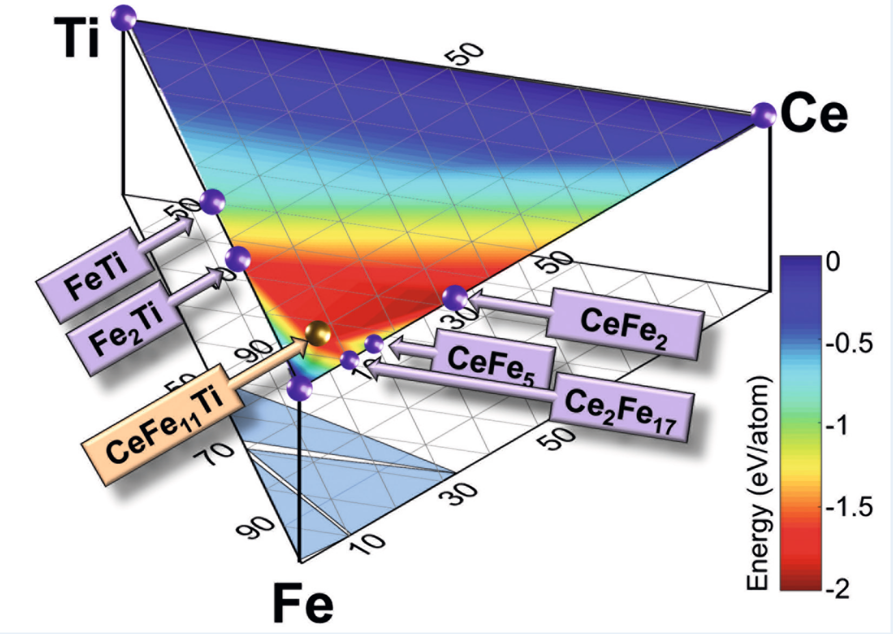


Fig. 2: *Heat map of the calculated free energies of formation for the Ce-Fe-Ti phases at T=1500 K.*

also severe challenges. Most critical is the formation of magnetically detrimental Laves phases, such as $CeFe_2$. They tend to dominate the microstructure, retarding the crystallization of the desired hard magnetic phase.

We are using sophisticated *ab initio* based methods to calculate finite temperature phase stabilities. Employing state-of-the-art approaches for vibrational, electronic, and magnetic entropy contributions, the Helmholtz free energy is calculated for the desired hard-magnetic ternary phase and all relevant binary phases, as shown in Fig. 2. Consequently, the thermodynamic stability of $CeFe_{11}Ti$ as compared to a set of competing phases can be accurately evaluated [2]. The *ab initio* calculations predict a critical temperature below which a decomposition to Laves phases occurs, serving as a guideline for a thermodynamic processing.

In order to tailor these phase stabilities, we have considered the effect of quaternary additions. To explore Ce-Fe-Ti-X alloys for all 3d and 4d transition elements X, we developed an efficient screening method and were able to demonstrate that alloying elements such as Zn can decrease the critical temperature substantially, making the material system more attractive for applications. The study therewith demonstrates that the substitution of established hard magnets by more sustainable material systems, requires a careful analysis not only of the magnetic performance, but also of the thermodynamic stability.

References:

1. D. Bauer et al.: Technical report, U.S. Department of Energy (2011).
2. H. I. Sözen et al.: Phys. Rev. Mater. 3 (2019) 084407.

Authors: H. Sözen, T. Hickel (CM)

Non-toxic, Affordable Bulk Thermoelectrics for Clean Power Generation from Waste Heat

A third of the power consumed across the industry sector is lost as heat. Thermoelectric materials convert heat into electricity and can harvest this wasted heat to regenerate clean energy. Major drawbacks of current thermoelectric materials are their high price and content of toxic elements. Designing new material systems, which overcome those obstacles, is becoming an important research topic at the MPIE.

