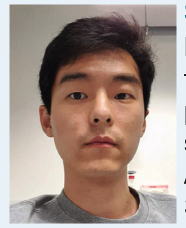
Scientists at the MPIE

Dr. Poulami Chakraborty works at the MPIE as a postdoctoral researcher in the group "Computational Phase Studies" since 2018. Her research focuses on the thermodynamics of hydrogen in metals and its role in embrittlement. Moreover, she studies planar defects and precipitation kinetics in aluminium alloys. Before joining the MPIE, Chakraborty did her PhD in physics at the S.N. Bose National Centre for Basic Sciences in Kolkata, India.

She is currently working on several projects together with Dr. Tilmann Hickel and Dr. Baptiste Gault. Her projects are funded through the ERC-SHINE grant of Dr. Gault. The grant aims to gain insights into the role of hydrogen in hydrogen storage materials and hydrogen-induced embrittlement. Chakraborty deals with the theoretical aspects of these interactions by studying solute-hydrogen interactions at the atomic level. One of her current projects is about the thermodynamics and kinetics of planar defects in aluminium. She also studies the interaction of hydrogen with the segregation of solutes at the grain boundaries and their binding in precipitates. Another project involves the investigation of planar defects in zirconium and its hydride phases.

Selected Publications:

1. P. Chakraborty, A. Chakrabarty, A. Dutta, T. Saha-Dasgupta: *Soft MAX phases with boron substitution: A computational prediction.* Phys Rev Mater 2 (2018) 103605.
2. P. Chakraborty, T. Das, D. Nafday, L. Boeri, T. Saha-Dasgupta: *Manipulating the mechanical properties of Ti_2C MXene: Effect of substitutional doping.* Phys Rev B 95 (2017) 184106.
3. P. Chakraborty, A. Moitra, T. Saha-Dasgupta: *Effect of hydrogen on degradation mechanism of zirconium: A molecular dynamics study.* J Nucl Mater 466 (2015) 172.



Se-Ho Kim joined the MPIE in 2018 after finishing his master program in materials science at the Korea Advanced Institute of Science and Technology in Daejeon, South Korea. He is currently doing his PhD in the "Atom Probe Tomography" group of Dr. Baptiste Gault.

In the framework of the ERC-Shine grant, Kim analyzes nanostructures including nanoparticles, nanosheets, and nanowires that are applicable in the hydrogen economy. He develops new methodologies to not only visualize the 3D morphology of these nanostructures but also measure their chemical distribution using atom probe tomography. This is specifically relevant, as trace impurities or dopants are often decisive for the functional properties of the materials. Kim also works together with the "Nanoanalytics and Interfaces" MPIE group. Together, they successfully quantified and located doped elements within as-synthesized nanostructures such as TiO_2 nanowires and MoS_2 nanosheets. They are able to show how the material's synthesis affects the integration of chemical impurities, which in turn affect the performance of the nanostructures.

Selected Publications:

1. J. Lim, S.-H. Kim, R. A. Armengol, O. Kasian, P.-P. Choi, L. T. Stephenson, B. Gault, C. Scheu: *Atomic-Scale Mapping of Impurities in Partially Reduced Hollow TiO_2 Nanowires.* Angew Chem 59 (2020) 5651.
2. S.-H. Kim, R Sahu, O.Kasian, L. T. Stephenson, C. Scheu, B. Gault: *Direct Imaging of Dopant and Impurity Distributions in 2D MoS_2.* Adv Mater 32 (2020) 1907235.
3. S.-H. Kim, K. Jang, P. W. Kang, J.-P. Ahn, J.-B. Seol, C.-M. Kwak, C. Hatzoglou, F. Vurpillot, P.-P. Choi: *Characterization of Pd and Pd@ Au core-shell nanoparticles using atom probe tomography and field evaporation simulation.* J Alloy Compd 831 (2020) 154721.

Selected Publications

Computational Materials Design (CM):

L.-F. Zhu, F. Körmann, A.V. Ruban, J. Neugebauer, B. Grabowski: *Performance of the standard exchange-correlation functionals in predicting melting properties fully from first principles. Application to Al and magnetic Ni.* Phys Rev B 101 (2020) 144108.

M. Ashton, A. Mishra, J. Neugebauer, C. Freysoldt: *Ab initio description of bond breaking in large electric fields.* Phys Rev Let 124 (2020) 176801.

