PART IV.

GENERAL INFORMATION AND STATISTICS

Boards, Directors, Max Planck Fellows, External Scientific Members and Guest Scientists

Supervisory Board (2012)

Prof. Dr.rer.nat. Peter GRUSS (chairman)
Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V., Munich

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Prof. Dr.-Ing. Werner HUFENBACH
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ArcelorMittal, Maizières-lès-Metz Cedex, France

Prof. Dr.-Ing. Ernst M. SCHMACHTENBERG
Rheinisch-Westfälische Technische Hochschule Aachen, Aachen

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Ministerium für Innovation, Wissenschaft und Forschung: Institutionelle Forschungsförderung, Düsseldorf

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Ruhr-Universität Bochum, Bochum

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Bundesministerium für Bildung und Forschung: Referat 511 - Neue Werkstoffe und Nanotechnologie, Bonn

Scientific Advisory Board (2012)

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ThyssenKrupp Steel Europe AG, Duisburg

Prof. Dr.-Ing. Bernd ISECKE
Bundesanstalt für Materialforschung und -prüfung, Berlin

Prof. Dr. Philippe MARCUS
Ecole Nationale Supérieure de Chimie de Paris, France

Prof. Dr. Tresa M. POLLOCK
University of California, Santa Barbara, CA, USA

Dr. Benedikt RITTERBACH
Salzgitter Mannesmann Forschung GmbH, Salzgitter

Dr. André SCHNEIDER
Vallourec & Mannesmann Deutschland GmbH, Düsseldorf

Dr. Peter SCHWAB
voestalpine AG, Linz, Austria

Dr.-Ing. Michael STEINHORST (membership pending)
Tata Steel Research, Development & Technology, Ijmuiden, The Netherlands

Prof. Dr. Adrian SUTTON
Imperial College London, UK

Dr. Sven VANDEPUTTE
OCAS - Arcelor Research Industry Gent, Zelzate, Belgium

Directors, Max Planck Fellows, and External Scientific Members

Directors:

Prof. Dr.rer.nat. Gerhard DEHM (since Oct. 2012)
Prof. Dr.rer.nat. Jörg NEUGEBAUER (since Nov. 2004)
Prof. Dr.-Ing. Dierk RAABE (since July 1999) *
Prof. Dr.rer.nat. Martin STRATMANN (since Jan. 2000)

* chief executive since 29 Sep. 2010

Max Planck Fellow:

Prof. Dr.-Ing. Gunther EGGELER, Ruhr-Universität Bochum

External Scientific Member:

Prof. Dr. Mats HILLERT, Stockholm, Sweden
Prof. Dr. Reiner KIRCHHEIM, Göttingen

Guest Scientists

Computational Materials Design

Prof. Mark Asta (USA), University of California and Lawrence Berkeley National Laboratory, Berkeley, CA; July 2012

Klaus-Dieter Bauer (Austria), Johannes-Kepler-Universität Linz; Macke Scholarship Awardee; April to July 2011

Dr. Miguel Morales-Silva (USA), Lawrence Livermore National Lab; Aug to Sep. 2012

Jassel Majevadia (UK), Imperial College London; Jan. to Feb. 2012

Dr. Chris Race (UK); Alexander-von-Humboldt-Foundation; since Sep. 2011

Prof. George Smith (UK), University of Oxford; Nov. 2011

Prof. Adrian Sutton (UK), Imperial College London; Oct. 2011

Jianchuan Wang (China), Central South University, Changsha; Jan to Dec 2011

Siyuan Zhang (China), University of Cambridge, UK; German Academic Exchange Service (DAAD); Jan. 2011 to July 2012

Interface Chemistry and Surface Engineering

Dr. Waleed Azzam (Jordan), Tafila Technical University; German Research Foundation (DFG); June to Aug. 2011

Xiaxia Bai, M.Sc. (China), Graduate University of Chinese Academy of Sciences; PhD exchange student; since Sept. 2012

Dr. Ying Chen (China); Center for Electrochemical Sciences (CES), Bochum; Feb. 2010 to Sep. 2012

Prof. Chiafu Chou (Taiwan), Institute of Physics, Academia Sinica, Taipei; German Academic Exchange Service (DAAD); Feb. 2012

Jeyabharathi Chinnaya, M.Sc. (India), CSIR-Central Electrochemical Research Institute, Tamilnadu; German Academic Exchange Service (DAAD); Oct. 2011 to Sep. 2012

Prof. Pritam Deb (India), Tezpur University, Napaam, Sonitpur, Assam; Max Planck India Fellow; July to Aug. 2011

Ashwin Anthony Fernandes, B.Sc (India), National Institute of Technology Karnataka (NITK), Surathkal; German Academic Exchange Service (DAAD) Working Internships in Science and Engineering (WISE) fellow; May to July 2011

Chethana Gadiyar, B.Sc (India), National Institute of Technology Karnataka (NITK), Surathkal; German Academic Exchange Service (DAAD) Working Internships in Science and Engineering (WISE) fellow; May to July 2012

Julien Gagnon, B.Sc. (Canada), McGill University, Montreal; Research Internships in Science and Engineering (RISE) - German Academic Exchange Service (DAAD); May to Aug. 2012

Carolina Galeano, M.Sc., Max-Planck-Institut für Kohlenforschung, Mülheim; PhD exchange student, Jan. to Apr. 2012

Nejc Hodnik, M.Sc. (Slovenia), National Institute of Chemistry, Ljubljana; visiting PhD Student; Oct. 2010 to May 2011

Izzudin Hubby, M.Sc. (Indonesia), Research Center for Physics, Indonesian Institute of Sciences (LIPI), Jakarta; German Academic Exchange Service (DAAD); since May 2010

Dr. Maciej Krzywiecki (Poland), Assistant Professor, Institute of Physics, Silesian University of Technology, Gliwice; July to Aug. 2012

Huachu Liu, M.Sc. (China), School of Materials Science and Engineering, Shanghai University; State Scholar Fund of China; Oct. 2010 to Sept. 2011

Erin Martin, B.Sc. (USA), University of Missouri, Columbia, MU; Research Internships in Science and Engineering (RISE) - German Academic Exchange Service (DAAD); May to July 2012

Prof. Kamachi Mudali (India), Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamil Nadu; Max Planck scholarship; June 2012

Prince Nagra, B.Sc. (Canada), University of Toronto; Research Internships in Science and Engineering (RISE) - German Academic Exchange Service (DAAD); May to Aug. 2011

Dr. Christian Schwieger, Institute of Chemistry, Martin-Luther-Universität Halle-Wittenberg; Apr. 2012

Jonathon Witte, B.Sc. (USA), Harvey Mudd College, Claremont, CA; Research Internships in Science and Engineering (RISE) - German Academic Exchange Service (DAAD); May to Aug. 2011

Microstructure Physics and Alloy Design

Prof. Hamid Assadi (Iran), Tarbiat Modares University, Teheran; scholarship Alexander-von-Humboldt-Foundation (AvH); July 2011 to April 2012

Li-Hui Cheng, M.Sc. (Taiwan) National Taiwan University, Taipe; German Academic Exchange Service (DAAD); May to Oct. 2011

Prof. Shoji Goto (Japan), Akita University, Akita; scholarship Alexander-von-Humboldt-Foundation (AvH); Aug. to Nov. 2011 and May to June 2012

Dr. Nan Jia (China), Northeastern University, Shenyang; scholarship Alexander-von-Humboldt-Foundation (AvH); Nov. 2010 to June 2012

Dr. José A. Jiménez (Spain), Universidad Madrid and CENIM; July to Sep. 2011, Feb. to Mar. 2012 and July to Aug. 2012

Prof. Satoru Kobayashi (Japan), National Institute of Materials Sciences (NIMS), Tsukuba; Feb. to Mar. 2012

Julio Millán, M.Sc. (Venezuela) Universidad Simón Bolívar, Caracas; German Academic Exchange Service (DAAD); April 2008 to Mar. 2012

Dr. Motomichi Koyama (Japan), National Institute of Materials Sciences (NIMS), Tsukuba; Sep. to Oct. 2011

Prof. Riccardo Lebensohn (USA), Los Alamos National Laboratory, Los Alamos; Alexander-von-Humboldt Award (AvH); Feb. 2010 to Jan. 2011

Dr. Yujiao Li (China), on leave from University of Göttingen; Jan. 2011 to Sep. 2012

Dr. Sumantra Mandal (India), Indira Gandhi Centre for Atomic Research, Kalpakkam, Tamil Nadu; scholarship Alexander-von-Humboldt-Foundation (AvH); since Apr. 2012

Dr. Ross Marceau (Australia), The University of Sydney; scholarship Alexander-von-Humboldt-Foundation (AvH); since July 2011

Prof. Nobuo Nakada (Japan), Kyushu University, Fukuoka; Japan Society for the Promotion of Science (JSPS); Oct. 2011 to Sep. 2012

Dean Pierce, M.Sc. (USA), Vanderbilt University, Nashville; funding by DFG SFB 761 'Stahl *ab initio*'; Mar. to May 2011 and May to July 2012

Prof. Hugo Sandim (Brazil), Escola de Engenharia de Lorena, University of São Paulo, Lorena; Aug. 2011 to Feb. 2012

Dr. Maria Sandim (Brazil), Escola de Engenharia de Lorena, University of São Paulo, Lorena; Aug. 2011 to Feb. 2012

Dr. Rodrigo Siqueira (Brazil), Escola de Engenharia de Lorena, University of São Paulo, Lorena; July to Aug. 2011 and Mar. to April 2012

Prof. Bob Svendsen (USA/Germany), on leave from RWTH Aachen; since Mar. 2012

Dr. Yun Takahashi (Japan), Nippon Steel; Apr. 2011 to Mar. 2012

Dr. Cem Tasan (Turkey), M2i, Foundation Materials Innovation Institute, Delft, The Netherlands; Mar. 2010 to Jan. 2012

Dr. Ilana Timokhina (Australia), Deakin University, Geelong, Victoria; May to Dec. 2012

Yuki Toji, M.Sc. (Japan), JFE Steel Corp. Fukuyama; since Oct. 2011

Dr. Kim Verbeken (Belgium); Ghent University; scholarship of the Research Foundation Flanders; Oct. 2007 to Sep. 2012

Prof. Yuhua Wen (China), Sichuan University, Chengdu; scholarship Alexander-von-Humboldt-Foundation (AvH); Oct. 2010 to Sep. 2011

Prof. James E. Wittig (USA), Vanderbilt University, Nashville; funding by DFG SFB 761 'Stahl *ab initio*'; May to July 2012

Prof. Seonghoon Yi (Korea), Kyungpook National University, Daegu; Mar. 2011 to Feb. 2012

Dr. Han Zhang (China), Tsinghua University, Beijing; scholarship Alexander-von-Humboldt-Foundation (AvH); since Dec. 2011

Dr. Chengwu Zheng (China), Institute of Metal Research, Chinese Academy of Sciences, Shenyang; scholarship Alexander-von-Humboldt-Foundation (AvH); Mar. 2010 to Feb. 2012

Scientific Honours

2010 (not included in Scientific Report 2009/2010)

Dr. C. Herrera obtained the Best Poster Award at the 4th International Conference on Recrystallization and Grain Growth, Sheffield, UK, 4-9 July 2010.

Dr. A. Kostka was honourably mentioned in the micrograph competition “The Art behind the Science” at the International Microscopy Congress IMC 17, Rio de Janeiro, Brazil, Sep. 2010.

Prof. Dr. J. Neugebauer became an elected member of the North Rhine-Westphalian Academy of Sciences, Mar. 2010.

Prof. Dr. D. Raabe was called by the German Bundespräsident as a member of the German Science Advisory Board (Wissenschaftsrat), Febr. 2010.

N.H. Siboni passed his master thesis about “Statistical and quantum mechanical simulation of interstitials in metals: mechanisms and constraints for superabundant vacancy formation” with excellence. RWTH Aachen, Dec. 2010.

2011

V. Becker has achieved the 1st place in the Programming Competition 2010/2011 of the Mathe-dual e.V., Mar. 2011.

U. Benedikt won the 2nd Best Poster Prize on the 47th Symposium for Theoretical Chemistry, Sursee, Switzerland, Sep. 2011.

Dr. P. Choi has received the Golden Poster Award for the poster “Nanoscale characterization of TiAlN/CrN multilayer hard coatings” at the 5th International Union of Microbeam Analysis Societies meeting, Seoul, Korea, 22-27 May, 2011.

N.-N. Elhami and *Dr. S. Zaefferer* have won the 1st Poster Prize of the Royal Microscopical Society at the RMS-EBSD 2011 conference for the poster "Interpretation and application of cECCI Images for defect analysis in TWIP steels", London, UK, Mar. 2011.

The article by *Dr. B. Grabowski, Dr. T. Hickel, Prof. Dr. J. Neugebauer* “Formation energies of point defects at finite temperatures”, Phys. Status Solidi B 248 (2011) 1295, was selected for the front cover.

The article by *Dr. T. Hickel, Dr. B. Grabowski, Dr. F. Körmann* and *Prof. Dr. J. Neugebauer*, “Advancing DFT to finite temperatures: Methods and applications in steel design”; Psi-k Newsletter 105 was selected as highlight for the Psi-k newsletter, June 2011.

Dr. S.O. Klemm received the Dr. Klaus Seppeler Stiftungspreis 2011 of the GfKORR Deutsche Gesellschaft für Korrosionsschutz e.V., Nov. 2011.

Dr. F. Körmann passed his doctoral thesis “Magnetic systems studied by first-principles thermodynamics” with excellence, University of Paderborn, May 2011.

Dr. R. Marceau from Sydney (Australia) obtained an Alexander-von-Humboldt-Stipend and works at the institute since Aug. 2011.

Dr. K.J.J. Mayrhofer was awarded a grant about 1 million Euro from the Federal Ministry of Education and Research for his project "$ECCO_2$", Nov. 2011.

Dr. K.J.J. Mayrhofer received the Anton-Paar Prize (Junior scientist prize < 35) of the Austrian Chemical Society GÖCH, Linz, Austria, Sep. 2011.

Prof. Dr. D. Raabe was awarded the DGM Prize from the Deutsche Gesellschaft für Materialkunde as excellent researcher for outstanding scientific or scientific-technical achievements in materials science and materials engineering, 15 June 2011.

Dr. C. Race from London (UK) obtained an Alexander-von-Humboldt-Stipend and works at the institute since Sep. 2011.

Dr. F. Roters has successfully completed his habilitation at the RWTH Aachen, faculty 5: Georessourcen und Materialtechnik with the lecture: "Werkstoffe für den Computer von Morgen". His habilitation dissertation is entitled: "Advanced Material Models for the Crystal Plasticity Finite Element Method - Development of a general CPFEM framework". The right to teach (*venia legendi*) was granted for "Computational Material Science", Aachen, June 2011.

Dr. S. Sandlöbes has been awarded the Borchers-Plakette of the RWTH Aachen for her excellent doctoral thesis about "Untersuchungen zum Einsatz berührungsloser in-situ Messmethoden metallurgischer Gase". Aachen, 16 June 2011.

2012

Dr. O. Cojocaru-Mirédin is one of the winners of the competition "NanoMatFutur" with a grant of 1.3 million Euro, May 2012.

