Scientists at the MPIE

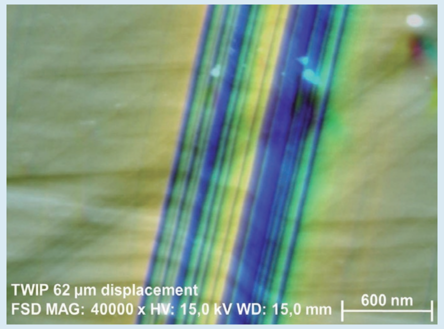
Dr. Pyuck-Pa Choi (35), born in South Korea, has been working in the department of Microstructure Physics and Alloy Design for two years. He is the group leader of the group "3D Atom Probe Tomography". This high-tech equipment, purchased at the MPIE in 2009, analyses steel down to an atomic scale. This special unit of equipment is one of only a handful within Europe. Choi's fields of interest range from the analysis of nanostructured materials to high-strength steel and compound semiconductors. Choi did his PhD on grain boundary segregation in nanocrystalline Al-Cu and Co-P alloys at the University of Göttingen. In 2011 he received the Golden Poster Award for his poster about "nanoscale characterization of TiAlN/CrN multilayer hardcoatings" at the 5th International Union of Microbeam Analysis Societies meeting in Seoul, Korea.

Natalie Tillack (22) has been working as a research fellow at the MPIE since 2009. She was working on her bachelor's thesis about "combined ab initio and kinetic Monte-Carlo studies on nano-precipitates in steels" in the department of Computational Materials Design. At the moment Tillack is working on her master's degree in physics at the Ruhr-University of Bochum and at the University of Oxford. She is investigating oxide-dispersion strengthened steels with ab initio methods. Therefore she is still working at the institute and travelling between Oxford and Duesseldorf on a regular basis. The Friedrich-Naumann-Foundation supports Tillack's studies and her stay abroad with a scholarship.

The MPIE's next top model

The importance of computational materials modeling has been increasing for the last decades. Models help to save experiments and hence time and money. They are becoming not only more sophisticated but also more detailed and exact. They can further help to understand processes on a microstructural scale and predict mechanical properties such as stress and strain behaviour.

How can we increase the safety of cars? This is a question which has been bothering scientists and car producers for several decades. The steels used in cars must be able to quickly absorb the shock energy of a crash. To do this, the material has to deform without breaking. The MPIE is developing a new model of TWIP steels (twinning induced plasticity). This kind of austenitic steel forms twins that lead to a prolonged characteristic hardening effect and an elongation at fracture of up to 60%. Moreover, TWIP steels are very light and thus help saving energy.



Nanotwins in Fe- 22 wt-% Mn- 0.6 wt-% C TWinning Induced Plasticity (TWIP) steel. Three separate forward scatter electron diodes produce individual RGB signals, allowing qualitative misorientation to be seen by color differences in the image.

A new model makes TWIP steels applicable in the automotive industry

Former problems that occurred during deformation processes could be solved soon. David Steinmetz, a PhD student and materials scientist at the MPIE, is developing a model for the strain hardening behavior of TWIP steels: "The model I am working on is based on microstructural investigations of grain size and dislocation structures, including twins and dislocation cells. New investigations have revealed the importance of these microstructural features within the network of deformation structure." Additionally, the model can accurately predict stress, strain and hardening behaviour over a temperature range of 400 Kelvin and it reveals that the high formability of TWIP steels is due to the interaction of twins and dislocations.

Desired properties are achieved by computational methods

The new model allows the understanding of the hardening behaviour of TWIP steels so that the automotive industry can save a lot of money and time. The simulation can teach us how to process sheets or to form crash-relevant parts of the car. The low stacking fault energy (SFE) of these high-manganese alloys, which is the key parameter for twinning, can nowadays be calculated by ab initio methods, performed in the department of Computational Materials Design headed by Prof. Jörg Neugebauer. In combination with the present model, this enables scientists of the MPIE to tailor the alloy composition and its SFE in order to achieve the desired macroscopic properties.