Interface Chemistry and Surface Engineering (GO):

D. Gohl, H. Rueß, S. Schlicht, A. Vogel, M. Rohwerder, K.J.J. Mayrhofer, J. Bachmann, Y. Román-Leshkov, J.M. Schneider, M. Ledendecker: *Stable and active oxygen reduction catalysts with reduced noble metal loadings through potential triggered support passivation.* Chem Electro Chem, in print.

B.H. Sun, W. Krieger, M. Rohwerder, D. Ponge, D. Raabe: *Dependence of hydrogen embrittlement mechanisms on microstructure-driven hydrogen distribution in medium Mn steels.* Acta Mater 183 (2020) 313.

Microstructure Physics and Alloy Design (MA):

A.J. Breen, L.T. Stephenson, B. Sun, Y. Li, O. Kasian, D. Raabe, M. Herbig, B. Gault: *Solute hydrogen and deuterium observed at the near atomic scale in high-strength steel.* Acta Mater 188 (2020) 108.

H. Zhao, L. Huber, W. Lu, N.J. Peter, D. An, F. De Geuser, G. Dehm, D. Ponge, J. Neugebauer, B. Gault, D. Raabe: *Interplay of chemistry and faceting at grain boundaries in a model Al alloy.* Phys Rev Let 124 (2020) 106102.

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

T. Meiners, T. Frolov, R.E. Rudd, G. Dehm, C.H. Liebscher: *Observations of grain-boundary phase transformations in an elemental metal.* Nat 579 (2020) 375.

S. Lee, M.J. Duarte, M. Feuerbacher, R. Soler, C. Kirchlechner, C.H. Liebscher, S.H. Oh, G. Dehm: *Dislocation plasticity in FeCoCrMnNi high-entropy alloy: quantitative insights from in situ transmission electron microscopy deformation.* Mater Res Lett 8 (2020) 216.

Selected Talks

Computational Materials Design (CM):

J. Neugebauer: *Modeling crystal growth and materials design in high dimensional chemical and structural configuration spaces.* German Conference on Crystal Growth DKT, Munich, Gemany, 11 - 13 Mar 2020.

J. Neugebauer: *Materials design in high dimensional chemical and structural configuration space.* TMS 2020 Annual Meeting & Exhibition, San Diego, USA, 23 - 27 Feb 2020.

Interface Chemistry and Surface Engineering (GO):

M. Rohwerder: *Zinc alloy coatings and nano-composite coatings for corrosion protection: From the basics to new challenges.* IIM NMD ATM 2019: Advanced Materials for Industrial and Societal Applications, Kovalam, Thiruvananthapuram, India, 13 - 16 Nov 2019.

M. Rohwerder: *Delamination of organic coatings: what are the rate determining processes?* EUROCORR, Seville, Spain, 9 - 13 Sep 2019.

Microstructure Physics and Alloy Design (MA):

S. Balachandran, D. Mayweg, Y. Qin, E. Norouzi, L. Morsdorf et al.: *Material alterations in intense mechanical and chemical contacts.* TMS 2020 Annual Meeting & Exhibition, San Diego, USA, 23 - 27 Feb 2020.

M. Diehl, N. Kusampudi, C. Kusche, D. Raabe, S. Korte-Kerzel: *Combining experiments, simulations and data science to understand damage in dual phase steels.* International Conference on Plasticity, Damage & Fracture, Riviera Maya, Mexico, 3 - 6 Jan 2020.

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

F. Stein, B. Distl, Z. Kahrobaee, M. Palm, K. Hauschild et al.: *Improvement of a CALPHAD database for the development of next generation TiAl alloys by targeted key experiments on high-temperature phase equilibria – The EU project ADVANCE.* TMS 2020 Annual Meeting & Exhibition, San Diego, USA, 23 - 27 Feb 2020.

M. J. Duarte, J. Rao, X. Fang, S. Brinckmann, G. Dehm: *Hydrogen-microstructure interactions at small scale by in-situ nanoindentation during hydrogen charging.* Nanobrücken 2020: A nanomechanical Testing Conference, Düsseldorf, Germany, 4 - 6 Feb 2020.