Prof. Dr. G. Dehm got an appointment for an extraordinary professorship (außerplanmäßige Professur) at the Ruhr-Universität Bochum, Nov. 2012.

Dr. M. Herbig has been selected for the best poster prize of the "Solid-State Interfaces II: Towards an Atomistic-Scale Understanding of Structure, Properties, and Behaviour through Theory and Experiment" Symposium at the TMS 2012 Annual Meeting & Exhibition in Orlando, FL, USA, Mar. 2012.

D. Korbmacher passed his master thesis "Dual scale modelling of hydrogen embrittlement" with excellence. Ruhr-University Bochum, Aug. 2012.

C. Jacobs was awarded the Azubipreis of the Max Planck Society for being the best apprentice in the district Duisburg/Solingen in the field of material testing. Munich, Sep. 2012.

Dr. F. Körmann obtained the Otto-Hahn-Medal of the Max-Planck Society, Düsseldorf, June 2012.

Dr. F. Körmann obtained the CALPHAD Poster Award, Berkeley, CA, USA, June 2012.

Dr. B. Lange passed his doctoral thesis "p-Dotierbarkeit von Galliumnitrid" with excellence. University of Paderborn, Aug. 2012.

Dr. S. Mandal from Kalpakkam (India) obtained an Alexander-von-Humboldt-Stipend and works at the institute since Apr. 2012.

Dr. K.J.J. Mayrhofer received the ISE Prize for Applied Electrochemistry (Junior scientist prize < 35) of the International Society of Electrochemistry ISE. Santiago de Queretaio, Sep. 2012.

Dr. K.J.J. Mayrhofer received the 'Innovationspreis des Landes NRW in der Kategorie „Nachwuchs"' (innovation award of the state NRW in the category "junior scientists"), Nov. 2012.

J. Meier obtained the Best Poster Prize of the 63rd Annual Meeting of the ISE in Prague, Czech Republic, Aug. 2012.

Prof. Dr. J. Neugebauer and *Prof. Dr. D. Raabe* have jointly received an ERC Advanced Grant for their research project SMARTMET from the European Research Council. The award is worth 3 million Euro, 24 Jan. 2012.

Prof. Dr. J. Neugebauer has been elected as member of the "DFG-Fachkollegium 302 Chemische Festkörper- und Oberflächenforschung, Theorie und Modellierung", Feb. 2012.

Prof. Dr. J. Neugebauer became a member of the IT strategy group of the Max Planck Society, Apr. 2012.

Prof. Dr. D. Raabe was elected as member and chairman of the Hochschulrat (Board of Governors) of RWTH Aachen University, Aachen, Nov. 2012.

A. Schuppert has received the 'Nachwuchspreis' of the association ZELLCHEMING (Zellstoff- und Papierchemiker und -Ingenieure e.V.), Wiesbaden, June 2012.

Dr. S.Y. Shin from Pohang (Korea) obtained an Alexander-von-Humboldt-Stipend and works at the institute since Apr. 2012.

N. Tillack passed her master thesis "Chemical trends in the yttrium-oxide precipitates in oxide dispersion strengthened steels: A first-principles investigation" with excellence. Ruhr University Bochum, Mar. 2012.

PD Dr. S. Zaefferer received an offer for a position as professor on the chair for electron microscopy and scientific director of the Center for Electron Nanoscopy, Technical University Kopenhagen, Denmark, Apr. 2012.

PD Dr. S. Zaefferer received an offer for a position as professor on the chair for physical metallurgy, Technical University Wien, Austria, May 2012.

Dr. H. Zhang from Beijing (China) obtained an Alexander-von-Humboldt-Stipend and works at the institute since Jan. 2012.

The *MPIE* was honoured by the Düsseldorf Chamber of Commerce and Industry (IHK Düsseldorf) for its excellent performance in occupational training (Nov. 2012).

Participation in Research Programmes

National:

BMBF (Federal Ministry of Education and Research)

Combinatorial electrocatalytic CO_2 reduction

Development of ferritic steels for high-temperature applications

Increase of competence in electrochemistry for electromobility

Novel corrosion protection coatings compatible with hot forming

Ultra-high resolution EPR spectroscopy on thin film silicon for solar cell research (EPR-Solar)

BMWi (Federal Ministry of Economics and Technology)

Hydrogen induced embrittlement of hardened cold rolls (IWAS)

Next Generation MKWS - Development of corrosion-resistant and expansion-adapted micro channel heat sinks for high-power diode lasers - Selection and qualification of materials

DAAD (German Academic Exchange Service)

Investigation of the behaviour of water in confined geometries

DFG (German Research Foundation)

Ab initio and atomistic calculations of complex bio-materials

Ab initio based description of hydrogen embrittlement

Ab initio description of temperature dependent effects in dimensionally constrained magnetic shape memory Heusler alloys (SPP)

Ab initio determination of free energies and derived properties (Heat capacities, vacancies, solvus boundaries) for selected Al alloys containing Si, Mg and Cu

Ab initio investigation of temperature-driven martensitic transformations: Case study for alkali earth metals

Ab initio study on the coupling of lattice and magnetic degrees of freedom and the role of interfaces in magneto-caloric materials

Algorithms for the fast materials-oriented simulation of process chains in forming technology (SPP 1204)

Antireflecting interlayers to increase transmission through thin metal films in spectroelectrochemical experiments

Atomic scale investigation of compositional changes at interfaces using Atom Probe Tomography

Atomic scale investigation of the kinetics of nano-precipitation in Fe–Si–Cu alloys using Atom Probe Tomography

Biomimetic photonic crystals with mechanochromic properties based on cuticular scales of the weevil *Entimus imperialis.*

Characterization and modeling of the interplay between grain boundaries and heterogeneous plasticity in titanium

Characterization of Cu(In,Ga)Se_2 thin-film solar cells by means of atom probe tomography

Constitutive modeling and microstructural validation for crystal plasticity finite element computation of cyclic plasticity in fatigue

Crustacean skeletal elements: variations in the constructional morphology at different hierarchical levels

Deformation mechanisms and local residual stresses in the system Fe–Mn–C (SFB)

Development and validation of a multiscale description of heterogeneous deformation and inter-crystalline fracture of molybdenum

Elastic effects on heterogeneous nucleation and microstructure formation

Elucidation of corrosion phenomena with high lateral resolution using scanning probe techniques

Experimental and theoretical investigations of the dynamics of collective phenomena in blood I: Idealized vesicle/fluid droplet models

Fine lamellar Fe–Al *in situ* composite materials: Microstructure and mechanical properties

Fundamental investigation of the mechanisms of deformation and recrystallisation of cold deformable Mg alloys micro-alloyed with rare earth elements and microstructure optimization for the development of a new class of Mg-alloys.

Heapocrates: Healing polymers for preventing corrosion of metallic systems

High resolution scanning electron back scatter diffraction experiments of local crystallographic orientation patterning during plastic deformation

Highly accurate calculation of parameters of the NMR spectroscopy, development, benchmarking and application

Investigation and characterization of the intermetallic phase formation of dissimilar FeAl-joints produced by fast laser-based joining processes with large temperature gradients

Investigation of local alloy compositions by atom probe tomography

Limits and controllability of the impurity level of titanium recycling alloys for further use

Local mechanical properties of Mn-based steels (SFB)

Manufacturing, structural characterization and investigation of the mechanical properties of ultra fine grained and nanocrystalline structured Fe_3Al–X (X=Cr, Ti) alloys

Materials World Network: Physically based approach for predicting and minimizing damage nucleation in metals

Mechanisms of self and impurity diffusion in Fe–Al intermetallic compounds

Microbially induced corrosion by sulfate-reducing bacteria

Microstructure mechanics and fundamentals of concurrent twinning and martensite formation (SFB)

Nanofluid mechanics

Quantum mechanically guided design of ultra strong glasses

Scale-bridging studies of the elastic contributions to nucleation and initial microstructure formation in the eutectic system Ti–Fe

Steel - *ab initio*: Quantum-mechanically guided design of new Fe-based alloys partial project: “Defects and residual stresses in Fe–Mn–C steels” (SFB 761/1 partial project C05)

Steel - *ab initio*: Quantum-mechanically guided design of new Fe-based alloys partial project: “*Ab initio* derivation of Gibbs enthalpies, stacking fault energies and boundary energies at finite temperatures” (SFB 761/1 partial project A02)

STM characterization of novel SAMs

Synthesis and characterization of reference materials (SFB)

Thermal stability of metal nitride superlattices studied by means of atom probe tomography

Helmholtz Society

Improving performance and productivity of integral structures through fundamental understanding of metallurgical reactions in metallic joints (IPSUS)

Ultra-high resolution EPR spectroscopy on thin film silicon for solar cell research (EPR-Solar)

Max Planck Society

Active coatings for corrosion protection (ASKORR)

Characterisation of iron oxide nanoparticles

Computational mechanics of polycrystals

International Max Research School (IMPRS) for Surface and Interface Engineering in Advanced Materials (SurMat)

Triple-M: Max Planck initiative on multiscale materials modeling of condensed matter

State of North Rhine-Westphalia

Center for Electrochemical Sciences (CES)

High-pressure Fe–Al steam turbine blade - Development of a processing route for fabrication of a high-pressure iron aluminide steam turbine blade

Innovative materials development for cutting tools by the strip casting manufacturing technique - Bladestrip

International:

Christian Doppler Society

Diffusion and segregation mechanisms during production of high strength steel sheet, Module I: Selective enrichmenet at hot and cold rolled strip

Diffusion and segregation mechanisms during production of high strength steel sheet, Module II: Pickling Module

Diffusion and segregation mechanisms during production of high strength steel sheet, Module III: Hydrogen Module

European Union

Adaptive nanostructures in next generation metallic materials: Converting mechanically unstable structures into smart engineering alloys (SMARTMET)

AlGaInN materials on semi-polar templates for yellow emission in solid state lighting applications

Novel concepts for molecular interface engineering and unravelling of structure/property relationships at electrified interfaces (MultiScAd)

Surface engineered InGaN heterostructures on N-polar GaN-substrates for green light emitters

Foundation Materials Innovation Institute

Development of full field gradient plasticity FEM code to predict constitutive material model for dual phase steels

Mobility of water and charge carriers in polymer/oxide/aluminium alloy interfaces

Mechanics of phase boundaries in multi-phase steels

RFCS

Advanced zinc-based hot dip coatings for the automotive application (AUTOCOAT)

High emissivity annealing technique (HEAT)

Hydrogen sensitivity of different advanced high strength microstructures (HYDRAMICROS)

New approaches to quantitative hydrogen analysis of coated steel products (COATHYDRO)

New developments and optimisation of high strength boron treated steels through the application of advanced boron monitoring techniques (OPTIBOS)

Steady reactivity in hot-dip coating by direct deposit of iron oxides

Sino-German Center for Research Promotion

Liquidus surfaces and reaction schemes of the ternary systems Cr–Al–Nb and Fe–Al–Nb: Experiments and thermodynamic modelling

Mechanisms of self and impurity diffusion in Fe–Al intermetallic compounds

Conferences, Symposia and Meetings Organized by the Institute

2011

T. Hickel and R. Spatschek co-organized the sessions “Thermodynamic modeling” and “Kinetics of phase transitions”, respectively, of the “Advanced Discussions, Current Developments” meeting, which took place at Ruhr-Universität Bochum, 10 and 11 Mar. 2011.

P. Choi organized the Bilateral Korean-German workshop between Korea Institute of Science and Technology (KIST) and MPIE, which was held at MPIE on 25 Mar. 2011. 10 lectures were given to about 50 participants.

T. Hickel and J. Neugebauer organized a focus meeting of the SPP1239 on "Fundamentals of shape-memory alloys" at MPIE Düsseldorf, 13 and 14 Apr. 2011.

A. Bobrowski and H. Bögershausen organized the conference “Mikroskopie und Präparation 2011 - MikPräp 2011” of the Gesellschaft für Materialografie Rhein - Ruhr (GMR²), Solingen, 14 Apr. 2011.

L. Lymperakis and R. Spatschek organized the Computational Materials Design Workshop in Attendorn, 6 to 8 July 2011.

S. Sandlöbes organized the meeting of the “Arbeitskreis Konstruktionswerkstoffe" of the “DGM Fachausschuss Mg” which took place at MPIE on 6 Oct. 2011.

M. Rohwerder organized and chaired the 220th ECS Meeting “Coatings for Corrosion Protection” in Boston, MA, USA, 9 to 14 Oct. 2011.

L. Lymperakis co-organized the SINOPLE Nitrid Workshop at the Harnack-Haus, Berlin, 12 and 13 Oct. 2011.

C. Freysoldt co-organized the EPR Solar Workshop at the Helmholtz-Zentrum Berlin, 13 and 14 Oct. 2011.

C. Freysoldt organized a workshop on “Modern developments in the *ab initio* description of charged systems for semiconductors and electrochemistry” at Ringberg castle, 23 to 26 Oct. 2011.

C. Tasan organized the “MPIE Workshop on Dual-Phase Steel”, which was held at MPIE on 24 Nov. 2011. 10 lectures were presented to about 80 participants from industry and universities.

2012

J. von Pezold organized the 1st Austrian-German workshop on Computational Materials Design in Kramsach, Austria, 23 to 27 Jan. 2012.

M. Palm organized and chaired the 20th meeting of the “Fachausschuss Intermetallische Phasen (FA-IP)” which was held at MPIE on 23 Feb. 2012. 6 talks were given to about 40 participants.

A. Erbe organized together with SENTECH Instruments the seminar "Thin Film Metrology" at the MPIE, 1 Mar. 2012.

J. Neugebauer organized a symposium at the DPG Spring Meeting on “Materials design on the atomistic scale: Experiment meets theory”, Berlin, 25 to 30 Mar. 2012.

T. Hickel and R. Spatschek co-organized the sessions “Thermodynamic modeling” and “Kinetics of phase transitions”, respectively, of the “Advanced Discussions, Current Developments” meeting, Ruhr-Universität Bochum, 26 and 27 Apr. 2012.

T. Hickel, C. Race, R. Drautz and J. Neugebauer organized a workshop on "*Ab initio* Description of Iron and Steel: Thermodynamics and Kinetics (ADIS)” at Ringberg castle, 29 Apr. to 5 May 2012.

M. Herbig organized the “MPIE Workshop on Hydrogen Embrittlement in Steels” at MPIE on 25 June 2012. 8 lectures were presented to about 120 participants from industry and universities.

P. Eisenlohr organized the “3rd International Symposium Computational Mechanics of Polycrystals” which was held in Bad Honnef on 28 and 29 June 2012. More than 20 talks were given to about 45 participants from 7 countries.

J. Neugebauer co-organized the Joint European Condensed Matter Conferences CMD-24 - CMMP-12 - ECOSS-29 - ECSCD-11, Edinburgh, UK, 3 to 9 Sep. 2012.

J. Neugebauer was a member of the Technical Committee at the Hydrogen Conference “Hydrogen-Materials Interactions”, Wyoming, WY, USA, 9 to 12 Sep. 2012.

J. Neugebauer co-organized the ECCOMAS Symposium “Computational design of functional thin films”, Wien, 10 to 14 Sep. 2012.

J. Neugebauer organized a symposium “Multiscale Modelling of Mechanical Properties” at the MSE Darmstadt, 25 to 27 Sep. 2012.