Imprint

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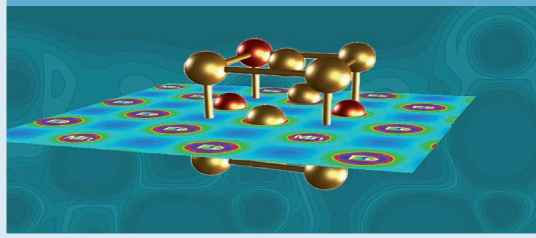
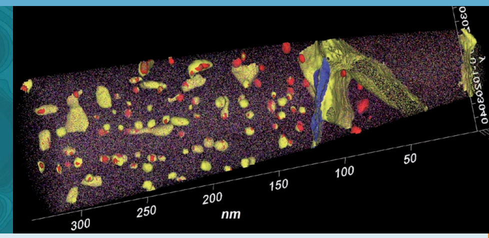
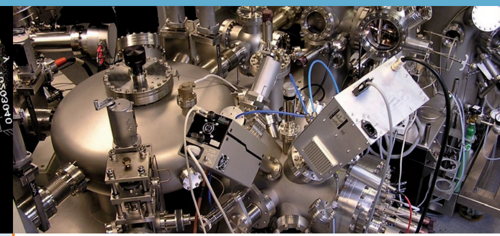


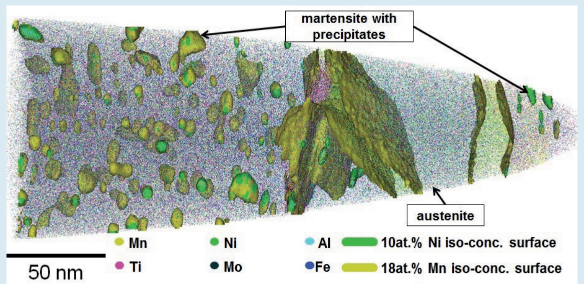




New high performance steel with potential applications in the automotive industry

Steel is the most important material for the automotive industry. 55% of the auto body components are made of steel. Optimizing the properties of those materials can reduce weight and costs enormously. A new class of steels developed at the MPIE, the "lean maraging TRIP steels", fulfills these requirements and offers potential applications in the automotive sector.

The requirements for steels applied in the automotive industry are manifold: strong steels are used for centre pillars, the part of a car installed next to the driver's door. On the other hand, the front part of a car must consist of strong and at the same time ductile material. Thus, in case of a crash, the shock energy can be absorbed and the driver is protected. Dr. Dirk Ponge, group leader at the MPIE, has achieved to combine both requirements in one class of new steel, named "lean maraging TRIP steels".



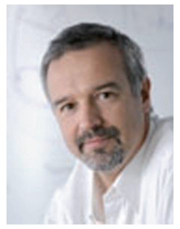
Result of an analysis by the 3D-atom probe. The martensitic and austenitic phases are visible. Even single atoms are recognized by this technique – each dot represents the location of one atom while the surfaces are regions of iso-concentration of a certain element.

Due to a high nickel content conventional maraging steels are very strong and used in air plane landing gear. The term maraging merges 'martensite' and 'aging'. The name is derived from a special heat treatment (aging) which strengthens an already quite strong martensite structure. "The use of a high amount of nickel results in a strong steel, but also caused an expensive production." That's why Ponge reduced the nickel content and found a surprising effect.

Combination of strength and ductility

During heat treatment, the formation of intermetallic precipitations causes an increase in strength. At the same time austenite is formed which is the reason for the increase in ductility and the basis for a second effect: the TRIP effect. TRIP stands for transformation induced plasticity. Triggered by a deformation process, a phase transformation from metastable austenite to martensite takes place in the material. This leads to an increase in strain hardening rate and enables to reach high elongations. With both these effects occurring, one obtains a good combination of

EDITORIAL



Dear Reader,

This newsletter provides information about recent developments at our institute, addressing main research achievements, technological breakthroughs, and new instrumentation that is available in Düsseldorf. While our bi-annual scientific report and our homepage (www.mpie.de) give a more comprehensive view into the details of our research projects this newsletter intends to build a bridge between basic science and application. We also want to make you more familiar with the team that stands behind the work. The newsletter appears twice a year and will be available on our homepage, too.