The Laplace Project

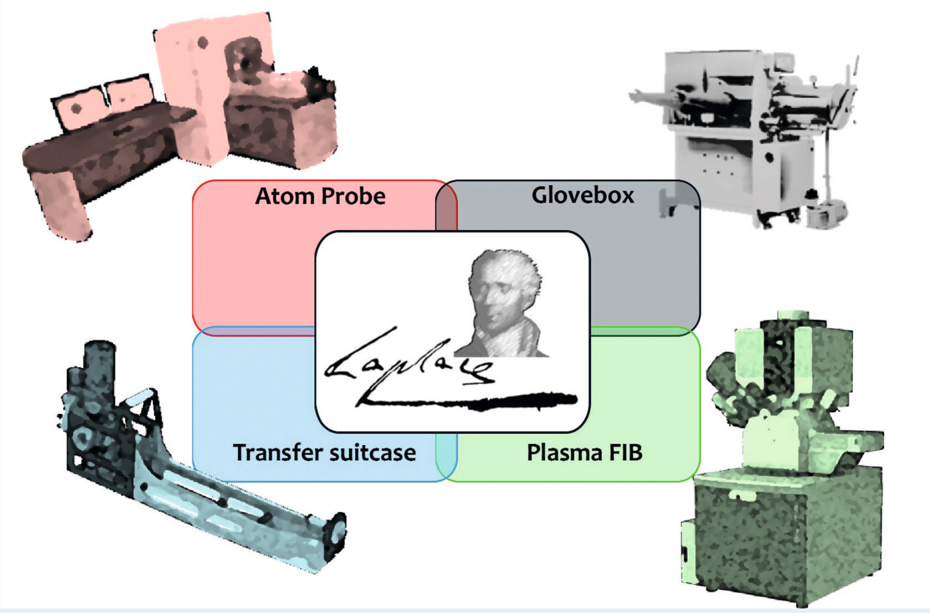


Fig. 1: *Combining different techniques and equipment to precisely determine the chemical composition and position of every atom in a sample.* © Baptiste Gault, Max-Planck-Institut für Eisenforschung GmbH

In 1814, Pierre-Simon Laplace postulated that if at any moment a "demon" could know the position and momentum of each and every one of the atoms in the universe, it would know everything about their past and their future. Inspired by this idea, we started putting together infrastructure enabling the correlation of multiple microscopy techniques on the same specimen. The idea being then that if we can gain insights into the structure of a specimen from electron microscopy, and combining this information with atom probe enables us to get close to knowing rather precisely what all the atoms within the material are and where they are located.

We hence pursued this concept and developed the infrastructure for the Laplace project: an atom probe, a scanning-electron microscope equipped with a focused-ion beam (SEM-FIB) and a glove-box, all interconnected via ultra-high-vacuum transfer suitcases. The idea was to enable successive imaging and atom probing while minimising the contamination associated with taking the specimen out of the vacuum and transporting it into another microscope in ambient atmosphere conditions. An additional feature was to perform the imaging and possibly the preparation of the specimens, as well as these transfers at cryogenic temperature.

This platform is versatile and additional devices are still being developed as we speak. The Max Planck Society supported the project with the purchase of a new atom probe and the associated development cost, as well as some of the scientists that are working to enable these breakthrough methodologies. The Federal Ministry of Education and Research supported the purchase of the SEM-FIB. For this latter instrument, we selected a Xe-Plasma FIB, instead of the more typical gallium-based instrument to mill larger volumes from a broader variety of materials. New research enabled by the infrastructure was the search for hydrogen in metals, which is the core topic of my ERC-Consolidator grant SHINE.

Imprint

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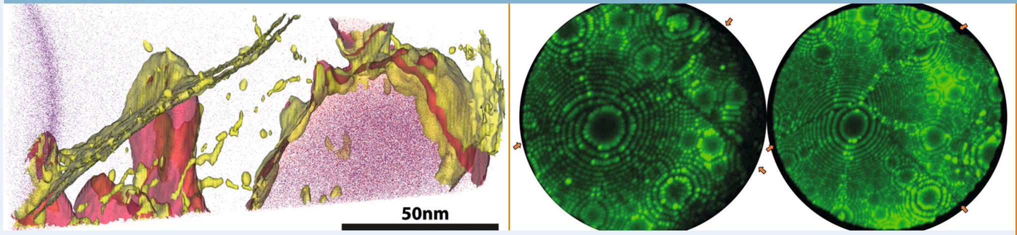
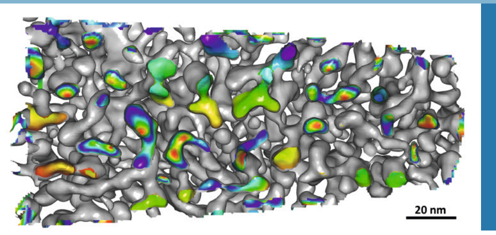
Max-Planck-Str. 1
40237 Düsseldorf
www.mpie.de