J. Neugebauer co-organized a joint symposium “Thermodynamic Concepts in Materials & Process Design” at the MMM Singapore, 15 to 19 Oct. 2012.

Institute Colloquia and Invited Seminar Lectures

2011

P. Rehak, Brno University of Technology, Brno, Czech Republic: Study of Dynamical Stability of Crystals (5 Jan. 2011)

W. Shan, University of Hannover: Coupled Finite Element-Lattice Static Model, with Adaptivity (10 Jan. 2011)

S. Brinckmann, Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum: Towards Combining Molecular Dynamics and Discrete Dislocation Dynamics (31 Jan. 2011)

H.J. Maier, Universität Paderborn: Microstructure and Mechanical Properties of Conventional and Magnetic Shape Memory Alloys (2 Feb. 2011, Colloquium)

N. Marzari, University of Oxford, UK: Simple Solutions to Complex Problems: Towards High-Throughput Screening of Novel Thermoelectrics and Ferroelectrics (14 Feb. 2011)

J. Repper, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), TU München: Intergranular Residual Stress Studies and More by Neutron Diffraction (15 Feb. 2011)

P.V. Satyam, University of Bremen: Compositional Analysis of SiGe Nanostructures by Electron and Ion Scattering Methods (16 Feb. 2011)

V. Komanicky, Safarik University, Kosice, Slovakia: Electrocatalysis on Precisely Tailored Nano-Sized Model Systems (23 Feb. 2011)

J. Senger, Karlsruhe Institute of Technology (KIT): Discrete Dislocation Dynamics Simulations of Mechanical Properties in Micrometer Sized Pillars (24 Feb. 2011)

M.J. Duarte Correa, Cinvestav IPN, Querétaro, Mexico and Universitat Politècnica de Catalunya, Castelldefels, Spain: Preparation and Characterization of Structure and Stability of Different Metallic Glasses (3 Mar. 2011)

L. Ismer, University of California, Santa Barbara, CA, USA: Point-Defect-Mediated Dehydrogenation of AlH_3, (8 Mar. 2011)

A. Terfort, Goethe-Universität Frankfurt/Main: Self-Assembled Monolayers as Functional Materials (15 Mar. 2011, Colloquium)

M. Griebel, Universität Bonn: Numerical Simulation in Material Science and Nanotechnology (24 Mar. 2011)

G. Schütz, Max-Planck-Institut für Intelligente Systeme, Stuttgart: X-Ray Microscopy in Material, Environmental Science and Biology (31 Mar. 2011)

G. Dehm, Montanuniversität Leoben, Austria: New Insights in Plasticity of Metals by Highly Localized *in situ* Measurements (1 Apr. 2011, Colloquium)

T. Schena, Forschungszentrum Jülich: Tight-Binding Treatment of Complex Magnetic Structures in Low-Dimensional Systems (1 Apr. 2011)

C. Scheu, Ludwig-Maximilians Universität München: Atomic Scale Analysis of Nanostructures and Interfaces (19 Apr. 2011, Colloquium)

S. Baldelli, University of Houston, TX, USA: Sum Frequency Generation Vibrational Spectroscopic Imaging of Monolayers on Surfaces (28 Apr. 2011)

I. A. Abrikosov, Linköping University, Sweden: Towards Predictive Theory for *ab initio* Simulations of Materials Properties (4 May 2011)

S. Chakraborty, Ruhr-Universität Bochum: Silicon Revisited with an *ab-initio* Approach (1 June 2011)

S. Wege, Leibnitzinstitut für Werkstoffwissenschaft (IfW), Dresden: Method for Determination of Strain in Polycrystals using EBSD (9 June 2011)

E. Quandt, Institute for Materials Science, Christian-Albrechts-Universität zu Kiel: Thin Film Smart Materials for Medical Applications (4 July 2011, Colloquium)

I. Bleskov, CIRIMAT-ENSIACET-INP, Toulouse, France: Theoretical Investigation of Elastic Properties of New Refractory RuAl-Based Alloys (5 July 2011)

F. Otto, Max Planck Institute for Mathematics in the Sciences, Leipzig: Pattern Formation in Micromagnetics (11 July 2011)

E. Spohr, University Duisburg-Essen: Simulating Proton Transfer to Metal Electrodes with Reactive Molecular Dynamics Trajectories (12 July 2011, Colloquium)

Y. Cui, Paris, France: p-type Doping and Codoping of ZnO Based on Nitrogen is Ineffective: An *ab initio* Clue (12 July 2011)

E. Kabliman, Vienna University of Technology, Austria: *Ab initio*-Based Mean Field Theory of the Site Occupation in the Fe-Cr Sigma Phase (18 July 2011)

A. Winkelmann, Max Planck Institute for Microstructure Physics, Halle: The Physics of EBSD (27 July 2011)

D. Haley, University of Oxford, UK: Curvature Flow for Dynamic Emitter Geometry in Atom Probe (29 Aug. 2011)

R.C. Reed, University of Birmingham, UK: Nickel-Based Superalloys: Construction, Use and Validation of Numerical Models (1 Sep. 2011, Colloquium)

H. Assadi, Tarbiat Modares Univerisity, Tehran, Iran: Cold Spray Technology - Thermal Spraying on the Verge of Metal Forming (5 Sep. 2011)

D. Lambrecht, University of California, Berkeley, CA, USA: Multi-Scale Electronic Structure Simulation of Soft Matter and Chemistry at Interfaces (16 Sep. 2011)

D. Usvyat, University of Regensburg: Towards an Accurate Theoretical Description of Physisorption: Periodic Local-Correlation Method (27 Sep. 2011)

L. Nykänen, University of Jyväskylä, Finland: Chemistry of Carbon on Transition Metal Surfaces (27 Sep. 2011)

Y. Bar Sinai, Weizmann-Institut, Rehovot, Israel: Slow Rupture in a Generic Friction Model (29 Sep. 2011)

J.B. Seol, POSTECH Pohang University of Science and Technology, South Korea: 1. Role of Carbon Atoms on the Deformation Behavior of Strain-Induced Martensites in the High Mn Steels; 2. Atomic Scale Investigation on $(Fe,Mn)_3AlC$ Carbides Formed in High Aluminum Transformation-Induced-Plasticity Steels by Atom Probe Tomography (29 Sep. 2011)

P. Sofronis, International Institute for Carbon-Neutral Energy Research, Kyushu University, Fukuoka, Japan, and University of Illinois at Urbana-Champaign, IL, USA: International Institute for Carbon-Neutral Energy Research - Outline and Future Perspectives (6 Oct. 2011)

K. Tsuzaki, National Institute for Materials Science (NIMS), Tsukuba, Japan: Structural Materials Research at NIMS (10 Oct. 2011)

S. Kobayashi, National Institute for Materials Science (NIMS), Tsukuba, Japan: The Effect of Grain Boundary Precipitates on High Temperature Strength in Fe_3Al Based Alloys (11 Oct. 2011)

D. Rettenwander, Universität Salzburg, Austria: Computational Characterization of Methionine Radicals (17 Oct. 2011)

A. Sutton, Imperial College London, UK: The Theory of Grain Boundary Structure in Single-Component and Multi-Component Crystals (18 Oct. 2011, Colloquium)

S. Naghavi, Johannes Gutenberg Universität Mainz: Elastic Properties of Heulser Compounds from First-Principle Calculations (19 Oct. 2011)

W.A. Curtin, Brown University, Providence, RI, USA: From Atoms to Ductility: the Mechanisms of Dynamic Strain Aging and its Impact on Ductility in Al-Mg Alloys (7 Nov. 2011)

W.A. Curtin, Brown University, Providence, RI, USA: First-principles Predictions of Solute Strengthening in Al and Mg Alloys (8 Nov. 2011)

M. Mehring, Technische Universität Chemnitz: Molecular Precursors and Clusters for the Synthesis of Metal Oxides and Organic-Inorganic Hybrid Materials Containing Bismuth (8 Nov. 2011, Colloquium)

G. Smith, University of Oxford, UK: Where are the Carbon Atoms in Martensite? (15 Nov. 2011, Colloquium)

A. Klamt, COSMOlogic GmbH&CoKG, Leverkusen, and University of Regensburg: COSMO-RS, the Bridge from Quantum Chemistry to Fluid Phase Thermodynamics (16 Nov. 2011)

G. Smith, University of Oxford, UK: Where are the Carbon Atoms in Martensite? Continued (17 Nov. 2011)

D. Zaytsev, Ural Federal University Ekaterinburg, Russia: The Relationship between Mechanical Properties and Microstructure of Human Tooth Hard Tissues (22 Nov. 2011)

J. Takahashi, Advanced Technology Research Labs, Nippon Steel Corporation, Chiba, Japan: Application of Atom Probe Tomography Analysis to Traditional Issues of Steel Materials (23 Nov. 2011)

W. Poole, University of British Columbia, Vancouver, Canada: Developing Magnesium Materials for the Transportation Sector - An Overview of the Canadian Research Network, MagNET (28 Nov. 2011)

D. Holec, Montanuniversitaet Leoben, Austria: Electron Energy Loss near Edge Structures of AlN-Based Ternary Thin Films: Theory vs. Experiment (29 Nov. 2011)

P. Neumann, Mettmann, retired (former director at MPIE): Calculating the Giant Strains at the Intersections of Slip Bands (29 Nov. 2011, Colloquium)

G. Zimbitas, TU Delft, The Netherlands: Internal Oxidation of Binary Ni Alloys (29 Nov. 2011)

A. Chakrabarty, Trinity College Dublin, Irland: Role of Defects and Impurities in Ferromagnetic Oxides: An Electronic Structure Study (30 Nov. 2011)

K. Murgaeva, TU Bergakademie Freiberg: TEM Analysis of the Orientation Relationships and Interfaces in Nanocomposites (1 Dec. 2011)

R. Schuster, Karlsruhe Institute of Technology (KIT), Karlsruhe: Electrochemical Microcalorimetry (6 Dec. 2011, Colloquium)

M. Rizzi, Ecole Polytechnique Federale de Lausanne, Switzerland: Carbon Dioxide Adsorption and Hydrogenation on Nickel-Based Surfaces: A First Principles Study (7 Dec. 2011)

P. Dey, Indian Institute of Technology Guwahati, India: Effect of Random Disorder on Superconductivity (13 Dec. 2011)

M. Militzer, University of British Columbia, Vancouver, Canada: Multi-scale Modelling of Phase Transformations in Steels (14 Dec. 2011)

P. Neumann, Mettmann, retired (former director at MPIE): A Heavenly Beautiful Journey into Deep Space (15 Dec. 2011)

R. Sigel, University Fribourg, Switzerland: Adsorption and Diffusion Dynamics at Interfaces (16 Dec. 2011)

2012

S. Chentouf, University Paul Verlaine of Metz, France: *Ab initio* Study of the Effect of Ti and Zr Transition Metals Located in Bulk $D0_3$-Fe_3Al and $\Sigma5$ (310)[001] Grain Boundary (9 Jan. 2012)

C. Teichert, Montanuniversitaet Leoben, Austria: Atomic-Force Microscopy Based Electrical and Mechanical Characterization on the Nanometer Scale (10 Jan. 2012)

H. Riechert, Paul-Drude-Institut, Berlin: InGaN/GaN Nanowires on Si - A Viable Route towards LEDs on Si? (19 Jan. 2012)

Z. Strelcova, Central European Institute of Technology, Masaryk University, Brno, Czech Republic: From Bioinformatics to *ab-initio* Dynamics, From Supramolecules to Biomolecules (19 Jan. 2012)

S. Ringer, Australian Centre for Microscopy & Microanalysis, University of Sydney, Australia: Alloy Design guided by Advanced Atom Probe Tomography and Microstructure Characterisation (24 Jan. 2012)

C.-H. Fischer, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin: Spray-ILGAR (Ion Layer Gas Reaction) and Spray-Pyrolysis - Two Powerful Methods for the Deposition of High Quality Compact or Nano-Dot Thin Films (2 Feb. 2012)

E. Arzt, INM - Leibniz Institute for New Materials and Saarland University Saarbrücken, Germany: Bioinspired Mesotextured Surfaces for Active Surface Control (6 Feb. 2012, Colloquium)

P.K. Nayak, Weizmann Institute of Science, Rehovot, Israel: Effect of Material Disorder and Interfacial Energetics on Photovoltaic Efficiency (9 Feb. 2012)

J. Weissmüller, Technische Universität Hamburg-Harburg and Helmholtz-Zentrum Geesthacht: Novel Functional Materials Based on Nanoporous Metals (9 Feb. 2012)

K.-U. Neumann, Loughborough University, UK: A Structural and Electrical Resistivity Investigation of some Cr_2VX and $Ni_{2-x}Mn_{1+x}Ga$ Heusler alloys (28 Feb. 2012)

E. Spiecker, Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich-Alexander-Universität Erlangen-Nürnberg: Bridging Length Scales in Transmission Electron Microscopy of Materials (28 Feb. 2012)

A. Schlieter, Institute for Complex Materials IFW Dresden: Scale-Bridging Studies of the Elastic Contributions to Nucleation and Initial Microstructural Formation in the Eutectic Ti-Fe System (29 Feb. 2012)

K. Tsuchiya, National Institute for Materials Science (NIMS), Tsukuba, Japan: Improvement of Strength and Ductility by Heterogeneous Microstructures (5 Mar. 2012)

K. Verbeken, Ghent University, Belgium: Evaluation of Hydrogen Trapping in Iron-Based Alloys by Thermal Desorption Spectroscopy (5 Mar. 2012)

I. Watanabe, National Institute for Materials Science (NIMS), Tsukuba, Japan: Numerical Prediction of Deformed Microstructure Subjected to Plastic Forming with Two-Scale Finite Element Analysis (5 Mar. 2012)

T. Ohmura, National Institute for Materials Science (NIMS), Tsukuba, Japan: Indentation-Induced Plasticity of Metals with Various Lattice Defects (6 Mar. 2012)

R.C. Chiechi, University of Groningen, The Netherlands: Unconventional Tools for Constructing Tunneling Junctions from Self-Assembled Monolayers (13 Mar. 2012, Colloquium)

G. Bester, Max-Planck-Institut fürFestkörperforschung, Stuttgart: Frontiers in the Atomistic Modeling of Nanostructures (15 Mar. 2012)

G.P. Leyson, Brown University, Providence, RI, USA: Solute Strengthening from First Principles and Application to Al and Mg Alloys (20 Mar. 2012)

O. Cheiliakh, Pryazovskyi State Technical University, Mariupol, Ukraine: The Creation and Strengthening of New Effective Functional Metastable Alloys Based on Effect of Phase Transformations Induced by Deformation (3 Apr. 2012)

H. Kitaguchi, Oxford University, UK: Carbon and Carbides in Metals: Understanding the Effect of Carbon and Carbides on Mechanical Properties and Developing a Strategy to Achieve Full Carbon Quantification using EELS and APT (4 Apr. 2012)

S. Peljhan, Jozef Stefan Institute, Ljubljana, Slovenia: Simulations of BTAH and Cl Adsorption on Cu Surfaces: Towards Understanding the Corrosion Inhibition Action on the Atomic Level (11 Apr. 2012)

R. Groeger, Academy of Sciences of the Czech Republic, Institute of Physics of Materials, Brno, Czech Republic: Atomic-Level Foundations of the Plastic Deformation of bcc Metals (24 Apr. 2012)