Enjoy reading and best regards,

Prof. Dr. Dierk Raabe
(Chief Executive, MPIE)

Awards and achievements

Viviane Becker received the 1st prize in the programming competition 2011 of the Mathe-dual e.V. This society promotes dual apprenticeships in the field of mathematics, informatics and technical studies.

Dipl.-Ing. Nahid Elhami is the winner of the 1st poster prize at the Electron-Backscatter-Diffraction-Meeting 2011, a conference organized by the Royal Microscopical Society. On her poster Elhami explained the application of cECCI images for defect analysis in TWIP steels.

Dr. Sebastian Klemm received the "Dr. Klaus-Seppeler-Stiftungspreis" of the Dr. Klaus-Seppeler-Stiftung and the Gesellschaft für Korrosionsschutz e.V. (Society for Corrosion Protection) for his dissertation titled "Microelectrochemical characterization of Zn, ZnO and Zn-Mg alloys with online dissolution monitoring".

Dr. Chris Race from London received a scholarship of the Alexander von Humboldt Foundation and chose the MPIE for his research on the analysis of the structure of alloys with the help of simulations.

tensile strength and total elongation up to 30.000 MPa%. The intermetallic precipitations, which are responsible for the excellent properties are analysed with the 3-dimensional atom probe.

Optimisation by computational materials design

Currently, the development of these steels is being optimised. Ponge expects to further decrease the production costs and to improve the mechanical properties by modifying the alloy composition. This is performed in close cooperation with the department of Computational Materials Design. The department of Prof. Jörg Neugebauer is calculating with the means of quantum physics, which precipitations are formed in the material with respect to the composition. This improves the efficiency of the further development and reduces the number of experiments. A systematic and application-oriented development of the lean high-performance steels is on the way.

Selected lectures and publications

J. Neugebauer, R. Nazarov, B. Grabowski, F. Koermann, J. von Pezold, T. Hickel: "Fully ab initio description of point defect formation and properties at extreme temperatures". Spring Meeting of the Materials Research Society 2011, April 25th–29th, San Francisco, California.

D. Raabe: "Alloy design of nano-precipitate-hardened high-Mn maraging-TRIP". Keynote Lecture, The First International Conference on High Manganese Steels 2011, May 15th -18th, Seoul, Korea.

M. Stratmann: "Electrochemical design of novel zinc alloys for the corrosion protection of steel". 216th ECS Meeting 2009, October 4th-9th, Vienna, Austria.

H. Fabritius, C. Sachs, D. Raabe, S. Nikolov, M. Friák, J. Neugebauer: Chitin in the exoskeletons of Arthropoda: From ancient design to novel materials science, vol. 34, Chitin Aims & Scope Topics in Geobiology Book Series, Springer, 2011, Chitin: formation and diagenesis

F. U. Renner, G. A. Eckstein, L. Lymperakis, A. Dakkouri-Baldauf, M. Rohwerder, J. Neugebauer, M. Stratmann: In-situ Scanning Tunneling Microscopy Study of selective dissolution of Au3Cu and Cu3Au (001), Electrochimica Acta 56, 2011, 1694-1700

News and events

Visit of the state secretary

The North Rhine-Westphalian state secretary and head of the state chancellery Franz-Joseph Lersch-Mense visited the MPIE on June 15th. He was fascinated by the modern materials research which is done at the institute and confirmed that the institute is a center of innovation for the whole of North Rhine-Westphalia.

Foreground: Franz-Joseph Lersch-Mense, state-secretary & Dr. Sebastian Klemm, scientist at the MPIE.

Extended visitors' service for schools

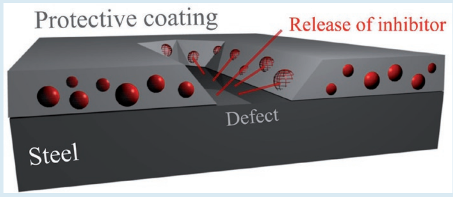
Several classes from the sixth form (Oberstufe) visited the MPIE this year. During their stay they gained insight into modern materials research performed at the institute. Several highlights were presented, e.g. the functionality of fuel cells.
The visitors' service for advanced classes in physics and chemistry has been established recently. It is planned to extend this service in the future.