Contact:
pr@mpie.de

Max-Planck-Institut für Eisenforschung GmbH





Atomic Insights into Complex Materials - High-end Atom Probe Tomography and the Story behind it -

Hi,

I'm Baptiste. I lead two research groups at the Max-Planck-Institut für Eisenforschung (MPIE). One is focused on atom probe tomography, and the other… well also on atom probe tomography but targeting specifically hydrogen and is funded by a Consolidator grant of the European Research Council that I was awarded in 2018. In short, in the group we develop and use this microscopy and microanalysis technique to investigate the composition of materials at the near-atomic scale to better understand how the nanoscale structure of a material influences its behaviour– with an aim to use this knowledge to guide the design of higher performing or more enduring materials.

I was invited to guest edit this newsletter as I was awarded the Leibniz Prize 2020 by the German Research Foundation.

Receiving the Leibniz Prize has been the greatest honour and, well, the greatest surprise. Thinking of my job, what comes to mind is a famous quote from Gary Lineker[1], who, in the 1990s, said "Football is a simple game, twenty-two men chase a ball for 90 minutes and at the end, the Germans always win". I see research as a team sport. In the end, women and men of different nationalities and disciplines together chase understanding of experimental and theoretical data, and at the end, Science wins. At the moment, Germany also wins often, thanks to the high level of support that we are getting – Germany is in the top 10 worldwide in terms of R&D expenditure per capita.

I love my job here at the MPIE. Our key strengths lie in the blend of expertise, in our collaborative spirits and the very talented and smart early-career scientists with whom we work. Atom probe has become part of, or central to a wide range of studies on material. I selected and will discuss just some amongst the very exciting work with which I had the chance to be involved.

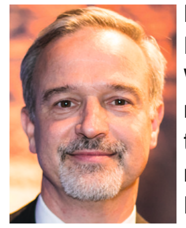
The past…

The Prize was awarded to me for my frontier work in atom probe tomography (APT) and the research that the technique enables. APT is unlike any other microscopy and microanalysis technique. In APT we peel off individual atoms from a specimen, measure their mass, attribute an elemental nature, e.g. is it Fe or Al or C or W, and then build a digital three-dimensional point cloud to reposition each of these atoms as close as possible to where they were originally located inside the material. From within this virtual 3D map, we can then dig and retrieve information. Sometimes this is done manually, sometimes through applying more advanced data extraction, including machine learning or other artificial

[1] Gary Lineker is a famous English football player of the 1980s.

➡

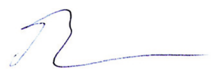
EDITORIAL



Dear Colleagues and Friends of the MPIE,

We have some very good news to share: Dr. Baptiste Gault, head of our research group "Atom Probe Tomography", was honoured this year with the Leibniz Award, the highest German research award. Dr. Gault is a worldwide leading scientist who pushes the technique of atom probe tomography (APT) to its limits. Already during his PhD studies, he implemented a pulsed-laser source on an atom probe, paving the way for the modern design of commercial APT instruments. He not only probes complex metallic materials at so far unprecedented resolution, but found a way to analyse with APT even biological materials, including proteins suspected to contribute to Alzheimer. His group works on connecting the vast amount of data from APT with machine learning techniques to accelerate and facilitate data extraction. And, one current big project, which is funded by the European Research Council, targets a crucial problem faced both by the steel industry and the hydrogen economy: the effect of hydrogen on metallic alloys. But, let him speak by himself in this very special newsletter edition.

Enjoy reading,



Prof. Dr. Dierk Raabe, managing director

Awards and Achievements

Dr. Lamya Abdellaoui, postdoctoral researcher in the group "Nanoanalytics and Interfaces", has been selected to be part of the organizing team of the "Virtual Thermoelectric Conference 2020". She is the only member from Germany in the team.

Dr. Stoichko Antonov, postdoctoral researcher from the USA, was honoured with a fellowship of the Alexander von Humboldt Foundation and is now working in the Group "Atom Probe Tomography".