S. Bargmann, University of Dortmund: Modeling and Simulation of Polycrystalline Metals Based on Extended Crystal Plasticity (2 May 2012)

J. Brillo, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln: Thermophysical Properties of Liquid Multicomponent Alloys (3 May 2012)

C. Peter, Max Planck Institute for Polymer Research, Mainz: Hierarchical Simulations of Polyelectrolyte Solutions in Contact with Calcite Surfaces (3 May 2012)

M. Korth, Universität Ulm: Computational High-Throughput Screening of Advanced Battery Electrolyte Solvents (7 May 2012)

A. Haschibon, Fraunhofer Institute for Mechanics of Materials IWM, Freiburg: Modeling and Simulation of Solid-Solid and Solid-Liquid Interfaces (10 May 2012)

K. Brandhorst, Institute for Advanced Simulation (IAS), Forschungszentrum Jülich: Mechanical Bond Strength Descriptors and Sparse Matrix Algebra (25 May 2012)

A. Dianat, TU Dresden: First-Principle Simulations of Materials Properties (4 June 2012)

U. Kamachi Mudali, Indira Gandhi Centre for Atomic Research, Kalpakkam, India: Superhydrophobic Way for Corrosion Protection of Metals and Alloys (21 June 2012)

C.G. Levi, University of California, Santa Barbara, CA, USA: Extending the Temperature Capability of Thermal Barrier Coatings: Fundamental Challenges and Possible Materials Solutions (26 June 2012)

A. Breidi, Chimie Métallurgique des Terres Rares, CNRS, Université Paris-Est, France: *Ab initio* Study of Topologically Close-Packed Phases (TCP) in Rhenium-Based Binaries (27 June 2012)

V. Subramanya Sarma, Indian Institute of Technology, Madras, India: Strategies for Improving the Ductility of Ultrafine Grained/Nanostructured Metals and Alloys (28 June 2012)

G. Winther, Technical University of Denmark, Lyngby, Denmark: Microstructure, Slip Systems and Plastic Anisotropy (2 July 2012)

A.A. Kornyshev, Imperial College London, UK: Ionic Liquids at Interfaces and in Confinement: From Fundamentals to the Physics of Supercapacitors and Electroactuators at the Nanoscale (3 July 2012, Colloquium)

I. Lauermann, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH: Synchrotron-Based Characterization of Surfaces and Interfaces in Chalcopyrite Thin Film Solar Cells (13 July 2012)

T. Furuta, Toyota Central R&D Labs., Inc., Aichi, Japan: Ideal Strength Metallic Materials (16 July 2012)

T. Maeshima, Toyota Central R&D Labs., Inc., Aichi, Japan: Microstructure of Al-TM (Transition Metal) System by Aggressive Use of Fe (16 July 2012)

A. Barnoush, Saarland University, Saarbrücken: Micro- and Nanomechanical Testing under Simulated Environmental Conditions (17 July 2012)

M. Zeleny, Aalto University School of Science, Finland: *Ab initio* Study of Magnetism of Manganese in Nanostructures and Thin Films (17 July 2012)

S. Korte, Friedrich-Alexander-Univerität Erlangen-Nürnberg: Plasticity in Hard Materials - Probing Deformation Mechanisms by Micromechanical Testing across Sizes and Temperatures (18 July 2012)

Z. Wang, Shenyang National Laboratory for Materials Science, Chinese Academy of Sciences, Shenyang, China: Aluminization Behavior and Austenitization Process of a Ferritic Heat-Resistant Steel with a Nanostructured Surface Layer (18 July 2012)

M. Asta, University of California and Lawrence Berkeley National Laboratory, Berkeley, USA: Dynamics of Grain-Boundary Motion Studied by *in-situ* Electron Microscopy and Molecular Dynamics Simulations (19 July 2012)

T. Maeshima, Toyota Central R&D Labs., Inc., Aichi, Japan: Prediction of Liquid Phase Behavior during the Rapid Transient Liquid Phase Bonding Process of Steel using Cementite Filler Metals (19 July 2012)

N. Wanderka, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin: Is AlCoCrCuFeNi High Entropy Alloy Suitable for High Temperature Application? Investigations by Transmission Electron Microscopy and Three Dimensional Atom Probe (19 July 2012)

S. Siebentritt, University of Luxembourg, Belvaux, Luxembourg: Kesterite - A New Material for Solar Cells (20 July 2012)

H. Noei, Ruhr-Universität Bochum: Vibrational Spectroscopic Studies on Metal Oxides and Metal-Organic Frameworks (24 July 2012)

M. Krzywiecki, Silesian University of Technology, Gliwice, Poland: Studies of CuPc Ultra-Thin Layers Deposited on Si (111) Substrates (26 July 2012)

A. Maljusch, Ruhr-Universität Bochum: Integrated Scanning Kelvin Probe - Scanning Electrochemical Microscopy System: Design, Development and Applications (26 July 2012)

C. Schön, Max-Planck-Institut für Festkörperforschung, Stuttgart: Energy Landscapes of Chemical Systems and the Modeling of Chemical Processes (27 July 2012, Colloquium)

X. Min, National Institute for Materials Science (NIMS), Tsukuba, Japan: Microstructure-Property Relationship for Ti–Mo β-Titanium Alloys and Fe–Mn–Si Shape Memory Alloys (6 Aug. 2012)

K. Nakano, National Institute for Materials Science (NIMS), Tsukuba, Japan: Analysis of the Initiation of Plastic Deformation in Fe-C Alloys (6 Aug. 2012)

K.A. Padmanabhan, University of Hyderabad, India: A Mechanism of Deformation for Disordered States of Matter (13 Aug. 2012)

J.-S. Lee, Hanyang University-ERICA, Ansan, South Korea: Advances in Processing of Ferrous PM Microcomponents using Nano Powders (17 Aug. 2012)

M. Morales-Silva, Lawrence Livermore National Lab, CA, USA: Quantum Monte Carlo Methods (21 Aug. 2012)

M. Morales-Silva, Lawrence Livermore National Lab, CA, USA: Application of QMC Methods: High-Pressure Hydrogen (22 Aug. 2012)

E. Povoden-Karadeniz, Vienna University of Technology: CALPHAD-Integrated Thermokinetic Simulation of Precipitate Evolution (28 Aug. 2012)

J. Vogelsang, SIKA AG, Zürich, Switzerland: Do New Concepts for Corrosion Protection have a Chance? (29 Aug. 2012)

B.-J. Lee, POSTECH, South Korea: Multi-Scale, Semi-Empirical Atomistic Approaches for Structural Materials Research (31 Aug. 2012)

D.J. Jarvis, New Materials & Energy Research, ESA, The Hague Area, The Netherlands: Metallurgy Europe (3 Sep. 2012)

M. Scott Shell, University of California, Santa Barbara, CA, USA: Understanding Peptide Self-Assembly with All-Atom and Coarse-Grained Simulations (3 Sep. 2012)

S. Lozano-Perez, Oxford University, UK: High-Resolution Characterisation of Stress Corrosion Cracking in Stainless Steels (7 Sep. 2012)

M. Ilhan, Universität Duisburg-Essen: *Ab initio* simulations of the onset of proton mobility in water-starved polymer electrolyte membrane pores (10 Sep. 2012)

N. Mattern, IFW Dresden: Phase-Separated Metallic Glasses (11 Sep. 2012)

A. Stierle, DESY Nanolaboratory, Hamburg: Oxidation of Alloys and *In-situ* X-Ray Diffraction: Subsurface Superlattice Disordering and the Role of Steps (20 Sep. 2012)

D. Evans, University of South Australia, Adelaide, Australia: Thin Film Coatings for Real World Applications: From Conducting Polymers to Transition Metal Alloys (21 Sep. 2012)

S. Brinckmann, Ruhr-Universität Bochum: Sequential and Concurrent Multiscale Simulations of Metal Fracture (24 Sep. 2012)

M. Katsnelson, Nijmegen University, The Netherlands: Graphene as a Prototype Membrane: Ripples, Puddles and Strain Engineering (2 Oct. 2012)

A.H. Romero Castro, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional (Cinvestav) Unidad Querétaro, Mexico: Designing Materials from Scratch: Probing Theoretical Methods (25 Oct. 2012)

V. Šima, Charles University Prague, Czech Republic: Recent Experience and Results Obtained with Spark Plasma Sintered FeAl Intermetallics in Prague (6 Nov. 2012)

M. Spiegel, Salzgitter Mannesmann Forschung GmbH, Duisburg: Material Requirements for the Energy Transition (6 Nov. 2012, Colloquium)

S. Neumeier, Friedrich-Alexander-Universität Erlangen-Nürnberg: γ'-Hardened Cobalt-Base Superalloys - A New Class of High Temperature Materials (19 Nov. 2012)

M.J. Cordill, Erich Schmid Institute of Materials Science, Austrian Academy of Sciences and Montanuniversität Leoben: Mechanical and Interfacial Behavior of Copper and Titanium Films on Polyimide at Elevated Temperatures (20 Nov. 2012, Colloquium)

S. Curiotto, Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), Aix-Marseille University, Marseille, France: Interfacial Morphologies and Orientation Relationships between Copper Crystals and Sapphire (22 Nov. 2012)

Lectures and Teaching at University

2011

A. Erbe, Ruhr-Universität Bochum: Physical Chemistry V: Molecular Reaction Dynamics, WS 2011/2012

T. Hickel, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, compact course, Mar. 2011

T. Hickel, R. Drautz, J. Neugebauer, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2011/2012

K.J.J. Mayrhofer, Ruhr-Universität Bochum: Advanced Methods in Electroanalytical Chemistry Part II, SS 2011 and Part I, WS 2011/2012

J. Neugebauer, Ruhr-Universität Bochum: Application and Implementation of Electronic Structure Methods, SS 2011

J. Neugebauer, Ruhr-Universität Bochum: Lecture of the International Max Planck Research School Surmat, Module T3 “Multiscale Modelling”, 2011

D. Raabe, RWTH Aachen: Micromechanics of Materials, SS 2011

M. Rohwerder, Ruhr-Universität Bochum: Werkstoffoberflächen und Korrosion, SS 2011

F. Roters, RWTH Aachen: Process- and Materials Simulation, WS 2011/2012

F. Roters: Modellierung von Verformungsvorgängen auf Basis der Kristallplastizität, DGM Fortbildung Modellierung und Simulation, ICAMS Bochum, 18 Nov. 2011

R. Spatschek, F. Varnik, Ruhr-Universität Bochum: Thermodynamics and Statistical Physics, compact course, May 2011

R. Spatschek, Ruhr-Universität Bochum: Stochastic Processes, SS 2011

R. Spatschek, F. Varnik, Ruhr-Universität Bochum: Thermodynamics and Statistical Physics, WS 2011/2012

S. Zaefferer, T. Hickel and U. Prahl, RWTH Aachen: Microstructures, Microscopy and Modelling, SS 2011

S. Zaefferer, University of Vienna, Austria: Fundamentals and applications of texture and EBSD-based orientation microscopy, compact course, Apr. 2011

2012

G. Dehm, Universität Salzburg: Materialwissenschaften 1, WS 2012/2013

A. Erbe, Ruhr-Universität Bochum: Spectroscopy of Surfaces and Interfaces, WS 2012/2013

T. Hickel, R. Drautz, J. Neugebauer, Ruhr-Universität Bochum: Introduction to Quantum Mechanics in Solid-State Physics, WS 2012/2013

G. Madsen, J. Neugebauer, Ruhr-Universität Bochum: Application and Implementation of Electronic Structure Methods, SS 2012

K.J.J. Mayrhofer, Ruhr-Universität Bochum: Advanced Methods in Electroanalytical Chemistry Part II, SS 2012 and Part I, WS 2012/2013

J. Neugebauer, Ruhr-Universität Bochum: Lecture of the International Max Planck Research School Surmat, Module T3 “Multiscale Modelling”, 2012

D. Raabe, RWTH Aachen: Micromechanics of Materials, SS 2012

M. Rohwerder, Ruhr-Universität Bochum: Werkstoffoberflächen und Korrosion, SS 2012

R. Spatschek, F. Varnik, Ruhr-Universität Bochum: Thermodynamics and Statistical Physics, WS 2012/2013

S. Zaefferer, T. Hickel and U. Prahl, RWTH Aachen: Microstructures, Microscopy and Modelling, SS 2012

Invited Talks at Conferences and Colloquia

2010 (not included in Scientific Report 2009/2010)

Choi, P.: *Characterization of $CuInSe_2$ and $CuInGaSe_2$ thin-film solar cells using atom probe tomography.* (Int. Conf. on Electronic Materials and Nanotechnology for Green Environment (ENGE 2010), Jeju Island, South Korea, 21 to 24 Nov. 2010).

Cojocaru-Mirédin, O.; Choi, P.; Würz, R.; Liu, T.; Raabe, D.: *Characterization of $CuInSe_2$ and $Cu(In,Ga)Se_2$ thin-film solar cells using atom probe tomography.* (Seminar talk at Centre for Solar Energy and Hydrogen Research (ZSW), Stuttgart, Germany, 02 Dec. 2010).

Fabritius, H.; Nikolov, S.; Hild, S.; Ziegler, A.; Friák, M.; Neugebauer, J.; Raabe, D.: *Design principles of arthropod cuticle evaluated experimentally and by ab initio-based multiscale simulations.* (Ringberg Symp. 2010, Molecular Bionics - From Biomineralization to Functional Materials, Ringberg Castle, Tegernsee, Germany, 03 to 06 Oct. 2010).

Freysoldt, C.: *Fully ab initio finite-size corrections for electrostatic artifacts in charged-defect supercell calculations.* (Psi-k Conf. 2010, Berlin, Germany, 12 to 16 Sept. 2010).

Friák, M.; Zhu, L.-F.; Dick, A.; Hickel, T.; Neugebauer, J.: *First-principles study of the Ti–Fe eutectic system.* (Seminar talk at Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic, 24 Sept. 2010).

Gerstl, S.S.A.: *Instrumentation and software; Reconstruction; Data analyses; Case study of advanced materials.* (Atom Probe Tomography - Workshop Part 4, 52nd Int. Field Emission Symp., University of Sydney, Australia, 05 to 08 July 2010).

Kostka, A.; Springer, H.: *Fundamental research on the role of intermetallic phases in Al-Fe joints.* (Improving Performance and Productivity of Integral Structures through Fundamental Understanding of Metallurgical Reactions in Metallic Joints - VI-IPSUS Summer School, Hamburg, Germany, 30 Aug. to 03 Sept. 2010).

Krüger, T.: *Mesoscopic modeling of red blood cell dynamics.* (Seminar talk on Theory of Complex Systems, Institute for Theoretical Physics, University of Heidelberg, Germany, 16 Dec. 2010).

Mayrhofer, K.J.J.: *The particle-size effect in electrocatalysis.* (Seminar talk at National Institute of Chemistry, Ljubljana, Slovenia, 08 Apr. 2010).

Neugebauer, J.: *Stahldesign in der Wunderwelt der Quantenmechanik.* (Open Day, Stahlzentrum, Düsseldorf, Germany, 04 Sept. 2010).