Michael Kulse shows the floating steel cast to pupils of the 'Freies Christliches Gymnasium'.

Smart as skin: intelligent corrosion protection

Annually the economic loss due to corrosion amounts to ca. 80 billion Euro in Germany[1]. Affecting various kinds of materials, there is a common interest to create protective systems that can withstand this phenomenon. In steel industry this is usually achieved by galvanizing with zinc, which dissolves rather than iron when it is in contact with corrosive media. The group of Dr. Michael Rohwerder aims at further optimising the system. Thus a more reliable and efficient protection is ensured.

Research in corrosion protection has been increasing since the 18th century, especially with respect to steel. Galvanizing is a common protective means, but during the production process initial corrosive spots are formed right at the cut-edge. The idea that is developed at the MPIE is to incorporate microcapsules, which are filled with corrosion inhibitor, e.g. polyphosphomolybdate, into the zinc coating. As soon as the steel sheet is cut, the zinc starts to corrode and dissolve. This is the starting shot for the intelligent, second protective system: the capsules are released from the zinc onto the steel and smeared along the surface by the cutting device. The inhibitor can be released and thus protects the steel surface.



The microcapsules filled with corrosion inhibitor are released when the steel sheet is cut.

Modification with thiols facilitates the integration into the zinc

"This is an intelligent protective system that automatically realises when and where corrosion happens, becomes active and stops again when the respective spot is healed", explains Dr. Rohwerder, group leader in the department of Interface Chemistry and Surface Engineering. It works like a scratch in the skin: it is detected, healed and the initial status is restored.

For preparing these smart coatings, three work steps must be performed: loading of the silica microcapsules with the inhibitor, sealing them to avoid premature leaching and finally incorporating the capsules into the zinc layer. The sealing procedure, however, has of course an immense influence on the release kinetics. By rinsing with water glass solution, the release is steady and slow. The incorporation into the zinc layer is the most difficult part. Unmodified, the hydrophilic particles are repulsed by the zinc and only adsorb on the surface. Tabrisur Rahman Khan, a PhD student from Bangladesh, has now fixed the problem. He modifies the particles with zinc affine functional groups, such as thiols, which make the solvation feasible.

Max-Planck & Fraunhofer collaboration on intelligent corrosion coatings

Everything solved? Well, not completely. For efficient protection, a higher loading of the pores with the inhibitor must be realised. This is the focus of current research. Additionally, the concept of intelligent corrosion coatings has been expanded to systems with polymer coatings. The joint project ASKORR (Aktive Schichten für den Korrosionsschutz, active coatings for corrosion protection) is a successful collaboration between the Max-Planck and the Fraunhofer Society in this field. Two Max-Planck and two Fraunhofer Institutes are sharing their competences with respect to nanocomposite coatings, agent containers, zinc coatings and the analysis of effective mechanisms in order to improve the protective coatings. "It is a huge challenge, but present results look very promising", states Rohwerder.

[1] Gesellschaft für Korrosionsforschung

Awards and achievements

Prof. Dr. Dierk Raabe received the DGM Award of the Deutsche Gesellschaft für Materialwissenschaften for his innovative work in the field of microstructure physics.

Dr. Franz Roters, group leader in the department of 'Microstructure Physics and Alloy Design, has successfully completed his habilitation at the RWTH Aachen. His habilitation thesis is titled "Advanced material models for the crystal plasticity finite element method – development of a general CPFEM framework".

Dr. Stefanie Sandlöbes received the "Friedrich-Wilhelm-Preis" of the Friedrich-Wilhelm-Stiftung and the "Borchers-Plakette" of the RWTH Aachen for her dissertation about investigations on the application of non-intrusive in-situ measurement methods for the analysis of metallurgical gases.

The MPIE's high performance computer cluster is ranking once again in the list "Top 500" of the worldwide best computers '. In Germany it is on rank 29.