Raquel Aymerich Armengol, PhD researcher in the group "Nanoanalytics and Interfaces", was awarded to join the 70th Nobel Laureate Meeting this year as an online event and next year in Lindau, Germany.

Dr. Martin Diehl's (in the photo) and **Dr. Franz Roters'**, review article on DAMASK, the modular plasticity simulation tool developed at the MPIE, was selected for the Hall of Fame of the journal Advanced Engineering Materials. Both are senior scientists in the department "Microstructure Physics and Alloy Design".

Dr. Ümit Güder, postdoctoral researcher from Turkey, was awarded a research fellowship of the Alexander von Humboldt Foundation and is currently working in the department "Microstructure Physics and Alloy Design".

intelligence techniques. The information gleaned from the data is mostly the local composition of the different microstructural features that are contained within the specimen. Sometimes, imperfect structural information can also be retrieved and used to help guide the reconstruction process or e.g. identify phases. APT has found application in physical metallurgy in semiconductors, both for academic and industrial research (Samsung in South Korea has more than half a dozen instruments now). The technique is gaining momentum in fields such as geology and, maybe, in the future, in the biological sciences.

I have been fortunate, over the course of my research career to work on almost all aspects of atom probe science. The Prize was given to me at least in part for what I initiated during my PhD, which was concerned with implementing an ultrafast laser source on an atom probe and deciphering the physics of the field evaporation process. The interaction between a coherent light pulse lasting only tens of femtoseconds and the APT specimen, that are only tens of nanometres and hence smaller than the light's wavelength, is indeed non-trivial. So non-trivial that most of the interpretation of the data within my PhD thesis was proven wrong in the following years. Yet, my pioneering work was a great enabler in the development of the technique, and pulse-laser sources are now implemented on nearly all commercial APT instruments. In the following years, as a postdoctoral scientist, I worked also on improving the approaches to build the tomographic reconstruction, and working on quantifying more precisely the spatial performance of the technique.

Another important aspect for me was to start using the technique for materials characterisation – an opportunity to start using my knowledge in materials science, but also to develop some more understanding of how materials behave – I worked on Al-alloys, steel, zirconium alloys, semiconductors amongst others. Over 2010–2012, alongside my colleagues at The University of Sydney, we wrote a book on

Fig. 1: *Cover of Physical Review Letters with our combined APT-TEM-atomistic simulations study.* © American Physical Society.

atom probe, which was the first one to be published for almost a decade. For me, it was a tremendous experience, allowing me to gather solid knowledge on all aspects of the technique.

Since joining the MPIE in 2016, I cannot think of a single aspect of this previous experience that has not been useful. I have had a chance to renew my interests in

- instrument development via the Laplace project (see p. 6)
- data mining, in part via our involvement in the BIGMAX network that links Max-Planck-Institutes interested in exploring machine-learning approaches to help design new materials
- theory of field evaporation and field ionisation with the development of the analytical-field-ion microscope
- and very many materials science projects, with an emphasis on understanding the fundamental processes that take place in complex, engineering materials, especially over the course of their use in service, insights that are necessary to guide design of future materials with enhanced lifetime and improved sustainability.