Neugebauer, J.: *Ab initio based multiscale modeling of advanced electronic, structural and biological materials.* (Colloquium talk at Montan-Universiät Leoben, Austria, 13 Dec 2010).

Raabe, D.; Fabritius, H.; Nikolov, S.; Petrov, M.; Friák, M.; Elstnerová, P.; Neugebauer, J.: *Ab initio based multiscale modeling of biological composites: Example of the exoskeleton of the lobster Homarus americanus.* (Colloquium talk at Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität München, Germany, 09 Nov. 2010).

Raabe, D.; Roters, F.; Dmitrieva, O.; Dick, A.; Hickel, T.; Zaefferer, S.; Ponge, D.; Neugebauer, J.: *Crystal mechanics of the martensitic transformation: crystal plasticity, ab initio models, experiments.* (Colloquium talk at Institute for Mechanics, University of Dortmund, Germany, 18 Nov. 2010).

Raabe, D.; Li, Y.J.; Choi, P.; Dmitrieva, O.; Kirchheim, R.; Ponge, D.: *Towards the limits of strength: Design and understanding of ultra high strength steels.* (Colloquium talk at Ludwig-Maximilians-Universität München, Germany, 19 Nov 2010).

Sandlöbes, S.; Zaefferer, S.: *Effect of RE elements on the deformation and recrystallization behaviour of Magnesium.* (Rare Earth Elements in Magnesium Alloys - MagNET Workshop 5, Vancouver, Canada, 27 to 28 Oct. 2010).

Sandlöbes, S.; Senk, D.: *Automatisierung im Stahlwerk durch in-situ Ab- und Prozessgasmessung.* (8th Aachen Colloquium on Maintenance, Diagnosis and Monitoring System (AKIDA), Aachen, Germany, 17 to 18 Nov. 2010).

Stratmann, M.: *Intelligent corrosion protection by conducting polymer based nanocomposite coatings.* (Gesellschaft Deutscher Chemiker - GDCh Colloquium, Oldenburg, Germany, 25 Nov. 2010).

Todorova, M.: *Corrosion from first principles: A new approach to construct electrochemical E-pH diagrams.* (Crystallographic Colloquium at Ludwig-Maximilians-Universität München, Germany, 29 Oct. 2010).

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Auer, A.A.: *Mathematical methods in quantum chemistry.* (Workshop on Mathematical Methods in Quantum Chemistry, Mathematical Research Institute, Oberwolfach, Germany, 26 June to 02 July 2011).

Auinger, M.: *Theory and experiment for high temperature metal-gas reactions.* (Seminar talk at Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA, USA, 11 Nov. 2011).

Choi, P.: *Characterization of advanced functional and structural materials using atom probe tomography.* (Inauguration Symp. for the Atom Probe Facilities, Eidgenössische Technische Hochschule Zürich, Switzerland, 06 Dec. 2011).

Choi, P.: *Study of local chemical gradients in advanced precipitation hardened steel using atom probe tomography.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 01 to 05 Aug. 2011).

Cojocaru-Mirédin, O.; Choi, P.; Abou-Ras, D.; Würz, R.; Raabe, D.: *Characterization of CI(G)S thin-film solar cells using atom probe tomography.* (37th IEEE Photovoltaic Specialists Conf. (PVSC), Seattle, WA, USA, 19 to 24 June 2011).

Cojocaru-Mirédin, O.; Choi, P.; Würz, R.; Abou-Ras, D.; Raabe, D.: *Explorer les interfaces à l'échelle atomique dans les cellules photovoltaïques CIGSe.* (Seminar talk at Commissariat à l'Energie Atomique et aux Energies Alternatives, Grenoble, France, 05 Dec. 2011).

Eisenlohr, P.; Diehl, M.; Roters, F.; Lebensohn, R.A: *Solving finite-deformation crystal elasto-viscoplasticity with a fast Fourier transformation-based spectral method.* (The Minerals, Metals & Materials Society - TMS Annual Meeting, San Diego, CA, USA, 27 Feb. to 03 Mar. 2011).

Eisenlohr, P.; Tjahjanto, D.D.; Kords, C.; Roters, F.; Raabe, D.: *A modular crystal plasticity framework applicable from single grain to component scale.* (The Minerals, Metals & Materials Society - TMS Annual Meeting, San Diego, CA, USA, 27 Feb. to 03 Mar. 2011).

Eisenlohr, P.; Roters, F.; Kords, C.; Diehl, M.; Lebensohn, R.A.; Raabe, D.: *Combining characterization and simulation of grain-scale plasticity in three dimensions.* (Electron Back Scattering Diffraction - EBSD Conf. 2011 of the Royal Microscopical Society (RMS), Düsseldorf, Germany, 28 to 30 Mar. 2011).

Eisenlohr, P.; Amberger, D.: *Creep-resistant Mg-alloys - benefits of an intermetallic phase skeleton.* (Materials Engineering Seminar, University of Kassel, Germany, 11 July 2011).

Eisenlohr, P.; Tjahjanto, D.D.; Kords, C.; Roters, F.; Raabe, D.: *A modular crystal plasticity framework applicable from single grain to component scale.* (XI Int. Conf. Computational Plasticity, Barcelona, Spain, 07 to 09 Sept. 2011).

Erbe, A.: *Thin amorphous oxides and intermediates in chemical reactions: Challenging problems in interface science probed with photons.* (Mini-Workshop on Surface Science for Inauguration of the Turkish Surface Science Society, Ankara, Turkey, 23 May 2011).

Erbe, A.: *Oberflächendesign für empfindliche ATR-Spektroskopie in Modellexperimenten zum Verständnis der Korrosion.* (User meeting - Bruker Optics, Ettlingen, Germany, 22 Nov. 2011).

Fabritius, H.; Nikolov, S.; Hild, S.; Ziegler, A.; Friák, M.; Neugebauer, J.; Raabe, D.: *Mechanical design principles of crustacean cuticle evaluated experimentally and by ab initio-based multiscale simulations.* (Colloquium talk at Institut de Mécanique des Fluides et des Solides (IMFS), Centre national de la recherche scientifique - CNRS, Strasbourg, France, 17 Mar. 2011).

Fabritius, H.; Nikolov, S.; Hild, S.; Ziegler, A.; Friák, M.; Neugebauer, J.; Raabe; D.: *Design principles of crustacean cuticle: From molecules to skeletal elements.* (Workshop „From Nanoparticle Assembly to Functional Polymer Components", Department of Geo- and Environmental Sciences, Ludwig-Maximilians-Universität München, Germany, 08 July 2011).

Freysoldt, C.; Pfanner, G.; Neugebauer, J.: *The dangling-bond defect in amorphous silicon: Insights from theoretical calculations of the EPR parameters.* (Workshop "Advanced EPR for material and solar energy research", Berlin, Germany, 13 to 14 Oct. 2011).

Friák, M.; Zhu, L.-F.; Dick, A.; Udyansky, A.; von Pezold, J.; Emmerich, H.; Neugebauer, J.: *On selected methodological challenges at the interface between quantum-mechanical approaches and phase-field modeling methods in computational materials science*. (Spring Meeting of the German Physical Society (DPG), Dresden, Germany, 14 to 18 Mar. 2011).

Friák, M.; Nikolov, S.; Petrov, M.; Elstnerová, P.; Sachs, C.; Fabritius, H.; Ma, D. ; Lymperakis, L.; Hild, S.; Zigler, A.; Raabe, D.; Neugebauer, J.: *Ab initio based study of multi-scale elastic oproperties of hierarchical biocomposites*. (Multiscale Computational Biomechanics - CECAM Workshop, Zürich, Switzerland, 13 Apr. 2011).

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Gutierrez-Urrutia, I.; Dick, A.; Hickel, T.; Neugebauer, J.; Raabe, D.: *Understanding TWIP steel microstructures by using advanced electron microscopy and ab initio predictions.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 01 to 05 Aug. 2011).

Gutierrez-Urrutia, I.; Raabe, D.: *The influence of planar slip and deformation twinning on mechanical behavior in TWIP steels.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 01 to 05 Aug. 2011).

Gutierrez-Urrutia, I.; Raabe, D.: *Study of deformation twinning and planar slip in a TWIP steel by electron channelling contrast imaging in a SEM.* (Int. Conf. on the Textures of Materials - ICOTOM 16, Bombay, India, 12 to 17 Dec. 2011).

He, C.; Stein, F.; Palm, M.; Voß, S.: *Thermodynamic assessment of the Fe-Nb and Fe-Al-Nb system.* (3rd Sino-German Symp. on Computational Thermodynamics and Kinetics and their Applications to Solidification and Solid-State Phase Transformation, Xi'an/Shaanxi, China, 20 to 24 June 2011).

Hickel, T.; Körmann, F.; Grabowski, B.; Dick, A.; Neugebauer, J.: *First principles concepts to calculate thermodynamic properties of magnetic materials.* (Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Advanced Discussions, Ruhr-Universität Bochum, Germany, 10 to 11 Mar. 2011).

Hickel, T.; Grabowski, B.; Körmann, F.; Dick, A.; Neugebauer, J.: *Computational phase studies: Deriving free energies and phase transitions from first principles.* (Centre Européen de Calcul Atomique et Moléculaire - CECAM Workshop 442: Materials Informatics: Tools for Design and Discovery, Lausanne, Switzerland, 23 to 25 May 2011).

Hickel, T.; Grabowski, B.; Nazarov, R.; Sandschneider, N.; Neugebauer, J.: *Ab initio determination of point defects and derived diffusion properties in metals.* (3rd Sino-German Symp., Xi'an/Shaanxi, China, 20 to 25 June 2011).

Hickel, T.: *Ab-initio Modellierung von Stählen.* (Joint Colloquium of the SFB 761 and SFB 799 at Technische Universität Bergakademie, Freiberg, Germany, 05 Sept. 2011).

Hickel, T.; Ismer, L.; Nazarov, R.; von Pezold, J.; Friák, M.; Neugebauer, J.: *Ab initio investigation of hydrogen solubility and mobility in steels: Indentification of hydrogen related mechanisms in steels.* (Steel Hydrogen Conf., Gent, Belgium, 28 to 29 Sept. 2011).

Hickel, T.; Al-Zubi, A.; Neugebauer, J.: *Ab initio based prediction of phase diagrams: Application to magnetic shape-memory alloys.* (9th Materials Day at Ruhr-Universtät Bochum, Germany, 15 Nov. 2011).

Hickel, T.; Glensk, A.; Grabowski, B.; Neugebauer, J.: *Ab initio up to the melting point: Integrated approach to derive accurate thermodynamic data for Al alloys.* (European Aluminium Association, European Aluminium Technology Platform, Working Group 5: Predictive Modelling, 5th Workshop: Ab initio modelling, Aachen, Germany, 01 Dec. 2011).

Jia, N.; Raabe, D.; Zhao, X.: *Experiments and modeling on the development of deformation textures in f.c.c. materials.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 01 to 05 Aug. 2011).

Kords, C.; Eisenlohr, P.; Roters, F.; Raabe, D.: *Dislocation flux in three-dimensional crystal plasticity.* (9th Int. Conf. of Numerical Analysis and Applied Mathematics, Halkidiki, Greece, 18 to 25 Sept. 2011).

Kostka, A.; Song, J.; Raabe, D.; Veehmayer, M.: *Explosive cladding of Titanium to low carbon steel: Microstructure and properties.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 01 to 05 Aug. 2011).

Mayrhofer, K.J.J.: *IL-TEM for the investigation of nanoparticle corrosion.* (Seminar talk at Rheinische Friedrich-Wilhelms-Universität, Bonn, Germany, 14 Jan. 2011).

Mayrhofer, K.J.J.: *Degradation of carbon-supported fuel cell catalysts.* (Fundamentals and Developments of Fuel Cells - Conf. 2011, Grenoble, France, 19 to 21 Jan. 2011).

Mayrhofer, K.J.J.: *Elektrochemische Hochdurchsatzuntersuchungen mit gekoppelter online Analytik.* (4. Corrosion Protection Symp. - Corrosion protection by coatings in theory and practice, Trent, Rügen, 25 to 27 May 2011).

Mayrhofer, K.J.J.: *Electrocatalysis of PEM fuel cell reactions - Fundamental investigations for real applications.* (9th European Symp. on Electrochem. Engineering, Chania, Greece, 19 to 23 June 2011).

Mayrhofer, K.J.J.: *Catalysis in electrochemical reactors - Fundamental investigations for real applications.* (Seminar talk at Fritz-Haber-Institut of the Max Planck Society (MPG), Berlin, Germany, 22 Aug. 2011).

Mayrhofer, K.J.J.; Hartl, K.; Katsounaros, I.; Meier, J.C.; Hodnik, N.; Arenz, M.: *Activity and stability of Pt-alloy nanoparticles for fuel cell reactions.* (14. Austrian Chemistry Days, Linz, Austria, 26 to 29 Sept. 2011).

Mayrhofer, K.J.J.: *Online investigation of the stability of electrode materials by coupling of SFC-ICP-MS.* (Seminar talk at University of Ulm, Germany, 10 Dec. 2011).

Neugebauer, J.: *Ab initio based modeling of metallic alloys: From a predictive thermodynamic description to tailored mechanical properties.* (Colloquium talk at University of California-Santa Barbara, CA, USA, 23 Feb. 2011).

Neugebauer, J.: *Materials design based on ab initio thermodynamics: Development of accurate and efficient multiscale strategies.* (Spring Meeting of the German Physical Society (DPG), Dresden, Germany, 14 to 18 Mar. 2011).

Neugebauer, J.: *Fully ab initio description of point defect formation and properties at extreme temperatures.* (Materials Research Society - MRS Spring Meeting 2011, San Francisco, CA, USA, 25 to 29 Apr. 2011).

Neugebauer, J.: *Ab initio guided design of materials for photonic applications.* (Colloquium talk at Tyndall University, Cork, Ireland, 10 May 2011).

Neugebauer, J.: *Accuracy and limitations of ab initio approaches in predicting free energies for binaries and unstable phases.* (CALculation of PHAse Diagrams - CALPHAD Workshop, Rio de Janeiro, Brasil, 22 to 27 May 2011).

Neugebauer, J.: *Overview of fundamentals of first principle calculation methods.* (Workshop "From first principles to multi-scale modeling of materials", Pontifícia Universidade Católica do Rio de Janeiro, Department of Engineering Materials, Rio de Janeiro, Brasil, 27 May to 01 June 2011).

Neugebauer, J.: *Ab initio description of alloying effects on extended defects and interfaces.* (Alloying Element Effects on Migrating Interfaces - Alemi Workshop, Vancouver, Canada, 07 to 08 June 2011).

Neugebauer, J.: *Thermodynamic data from first principles: Achievements and challenges.* (Sino-German Symp., Xi'an/ Shaanxi, China, 20 to 24 June 2011).

Neugebauer, J.: *Ab initio thermodynamics: From catalytic surfaces to high-strength steels.* (Frontiers in InterfacE Science - Theory And Experiment Symp. - FIESTAE, Berlin, Germany, 29 June to 01 July 2011).

Neugebauer, J.: *Ab initio guided design of materials with superior mechanical properties.* (Colloquium talk at Institute of Technology, Karlsruhe, Germany, 12 July 2011).

Neugebauer, J.: *Ab initio guided materials characterization and design.* (Science Vision for the European Spallation Source (ESS), Bad Reichenhall, Germany, 10 to 12 Oct. 2011).