Thermoelectrics can generate electricity from a heat source through the Seebeck effect: a temperature difference leads to a difference in voltage. The efficiency of the conversion can be increased by introducing microstructural defects that efficiently scatter phonons, i.e. the carriers of lattice vibrations and hence heat, but do not affect much the movement of electrons thus maintaining good electrical conductivity. Together with national and international partners, members from the group Nanoanalytics and Interfaces (NG) and the MA department have discovered that the specific structure and composition of planar defects in an as-quenched $AgSbTe_2$ mosaic crystal make them effective to scatter sites for phonons leading to a considerable reduction of the lattice thermal conductivity. A combination of electron channeling contrast imaging (ECCI) in a scanning electron microscope [1], atom probe tomography and high-resolution imaging transmission electron microscopy was used to understand these mechanisms.

This preliminary joint work led us to establish a new joint activity with 6 early-career scientists working closely together across departments, under the leadership of Dr. Siyuan Zhang and Dr. Ting Luo, to develop new thermoelectric materials. We have identified a set of intermetallic compounds, Heusler and Half-Heusler alloys, which we are currently synthesizing using our combinatorial high-throughput metallurgical laboratory. We use our knowledge of metallurgical processing to control the introduction of defects in the microstructure and use advanced microscopy and microanalysis to

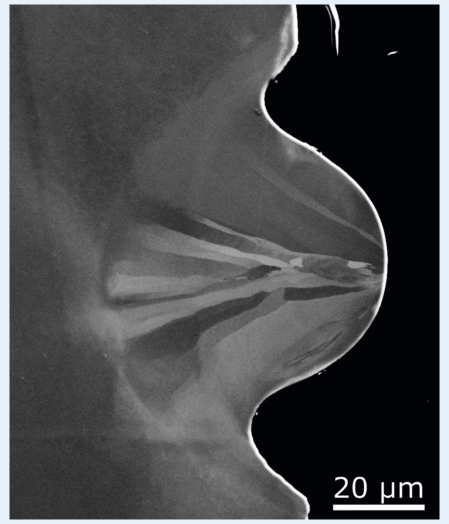


Fig. 1: *Arc melted Fe_2VAl alloy after laser surface remelting (power 200 W, speed 1400 mm/s, focus size 90 µm). Credit Leonie Gomell*

investigate the materials from the millimeter to the atomic scale. A first example is shown in the figure below, where we have used the in-house selective laser melting, typically used for 3D printing, to modify the local grain structure in a Fe_2AlV Heusler alloy. We are currently using our microscopy and microanalysis toolbox to determine which of the introduced defects most effectively reduce the thermal conductivity, helping us guide the design of future materials and devices.

References:

1. L. Abdellaoui, S. Zhang, S. Zaefferer, R. Bueno Villoro, A. Baranovski, O. Cojocaru-Mirédin, Y. Yu, Y. Amouyal, D. Raabe, G.J. Snyder: Acta Mater 178 (2019).

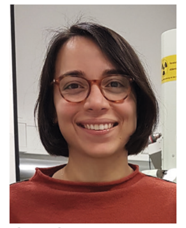
Authors: B. Gault (MA) & C. Scheu (NG)

Awards and Achievements

Kevin Schweinar, PhD student in the group "Atom Probe Tomography", has won the M&M Scholar Award 2019.

The Max Planck Society's (MPG) Senate reelected **Prof. Martin Stratmann**, director of the department "Interface Chemistry and Surface Engineering", as President of the MPG.

Po-Yen Tung, PhD student in the group "Material Science of Mechanical Contacts", was awarded with the Taiwanese Government Scholarship to Study Abroad.



Ceren Yilmaz, PhD student in the group "Microscopy and Diffraction", has won the Best Poster Award at the 7th International Conference on Recrystallization and Grain Growth in Ghent, Belgium.

Dr. Huan Zhao (see photo), **Dr. Baptiste Gault** and **Prof. Dierk Raabe** from the department "Microstructure Physics and Alloy Design" have been honoured with the TMS Light Metals Subject Award – Aluminum Alloys.