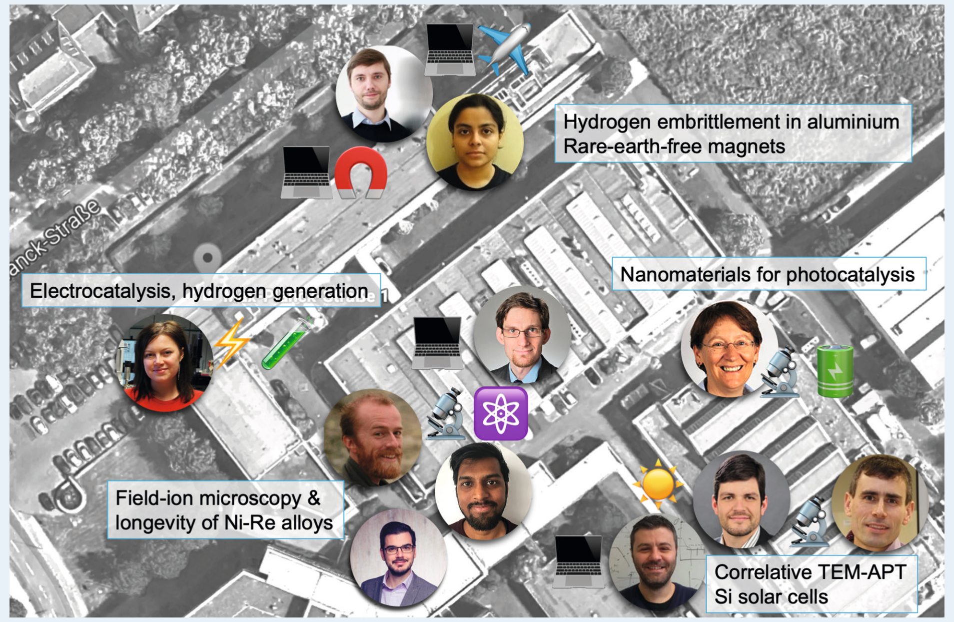


Fig. 2: *Some of the research collaborations that involve atom probe tomography across the MPIE.* © Baptiste Gault, Max-Planck-Institut für Eisenforschung GmbH

Complementing APT with TEM and complementing TEM with APT

Since before I joined, one of the key areas that the MPIE had been pushing was complementing APT with transmission electron microscopy (TEM) and complementing TEM with APT, in part through the work of Dr. Michael Herbig. This, in part, motivated the Laplace Project, but also is at the core of my work with Prof. Christina Scheu's and Dr. Christian Liebscher's groups. Our collaboration led to having atom probe tomography and high-resolution transmission electron microscopy on the cover of Physical Review Letter – one of the most prestigious scientific journals (see Fig. 1). This work was focused on understanding the behaviour of minor impurities in silicon, which are known to affect the performance of solar cells. We combined information on the intimate structure of grain boundaries with their local composition from atom probe. With the aid of atomistic simulations performed by Dr. Liverios Lymperakis from the Computational Materials Design Department, we concluded on the critical role of strain on the segregation of impurities at specific locations along the grain boundary facets or their junctions [1].

With Christina, we keep working closely on a range of functional materials, often also in collaboration with Dr. Olga Kasian (formerly department "Interface Chemistry and Surface Engineering", now at the Helmholtz Zentrum Berlin). We combine APT and TEM for compositional and structural analyses, and use that information to understand catalytic or electrocatalytic processes, with an aim to help design materials with better performance and enhanced longevity. Materials of interest here find application in the hydrogen economy, for water splitting for instance [2; 3], or nanomaterials, which are frontier applications of APT [4; 5].

Bridge to atomistic simulations

A key strength of APT is its compatibility in scale with atomistic simulations. Let me here mention joint projects with Drs. Tilmann Hickel and Christoph Freysoldt from the Computational Materials Design Department. With Tilmann, we work closely on hydrogen embrittlement in aluminium, which is at the core of the ERC-funded project of Dr. Chakraborty (see p. 5). We have used insights from APT to guide *ab initio* simulations to better understand the influence that hydrogen can have on grain boundaries in alloys that find application in the aerospace industry. We also work on trying to better understand the influence of the microstructure on the magnetic properties of rare-earth free magnets.

With Christoph, we worked on explaining the contrast between atoms of different species in field-ion microscopy using density-functional theory under intense electrostatic-field conditions. Drs. Leigh Stephenson & Shyam Katnagallu started exploring the possibility of re-visiting field-ion microscopy and combining it with time-of-flight mass spectrometry [6]. We designed an experiment using a binary Ni-Re alloy that had been subject to creep deformation at high temperature, and is core to our activity in superalloys, led by Dr. Paraskevas Kontis. They visualised bright atoms specifically at crystal defects. Christoph's input allowed us to interpret the contrast, which was then verified by experiments (see Fig. 3). This feedback loop between experiments and theory was crucial to really understand the results for the first time that Re was directly observed to be segregating to dislocations in this alloy system. This helped in rationalising a 40-year-long engineering observation that Re increases the creep lifetime of Ni-based superalloys, and gave evidence of a similar effect in complex alloys by combining electron microscopy, atom probe and atomistic phase-field simulations [7].

The future…?