Neugebauer, J.: *Doping and growth issues in group-III nitrides: An ab initio perspective.* (Workshop on III-Nitrides Growth, Characterization and Simulation, Berlin, Germany, 12 to 13 Oct. 2011).

Neugebauer, J.: *Ab initio based modeling of structural materials with superior properties: From a predictive thermodynamic description to tailored mechanical properties.* (European Congress on Advanced Materials and Processes - EUROMAT 2011, Montpellier, France, 12 to 15 Sept. 2011).

Neugebauer, J.: *Fully ab initio determination of free energies: Methodological challenges and applications.* (Conf. on Computational Physics - CCP2011, Gatlinburg, TN, USA, 30 Oct. to 03 Nov. 2011).

Neugebauer, J.: *Fully ab initio determination of free energies: Achievments and challenges.* (Scientific Group Thermodata Europe - SGTE Workshop, Herzogenrath/Aachen, Germany, 05 to 06 Dec. 2011).

Palm, M.: *Hochleistungswerkstoffe auf Basis intermetallischer Phasen.* (Materials Forum Rhein-Main, Deutsche Gesellschaft für Materialkunde e.V. - DGM, Hanau, Germany, 14 Mar. 2011).

Palm, M.; Krieg, R.: *Neutral salt spray testing on Fe–Al and Fe–Al–X.* (FeAl2011, Discussion Meeting on the Development of Innovative Iron Aluminium Alloys, Lanzarote Canary Islands, Spain, 05 to 07 Oct. 2011).

Pérez-Prado, M.T.; Boehlert, C.; Llorca, J.; Gutiérrez-Urrutia, I.: *In-situ analysis of deformation and recrystallization mechanisms.* (European Congress on Advanced Materials and Processes - EUROMAT 2011, Montpellier, France, 25 to 29 Sept. 2011).

Ponge, D.; Millán, J.; Yuan, L.; Sandlöbes, S.; Kostka, A.; Choi, P.; Hickel, T.; Neugebauer, J.; Raabe, D.: *Nanostructuring of 100 thousand tons.* (Gesellschaft Deutscher Chemiker - GDCh Colloquium, Universität Duisburg-Essen, Essen, Germany, 30 Nov. 2011).

Raabe, D.: *Designing structural metallic materials by combining ab-initio models, atomic scale characterization, and synthesis.* (Colloquium talk at Physics Department, University of Mainz, Germany, 10 May 2011).

Raabe, D.; Ponge, D.: *Alloy design of nanoprecipitate-hardened high-Mn maraging-TRIP.* (The First Int. Conf. on High Manganese Steels, Seoul, South Korea, 15 to 18 May 2011).

Raabe, D.; Roters, F.; Zaefferer, S.; Zambaldi, C.; Demir, E.; Zaafarani, N.; Diehl, M.; Lebensohn, R.A.; Eisenlohr, P.: *Computational crystal plasticity.* (Colloquium talk at Korea Institute of Science and Technology (KIST), Seoul, South Korea, 16 May 2011).

Raabe, D.: *Atomistic understanding of hundred-thousand tons.* (Bernkastel-Kues Workshop "Possibilities and Limitations of Quantitative Materials Modeling and Characterization", Bernkastel-Kues, Germany, 30 May 2011).

Raabe, D.: *Moritaten aus dem Reich der Schmiede: Die Geschichte der Werkstoffe in 45 Minuten.* (Meeting Materials Testing 2011- New developments in materials testing, Berlin, Germany, 01 to 02 Dec. 2011).

Renner, F.U.: *Corrosion behaviour of Fe–Al(–X) alloys in steam.* (Deutsche Gesellschaft für Materialkunde - DGM, Technical Committee Meeting, Technische Universität Dresden, Germany, 08 Feb. 2011).

Renner, F.U.: *Oberflächen auf der atomaren Skala: Entlegierung als ein Beispiel aus der Korrosion.* (Colloquium talk at Technische Universität Hamburg-Harburg, Germany, 08 Sept. 2011).

Rohwerder, M.: *Controlling electronic and ionic mobility in coatings and at interfaces: Novel materials concepts for corrosion protection.* (The Electrochemical Society - 219th ECS Meeting, Montreal, Canada, 01 to 06 May 2011).

Rohwerder, M.: *On the role of micro- and nanostructure of conducting polymers in composite coatings for intelligent corrosion protection.* (The Electrochemical Society - 219th ECS Meeting, Montreal, Canada, 01 to 06 May 2011).

Rohwerder, M.: *Korrosionsschutz durch intelligente release-Systeme.* (4th Corrosion Protection Symp., Rügen, Germany, 25 to 27 May 2011).

Rohwerder, M.: *High-resolution detection of hydrogen: The hydrogen electrode in the dry.* (Simpósio Brasileiro de Eletroquímica e Eletroanalítica - XVIII SIBEEE, Bento Gonçalves-RS, Brazil, 28 Sept. to 01 Oct. 2011).

Rohwerder, M.: *High-resolution detection of hydrogen: The hydrogen electrode in the dry.* (Gesellschaft Deutscher Chemiker - GDCh Colloquium, Greifswald, Germany, 11 Oct. 2011).

Rohwerder, M.: *Scanning Kelvin probe for hydrogen detection with high sensitivity and lateral resolution.* (Seminar talk at Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Dortmund, Germany, 01 Dec. 2011).

Roters, F.; Eisenlohr, P.; Tjahjanto, D.D.; Kords, C.; Raabe, D.: *A modular crystal plasticity framework applicable from component to single grain scale.* (Int. Union of Theoretical and Applied Mechanics - IUTAM Symp., Linking Scales in Computations: From Microstructure to Macro-scale Properties, Pensacola, FL, USA, 17 to 19 Mar. 2011).

Roters, F.; Tjahjanto, D.D.; C. Kords, C.; Eisenlohr, P.; Raabe, D.: *A modular crystal plasticity framework applicable from component to single grain scale.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 31 July 2011).

Sandlöbes, S.; Friák, M.; Dick, A.; Zaefferer, S.; Pei, Z.; Neugebauer, J.; Raabe, D.: *Combining ab initio calculations and high-resolution experiments to understand advanced Mg alloys.* (German-Korean Workshop on the "Production and industrial applications of semi-finished Mg products", Irsee, Germany, 02 to 09 Feb. 2011).

Sandlöbes, S.; Friák, M.; Dick, A.; Zaefferer, S.; Pei, Z.; Neugebauer, J.; Raabe, D.: *The effect of rare earth elements on the mechanical properties of Mg - Theory and experiment.* (Rare Earth Elements in Magnesium Alloys - MagNET Workshop 6, Hamilton, Canada, 07 to 08 Nov. 2011).

Spatschek, R.: *Kinetics of phase transitions.* (Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Advanced Discussions, Ruhr-Universität Bochum, Germany, 10 to 11 Mar. 2011).

Spatschek, R.: *Continuum modeling of metals at high temperatures.* (Seminar „Numerische Mathematik und Mechanik", Universität Duisburg-Essen, Essen, Germany, 12 Dec. 2011).

Stein, F.: *Fe–Al-based materials: Phase diagrams, properties, and potential for applications.* (Seminar talk at University of Vienna, Austria, 08 Apr. 2011).

Stein, F.: *Experimental determination of phase diagrams as a basis for materials development.* (Seminar talk at University of Nanning, Guangxi, China, 15 Nov. 2011).

Steinmetz, D.; Zaefferer, S.: *Currents state of the art in EBSD: Possibilities and limitations.* (Seminar talk at Ludwig-Maximilians-Universität München, Germany, 06 May 2011).

Stratmann, M.: *Coatings for corrosion protection: An overview of current issues.* (The Electrochemical Society - 220th ECS Meeting, Boston, MA, USA, 09 to 14 Oct 2011).

Todorova, M.: *Stability of polar ZnO(0001) surfaces in dry and humid atmosphere.* (The Thomas Young Centre - TYC Workshop ''Thermodynamics and kinetics of dopants, defects and adatoms at surfaces'', University College London, UK, 22 to 24 June 2011).

Todorova, M.: *Stabilisation of polar ZnO(0001) surfaces in dry and humid environment.* (Theory Seminar at Fritz-Haber-Institut of the Max Planck Society (MPG), Berlin, Germany, 08 Sept. 2011).

Todorova, M.: *Extending the concept of semiconductor defect chemistry to electro-chemistry: Constructing electrochemical E/pH diagrams based on ab-initio calculations.* (Workshop ''Modern developments in the ab initio description of charged systems for semiconductors and electrochemistry", Ringberg Castle, Tegernsee, Germany, 25 Oct. 2011).

von Pezold, J.: *Understanding embrittlement in metals: A multiscale study of the hydrogen enhanced local plasticity (HELP) mechanism.* (Seminar for Materials Research at Max-Planck-Institut für Plasmaforschung, Garching, Germany, 17 Feb. 2011).

Zaefferer, S.: *Diffraction techniques in the scanning electron microscope: Making SEM a universal tool for microstructure research*. (Spring Meeting of the German Physical Society (DPG), Dresden, Germany, 14 Mar 2011).

Zaefferer, S.: *Advanced applications of SEM-based diffraction techniques.* (Int. Union of Microbeam Analysis Societies - IUMAS Conf., Seoul, South Korea, 26 May 2011).

Zaefferer, S.: *Electron diffraction-based techniques in the SEM: Do they give you everything you ever wanted to know about your sample?* (14th Int. Conf. on Emergency Medicine - ICEM 2012, Wisła, Poland, 29 June 2011).

Zaefferer, S.; Jäpel, T.; Tasan, C.; Konijnenberg, P.: *Detailed observation of martensite transformation and twinning in TRIP and TWIP steels using advanced SEM diffraction techniques*. (Int. Conf. on Martensitic Transformations - ICOMAT 2011, Osaka, Japan, 07 Sept. 2011).

Zaefferer, S.: *Comprehensive 5-parameter grain boundary description: How to measure it, how to display it and how important is it?* (Int. Conf. on Martensitic Transformations - ICOTOM 16, Mumbai, India, 15 Nov. 2011).

Zheng, C.W.; Raabe, D.; Li, D.Z.: *Numerical simulation of dynamic strain-induced austenite-ferrite transformation and post-dynamic kinetics in a low carbon steel.* (Int. Conf. on Processing & Manufacturing of Advanced Materials - THERMEC 2011, Québec, Canada, 01 to 05 Aug. 2011).

Zhu, L.-F.; Friák, M.; Dick, A.; Hickel, T.; Neugebauer, J.: *Ab initio study of the Ti–Fe eutectic system.* (Erich-Schmid-Colloquium 2011, Erich Schmid Institute of Materials Science (ESI), Austrian Academy of Sciences, Leoben, Austria, 15 Feb. 2011).

2012

Albrecht, M.; Markurt, T.; Schulz, T.; Lymperakis, L.; Duff, A.; Neugebauer, J.; Drechsel, P.; Stauss, P.: *Dislocation mechanisms and strain relaxation in the growth of GaN on silicon substrates for solid state lighting* (Conf. on Extended Defects in Semiconductors - EDS 2012, Thessaloniki, Greece, 24 to 29 June 2012).

Auinger, M.: *Experimental studies and theoretical calculations on the formation of nitrides and oxides during selective oxidation in binary iron-alloys.* (8th Int. Symp. on High-Temperature Corrosion and Protection of Materials, Les Embiez, France, 20 to 25 May 2012).

Auinger, M.: *What do we know about internal oxidation in hot-rolled steels? - A theoretical study and its experimental verification.* (Seminar talk at Interdisciplinary Center for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany, 09 July 2012).

Auinger, M.: *Internal oxidation and nitridation of hot rolled steels - A theoretical study and its experimental verification.* (Gunnar Eriksson Symp. & GTT, The Single Source for Thermochemistry Tool - Workshop on Thermodynamic Simulations in Industry, Herzogenrath/Aachen, Germany, 11 to 13 July 2012).

Berezkin, A.V.; Biedermann, P.U.: *Multiscale simulation of PU coatings.* (Badische Anilin- & Soda-Fabrik - BASF Seminar, Ludwigshafen, Germany, 24 Apr. 2012).

Chen, Y.; Schneider, P.; Erbe, A.: *Investigation of electrochemical oxide growth on zinc by spectroscopic ellipsometry: An example of in operando spectroscopy.* (Int. Symp. on Electrochem. Micro & Nanosystem Technologies - EMNT 2012 - 9th Int. Symp. on Electrochem. Micro & Nanosystem Technologies, Linz, Austria, 15 to 17 Aug. 2012).

Choi, P.: *Overview of atom probe tomography research at MPIE.* (Material physics seminar at the University of Göttingen, Germany, 09 Feb. 2012).

Choi, P.: *Atom probe characterization of CIGS solar cells.* (Seminar talk at the University of Luxembourg, Luxembourg, 06 Mar. 2012).

Cojocaru-Mirédin, O.; Schwarz, T.; Choi, P.; Würz, R.; Raabe, D.: *Exploring the internal interfaces at the atomic-scale in thin-film solar cells.* (Seminar talk at Helmholtz Zentrum Berlin (HZB), Germany, 25 Mar. 2012).

Cojocaru-Mirédin, O.; Schwarz, T.; Choi, P.; Würz, R.; Abou-Ras, D.; Dietrich, J.; Raabe, D.: *Exploring the internal interfaces at the atomic-scale in Cu(In,Ga)Se_2 thin-films solar cells.* (1st EU APT Workshop, CEA/MINATEC, Grenoble, France, 04 to 05 Oct. 2012).

Dehm, G.: *In situ micro-mechanical testing at variable temperatures* (12th European Nanomechanical User Group Meeting, University of Malta, 24-25 Oct. 2012).

Dehm, G.: *Prospects and experimental constraints of nano/micro-mechanical testing in materials science* (GDRiCNRS-Mecano General Meeting, Ecole des Mines, Paris, France, 30-31 Oct. 2012).

Dehm, G.; Imrich, P.J.; Kirchlechner, C.; Smolka, M.; Yang, B.; Motz, C.: *In situ micro- and nanomechanical electron microscopy studies of grain boundaries in Cu*. (MRS Fall Meeting 2012, Boston, MA, USA, 25-30 Nov. 2012).

Eisenlohr, P.: *Modeling and simulation of crystal plasticity.* (Chemical Engineering and Materials Science Seminar, Michigan State University, East Lansing, MI, USA, 04 Oct. 2012).

Erbe, A.: *Native and electrochemically grown oxides on metals: The dark side of semiconductor research.* (School for Contacts in Nanosystems Spring Workshop 2012, Niedersächsische Technische Hochschule, Goslar, Germany, 11 May 2012).

Fabritius, H.: *Biologische Verbundwerkstoffe: Korrelation von Struktur, Zusammensetzung und physikalischen Eigenschaften am Beispiel der Arthropodenkutikula.* (Inorganic Chemistry Colloquium, Faculty of Chemistry, Universität Duisburg-Essen, Duisburg, Germany, 17 Apr. 2012).

Friák, M.; Hickel, T.; von Pezold, J.; Zhu, L.-F.; Dick, A.; Counts, W.A.; Sandlöbes, S.; Udyansky, A.; Zaefferer, S.; Roters, F.; Ma, D.; Pei, Z.; Raabe, D.; Holec, D.; Šob, M.; Neugebauer, J.: *Combining ab initio modeling and advanced experimental techniques within multi-scale approaches to materials properties.* (Seminar Talk at Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic, 24 May 2012).

Friák, M.; Hickel, T.; Abbasi, A.; von Pezold, J.; Zhu, L.-F.; Dick, A.; Sandlöbes, S.; Udyansky, A.; Zaefferer, S.; Ma, D.; Pei, Z.; Raabe, D.; Neugebauer, J.: *Ab initio approaches to stacking fault energy calculations in Mg–Y alloys*. (National Institute for Materials Science - NIMS 2012 Conf., Tsukuba, Japan, 04 to 06 June 2012).

Friák, M.; Ma, D.; Elstnerová, P.; Neugebauer, J.; Raabe, D.; Schindlmayr, A.; Scheffler M.; Šob, M.: *Ab initio study of epitaxy-induced stressed states*. (European Congress on Computational Methods in Applied Sciences and Engineering - ECCOMAS 2012, Vienna, Austria, 10 to 14 Sept. 2012).

Grabowski, B.: *Ab initio prediction of materials properties up to the melting point.* (Seminar series “Condensed Matter and Materials Division”, Lawrence Livermore National Lab, Livermore, CA, USA, 01 Feb. 2012).

Grabowski, B.: *Ab initio prediction of materials properties up to the melting point.* (Seminar “Ab initio Description of Iron and Steel: Thermodynamics and Kinetics”, Ringberg Castle, Tegernsee, Germany, 29 Apr. to 04 May 2012).

Grabowski, B.; Tasan, C.: *SMARTMET project: Towards breaking the inverse ductility-strength relation.* (ThermoCalc Software Workshop, Aachen, Germany, 06 Sept. 2012).

Hafez Haghighat, S.M.; Schäublin, R.: *Atomistic simulation and transmission electron microscopy of obstacle strengthening in iron.* (Seminar talk at Sahand University of Technology, Tabriz, Iran, 01 May 2012).

Hafez Haghighat, S.M.; Eggeler, G.; Raabe, D.: *Dislocation dynamics simulation: methodology and applications.* (Seminar talk at Sahand University of Technology, Tabriz, Iran, 12 May 2012).

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Doctoral Theses

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Dr.rer.nat. A. Laaboudi: Sauerstoffreduktion auf Thiol-modifizierten Au(111)-Oberflächen (Ruhr-Universität Bochum)

Dr.-Ing. Ö. Özlem: Synthesis, characterisation and functionalisation of ZnO nanorods on metals (Ruhr-Universität Bochum)

2011

Dr.-Ing. G.N. Ankah: Investigations of the selective dissolution of $Cu_3Au(111)$: *In-situ* and *ex-situ* Characterization (Ruhr-Universität Bochum)

Dr.phil. B. Britton: Measurement of residual elastic strain and lattice rotations with high resolution electron backscatter diffraction (Oxford University, UK)

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J. Lu: Correlation of microstructure, composition and mechanical properties to function in the mandibles of arthropoda (RWTH Aachen)

E. Plancher: Strain measurement by high resolution EBSD (Ecole des mines de Saint-Etienne/EDF, France)

R. Seeger: Analysis of the subsurface microstructure of metal/metal hip joints by means of TEM and atom probe tomography (University of Duisburg-Essen, Duisburg)

Y. Wang: Comparative study of deformation and recrystallization mechanisms of $Mg_{97}Zn_1Y_2$ and MgY_3 at elevated temperatures (RWTH Aachen)

2012

N. Buller: Untersuchung der elektrochemischen reduktiven Desorption von Thiolen auf Goldelektroden mit spektroskopischer Ellipsometrie (Carl von Ossietzky Universität Oldenburg)

D. Hessling: Probing the interaction of grain boundaries and dislocation slip by nanoindentation (FH Düsseldorf)

D. Korbmacher: Dual scale modeling of hydrogen embrittlement (Ruhr-Universität Bochum)

M. Kuzmina: Study of equilibrium segregation of Mn and reversion of austenite in tempered medium manganese steels and its influence on impact toughness (RWTH Aachen)

A. Monas: Modeling of phase change materials for nonvolatile data storage using GPU simulations (Ruhr-Universität Bochum)

S. Qin: Experimental investigation on the relationship of grain boundary character and local carbon partitioning in a quench-and-partitioning (QP) steel (RWTH Aachen)

N. Tillack: Chemical Trends in the yttrium-oxide precipitates in oxide dispersion strengthened steels: A first-principles investigation (Ruhr-Universität Bochum)

M. Wang: Strain hardening behavior of high-Mn steels (RWTH Aachen)

J. Wang: Austenite reversion in 0.45C-13.5Cr martensitic stainless steels: Influence of Mn concentration and tempering conditions on the evolution of microstructure and mechanical properties (RWTH Aachen)

D. Yan: Determination of mechanical values and flow curves of high strength steels for automotive seat parts after painting process (RWTH Aachen)

J. Zhang: An approach to measure residual stress in TWIP steels using nanoindentation (RWTH Aachen)

Bachelor Thesis

2011

D. Korbmacher: Entwicklung von Kontinuumsmodellen zur Wasserstoffversprödung an Rissen (Ruhr-Universität Bochum)

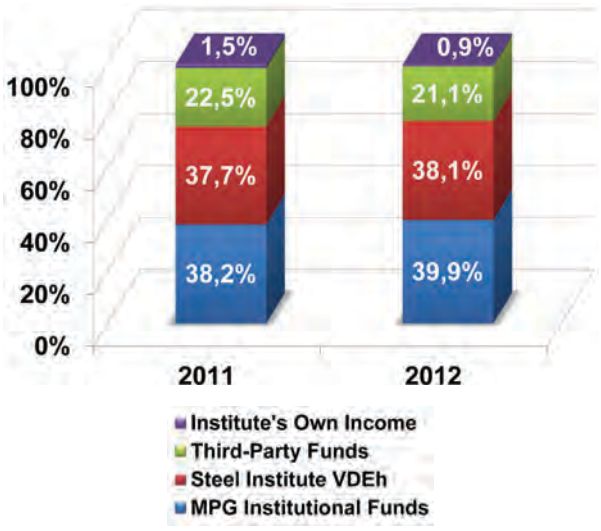
2012

F. Twiste: Untersuchung von Schmelzprozessen entlang von Korngrenzen mittels Greensfunktionsmethoden (Heinrich-Heine-Universität Düsseldorf)

Budget of the Institute

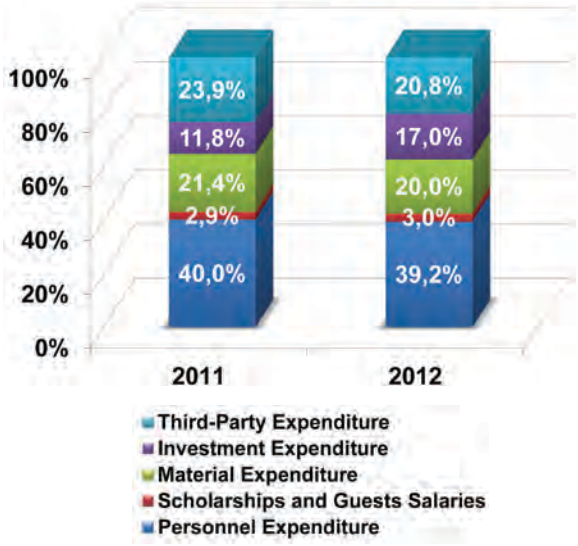
Revenue

(percentual contributions to total revenue without appointment-related investment funds and general reconstruction of the buildings; year 2012 data estimated)



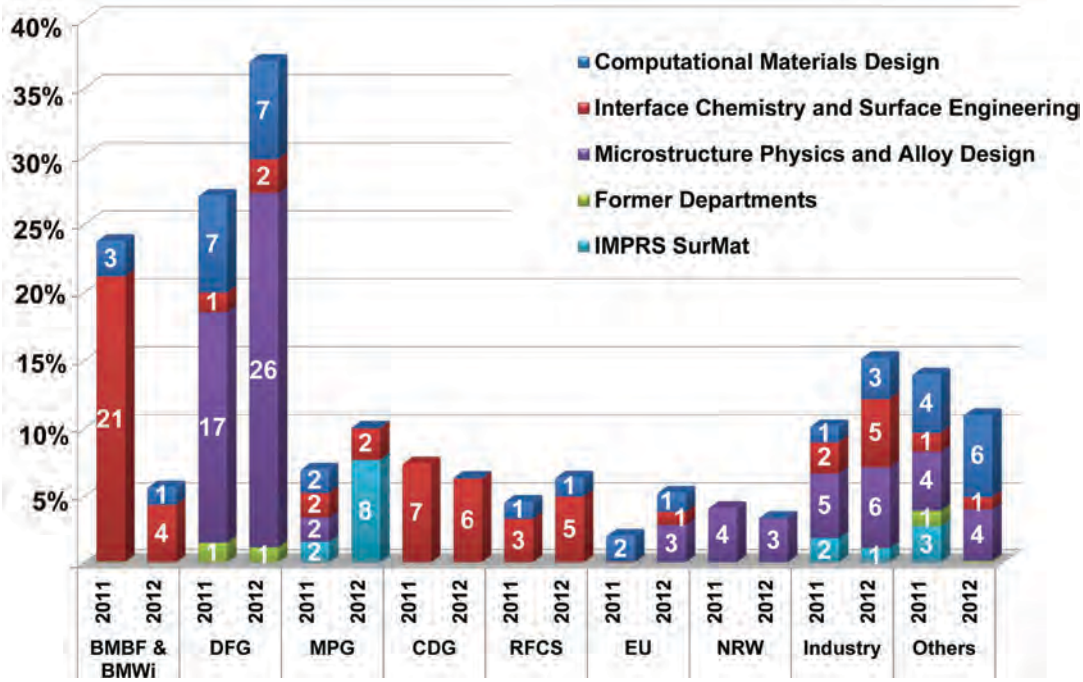
Expenditure

(percentual distribution of total expenditure; investments include large-scale apparatus, electronic data processing, appointment-related investments, separate investment for basic equipment; year 2012 data estimated)



Third-Party Funds

(percentual contributions to total revenue including personnel, materials, investments; year 2012 data estimated)



numbers are rounded percentage values

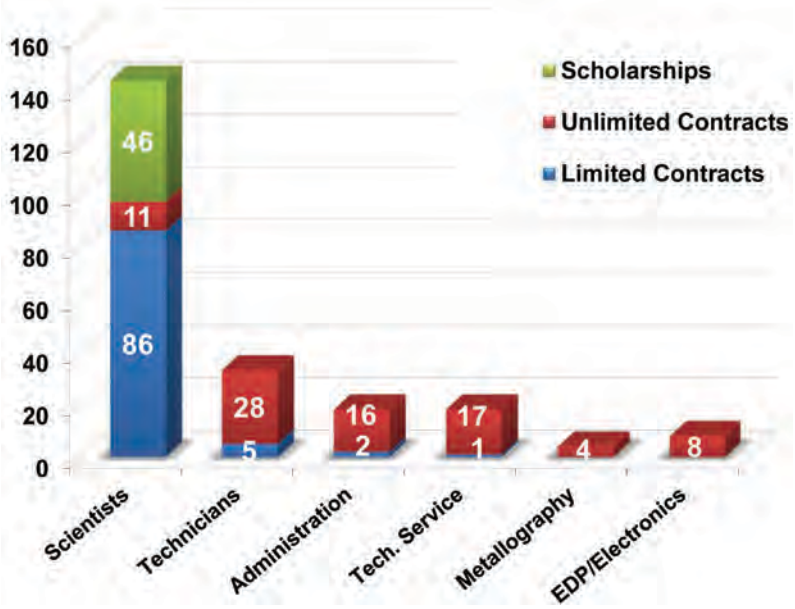
Former Departments:
Department of Materials Technology, Prof. G. Frommeyer, until Dec. 2008, and Department of Material Diagnostics and Steel Technology, Prof. A. Pyzalla, until Sep. 2008

BMBF: Federal Ministry of Science and Education
BMWi: Federal Ministry of Economics and Technology
DFG: German Science Foundation
MPG: Max Planck Society
CDG: Christian Doppler Society
RFCS: Research Fund for Coal and Steel
EU: European Union
NRW: State of North Rhine-Westphalia

Personnel Structure

Number of Occupied Scientific / Non-Scientific Positions

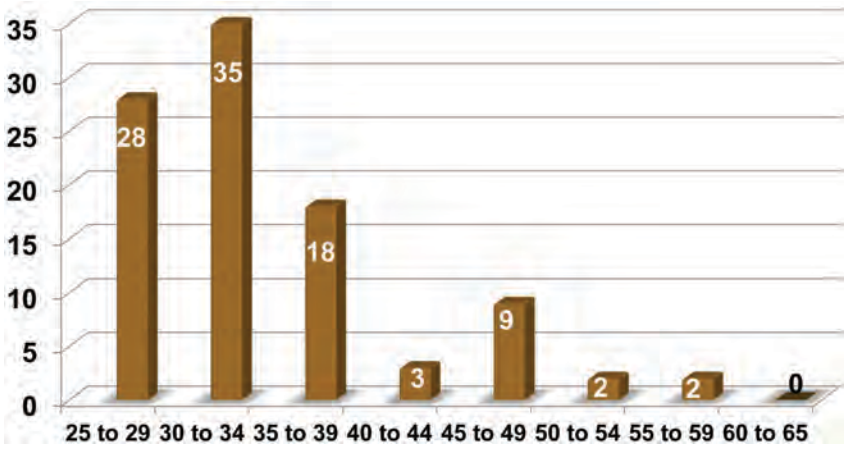
(Oct. 2012)



Additionally there were employed 15 interns and apprentices and 15 student research assistants.