One could wonder what is the next step in all this? To me, it is deploying the strength of atom probe to the analysis of liquids, liquid-solid interfaces and soft matter. Since the 1950s, several scattered investigations of biological materials by atom probe have been reported, but without a sustained effort that would have enabled true breakthroughs. In parallel, the development of cryo-TEM has initiated a revolution in the biological sciences, enabling to image proteins and viruses at an unprecedented resolution. Atom probe could, here again, provide precious and unique insights – an example is the presence of metallic species suspected to be involved in the Alzheimer disease. A few years ago, we started looking at such proteins in a collaboration with a group at Heinrich Heine University Düsseldorf. The grant from the Leibniz Prize will allow to complete this research, via cryo-specimen preparation, transport and analysis of frozen liquids, which can be used as carriers of such biological materials.

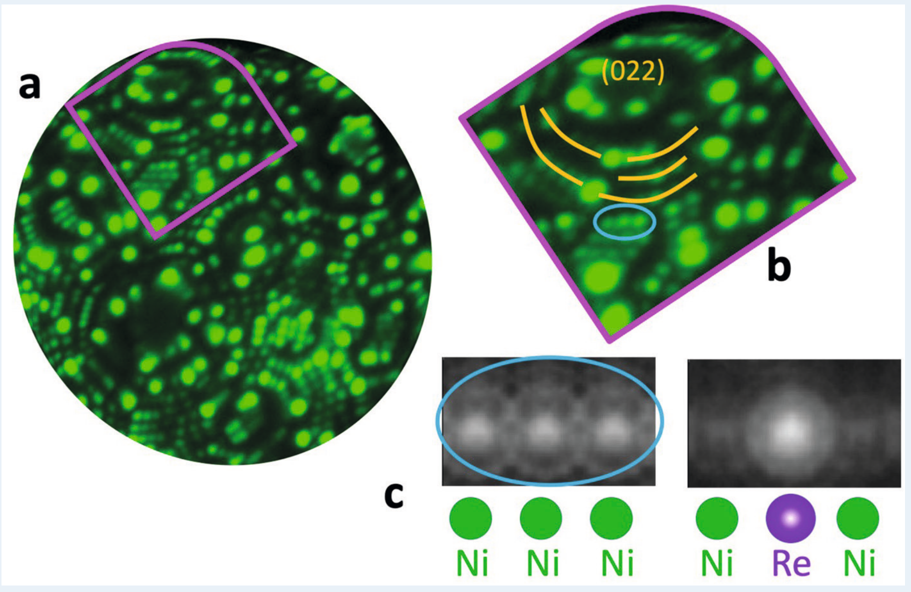


Fig. 3: *a) Field ion micrograph in which each bright spot is an individual atom. b) Close-up on a specific set of atomic planes, the yellow lines indicate that an extra half-plane is present: a dislocation induced by the plastic deformation. Two bright spots appear at the defect. c) Results from density-functional theory reveal that the imaged bright atoms correspond to Re-atoms [6].* © Baptiste Gault, Max-Planck-Institut für Eisenforschung GmbH

I really want to thank Prof. Dierk Raabe for opening the door for me to come back to research after spending some years at Elsevier, and do what I do best.

Un grand Dankeschön.

I want to say how grateful I am for the support I get from Sandy, my wife, who's been putting up with me for 20 years and with whom we have lived in 5 countries, and our lovely daughter Violette. To quote a great Canadian poet: "everything I do, I do it for you".

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5. J. Lim *et al.*: *Atomic-Scale Mapping of Impurities in Partially Reduced Hollow TiO_2 Nanowires*. Angew. Chemie - Int. Ed. 59 (2020) 5651.
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7. X. Wu *et al.*: Unveiling the Re effect in Ni-based single crystal superalloys. Nat. Commun. 11 (2020) 1.

Author: B. Gault (MA)

Awards and Achievements

The **MPIE** was elected into the board of the association "Wissensregion Düsseldorf e.V.".

Dr. Ting Luo, postdoctoral researcher from China, was awarded a research fellowship of the Alexander von Humboldt Foundation and is now working in the Group "Atom Probe Tomography".

Prof. Christina Scheu, head of the group "Nanoanalytics and Interfaces", has been elected as a new member of the review board "Production and Processing of Functional Materials" of the German Research Foundation.

Dr. Xuyang Zhou, postdoctoral researcher from China, received a research fellowship of the Alexander von Humboldt Foundation and is now working in the Group "Atom Probe Tomography".

Sophia-Helena Zwaka, head of the International Office, won the international research marketing competition of the German Research Foundation. Her concept "Coffee with Max Planck: Research Opportunities at the MPIE" is now being funded with 25,000 euros.