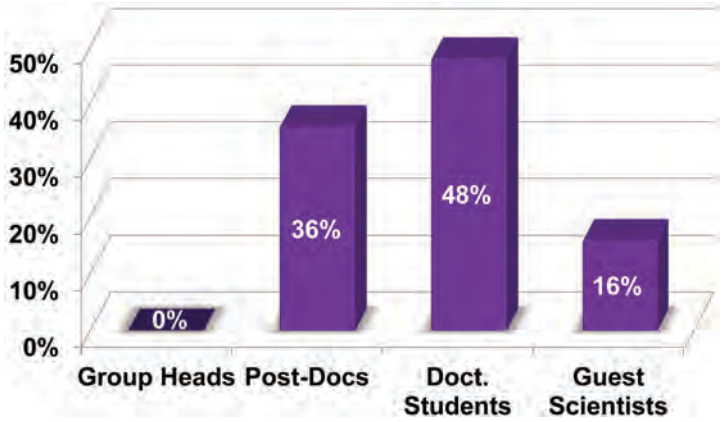
Age Distribution of Scientists

(Oct. 2012)



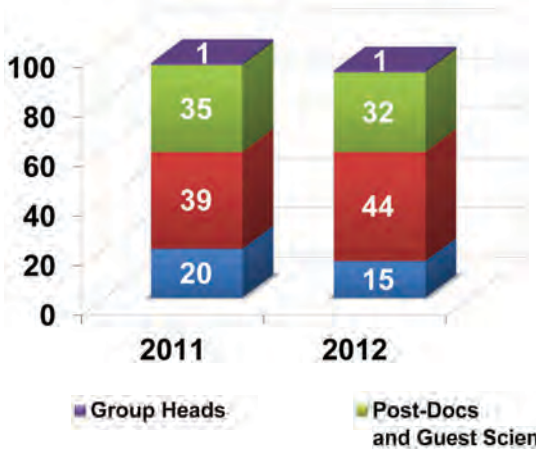
Female Scientists

(Oct. 2012, percentual numbers)

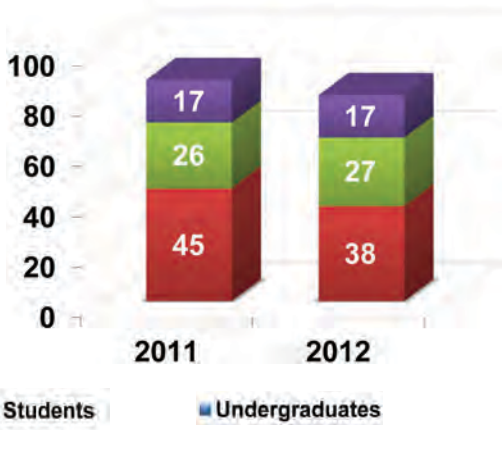


Number of Junior Scientists (year 2012 data estimated)

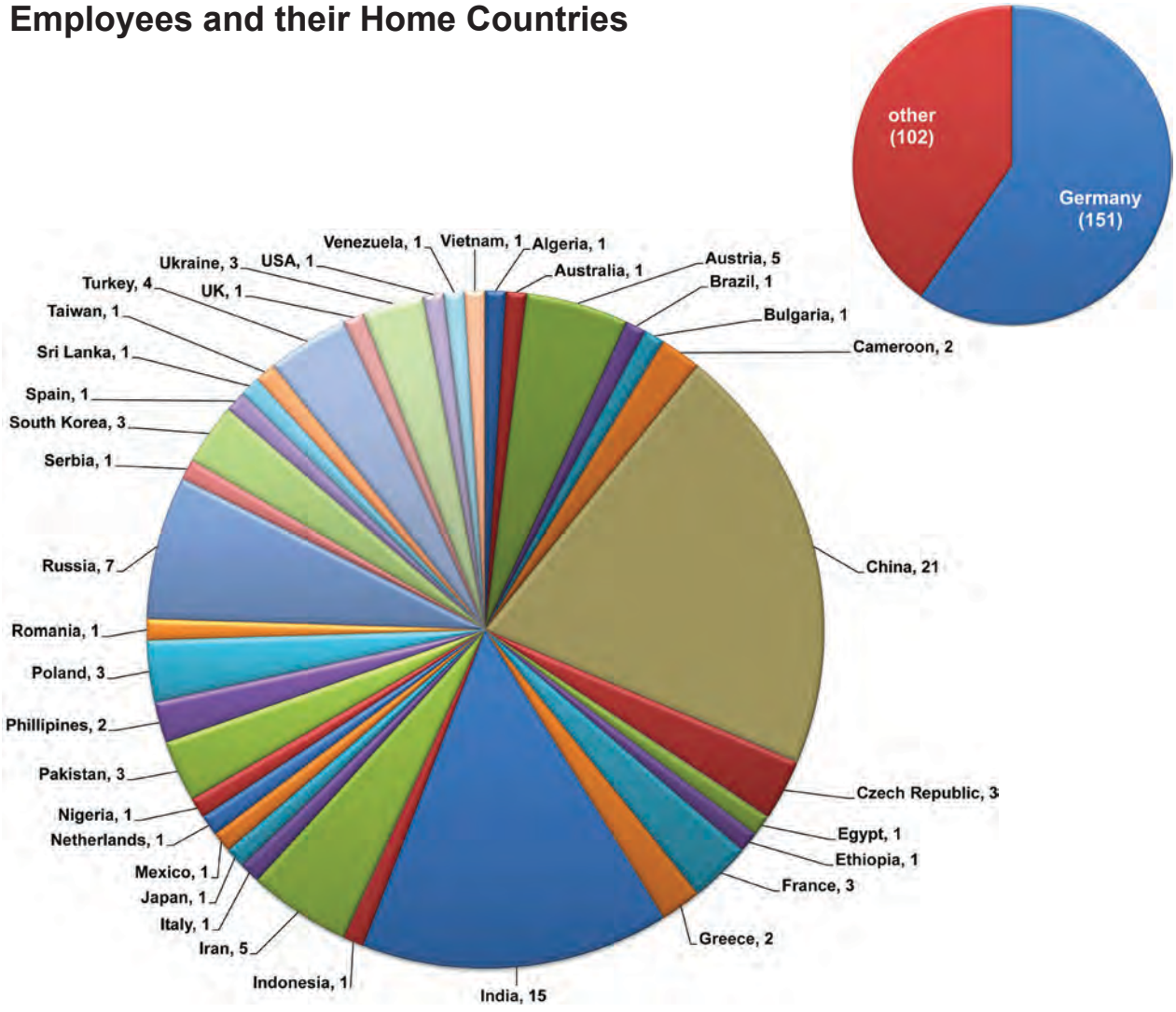
Financed via Third-Party Funds



Not Financed via Third-Party Funds



Employees and their Home Countries



The Institute in Public

Y. Ahmed Salem

Public Relations

During the last two years the importance of public relations (PR) was enforced at the MPIE by the appointment of a press officer in April 2011. In the following, some major events and activities at the MPIE are described briefly.

The MPIE in the Media

The number of published print and online articles about the MPIE could be more than tripled. This is not only due to the increased amount of published press releases but also to the creation of new mailing lists and a better internal communication which guarantees that important news are transported through the press officer to the public. In the following some important publications are named:

Fig. 1: *Amount of published print and online articles about the MPIE.*

- Rheinische Post: *"Humboldt-Stipendiaten zieht es nach Düsseldorf"*, 10 Aug. 2011
- Wirtschaftszeitung Aktiv: *"Stahl - was unsere Welt zusammenhält"*, 10 Sep. 2011
- Zeit: *"Auf höchstem Niveau"*, 13 Oct. 2011
- Westdeutsche Zeitung: *"Holländische Schüler im Max-Planck-Institut"*, 13 Oct. 2011
- Westdeutsche Zeitung: *"Eine Million Euro für das Max-Planck-Institut"*, 25 Oct. 2011
- Stahlmarkt: *"Düsseldorfer Stahlforscher überzeugten Worldsteel-Direktor"*, 01 Jan. 2011
- Stahl und Eisen: *"Computergestütztes Materialdesign optimiert Hüftimplantate"*, Volume 131, No. 11, 2011
- Umformtechnik: *"Metallforscher aus Düsseldorf und Japan kooperieren"*, Volume 4, 2011
- Max-Planck-Forschung: *"Die Rezeptur der Hummerschale"*, Volume 4, 2011
- Autocad-Magazin: *"Materialforschung: Superlegierungen für Triebwerke und die Energieversorgung von morgen"*, 07 Dec. 2011
- Maschinen Markt: *"Hochleistungsstähle erlauben Herstellung komplizierter Bauteile"*, 19 Dec. 2011
- Konstruktion und Entwicklung: *"Die Eigenschaftenvorhersager"*, Volume 01-02, 2012
- Innovationsreport: *"Intelligent corrosion protection"*, 03 May 2012
- Welt Kompakt: *"1,3 Millionen Euro für Forschung an Solarzellen"*, 01 June 2012
- Rheinische Post: *"Max-Planck-Preis für Fritz Körmann"*, 18 June 2012
- Süddeutsche Zeitung: *"Stahl aus dem Computer"*, 28 June 2012
- Stern.de: *"Stahl für übermorgen"*, 13 July 2012
- Stahl und Eisen: *"Stahl nach Maß - MPI-Wissenschaftler beim Ideenpark in Essen"*, Volume 132, No. 9, 2012

Promotion of Young Scientists

As the promotion of young scientists in the field of material sciences, physics and chemistry gets more and more important, the PR established new cooperations with neighbouring schools. Lab tours are offered for the pupils, as well as the possibility to do an internship in one of the scientific groups or in the apprenticeship working stations. The institute was not only frequently visited by pupils but also by students, often from abroad. In 2012 students of chemistry, applied physics, metallurgy and material sciences from the Universities of Leiden and Delft (The Netherlands), from the Western Australian School of Mines (Australia) and from the University of Leoben (Austria) paid a visit to the institute. They were especially interested in experiencing how an international research institute works and in getting into contact with scientists in the field of modern material sciences.

Additionally, the MPIE took part at the "Science Days 2012" of the Theodor Fliedner Gymnasium on March 1rst and 2nd. During these days, one of the MPIE scientists, Dr. Sebastian Klemm, presented his work to pupils of different ages in the school. The MPIE also presented its work about TiNb- alloys for hip replacement at the "Highlights der Physik" in Rostock from September 26th to October 2nd. This event is promoted by the Federal Ministry of Education and Research and the German Society of Physics (Deutsche Physikalische Gesellschaft) and aims at explaining physics to a broad public.

Fig. 2: *Scientists of the MPIE and the RWTH Aachen explained how computer simulations work at the ThyssenKrupp Ideenpark 2012.*

On November 11th 2011 the institute opened its doors for pupils during the Max Planck Day. This day is announced by the Max Planck Society and is dedicated to pupils of different ages. Pupils have the chance to get in touch with the nature of science and experience science by themselves. In the second half of August 2012 the institute was also a partner of the ThyssenKrupp Ideenpark in Essen, a technical fair for young and old. There, the department of Prof. Jörg Neugebauer together with the RWTH Aachen presented the collaborative research centre 761 "Stahl *ab initio*" and showed how computer simulations help to develop new steels.

VIP Visits

The institute had several VIP visits during the last two years. The North Rhine Westphalian state secretary Franz-Joseph Lersch-Mense visited the MPIE on June 15th 2011. He was fascinated by the work done at the institute and its unique structure as a public private partnership. Besides a lab tour where scientists of the MPIE explained their work, Lersch-Mense, Prof. Jörg Neugebauer, head of the department Computational Materials Design, Jürgen Kerkhoff, president of the Steel Institute VDEh and his vize-president Dr. Peter Dahlmann discussed the importance of Düsseldorf as a centre for research and talked about the diverse German research landscape.

Dr. Edwin Basson, CEO of the World Steel Organisation, paid a visit to the institute on September 20th 2011. Prof. Martin Stratmann, head of the department Interface Chemistry and Surface Engineering, explained how basic research in material sciences helps to develop new materials for the areas mobility, infrastructure and energy. Basson was impressed by the modern techniques used at the institute such as the three dimensional atom probe and the ultrahigh vacuum cluster.

On January 11th 2012, Thomas Jarzombek, member of the German Bundestag on behalf of the Christian Democratic Party (CDU), visited the MPIE on invitation of Prof. Stratmann. He was especially interested in the work of Dr. Karl Mayrhofer, head of the group Electrocatalysis. Mayrhofer got for his research project "ECCO$_2$ - combinatorial electrocatalytic CO$_2$ reduction" a funding of about one million euro from the Federal Ministry of Education and Research (BMBF). Jarzombek heard about this funding through a press release published by the MPIE.

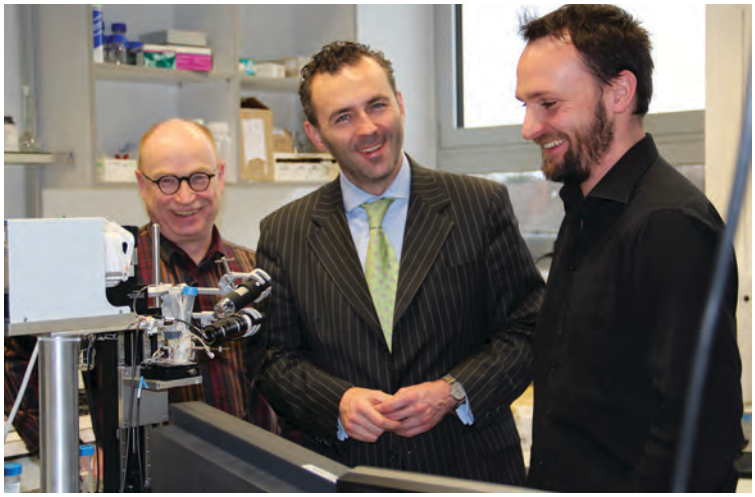
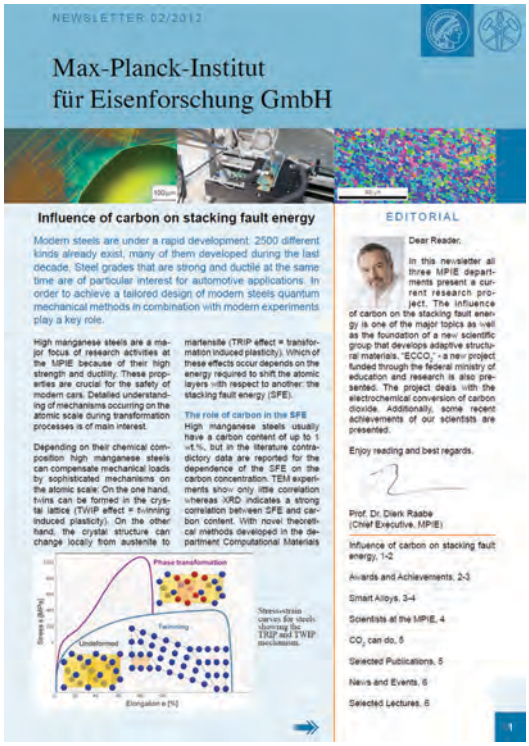


Fig. 3: *Dr. Karl Mayrhofer (right) and Prof. Martin Stratmann (left) explain to Thomas Jarzombek, member of the German Bundestag, how combinatorial electrocatalytic CO$_2$ reduction works.*

Newly Launched Newsletter

Since the beginning of 2012 the PR publishes a newsletter which appears twice a year and provides information about recent developments at the institute, addressing main research achievements, technological breakthroughs and new instrumentation. The newsletter intends to build a bridge between basic science and application. Additionally, the team that stands behind the work is presented.


NEWSLETTER 02/2012

Max-Planck-Institut für Eisenforschung GmbH

Influence of carbon on stacking fault energy

EDITORIAL

Fig. 4: *The newsletter of the MPIE appears twice a year and informs about recent research projects and the scientists behind the work.*

Research Presented in Multimedial Gateways

The PR of the MPIE engages in the Max Planck Science Gallery and the Max Planck Science Tunnel. These multimedial gateways into the world of modern research were recently established by the Max Planck Society and present, under regularly changing topics, many research projects of the Max Planck institutes. While the Science Gallery is installed in Berlin, the Science Tunnel is a mobile exhibition that started in 2012 in Paderborn and will travel e.g. through Russia, China and Brazil. The MPIE is represented through several

topics in these exhibitions. In the Science Gallery the topics multiscale simulations, corrosion, lightweight design and modern techniques of analysing materials are addressed. The last mentioned topic was also used for the Science Tunnel. There, a special focus lies on the three dimensional atom probe tomography and on up to date electron microscopy.

Fig. 5: *The ultrahigh vacuum cluster - a modern technique for analysing the surface of materials - is one of the topics presented at the Max Planck Science Gallery.*