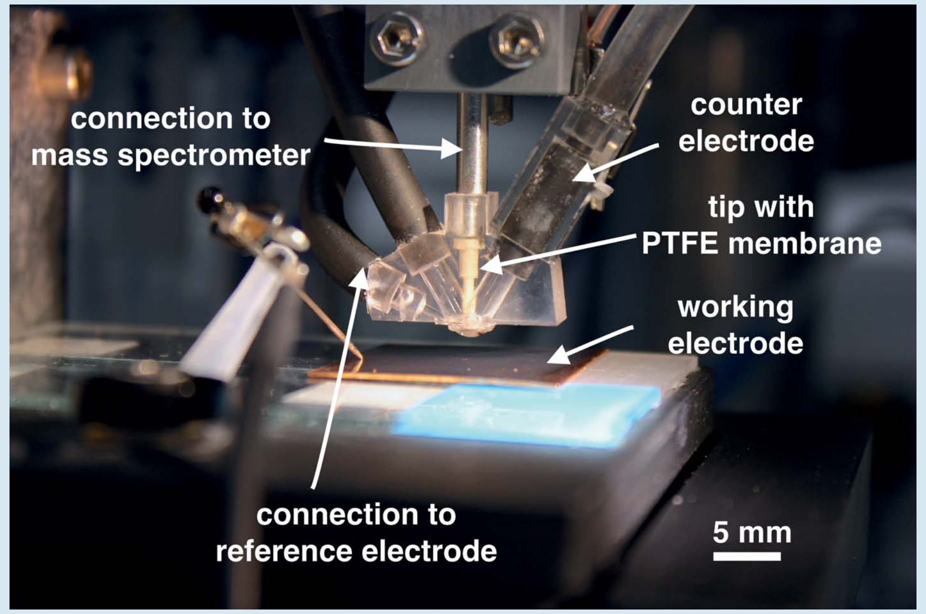
Scientists at the MPIE

Dr. Karl Mayrhofer is head of the group 'Electrocatalysis' within the department of 'Interface Chemistry and Surface Engineering' at the MPIE since 2010. At the same time he also teaches advanced methods in electroanalytical chemistry at the Ruhr University Bochum (Germany).

Before joining the MPIE, Dr. Mayrhofer worked as a postdoc on size-selected clusters as catalysts for fuel cell reactions at the Technical University of Munich. He pursued his PhD studies at the University of Vienna and the Lawrence Berkeley National Laboratory which is affiliated to the United States Department of Energy and located in Berkeley, California. In his thesis he analysed the oxygen reduction and carbon monoxide oxidation on platinum. Thereby he considered model as well as real systems for fuel cell electrocatalysts.

Karl Mayrhofer is especially renowned for his works on fuel cell and electrolysis technology and has been honoured with multiple science awards such as the "Science Award Electrochemistry 2013" which is sponsored by Volkswagen and BASF or the "Innovationspreis NRW 2012", an award of the state North Rhine Westphalia for innovative research, each endowed with 50.000€. His latest award is the "Dechema Preis 2014", an international award for excellent research in technical chemistry, engineering and biotechnology of the Max Buchner Society.

Current research projects with scientific and industrial partners are for example on new materials for water electrolysis – a project together with the Max Planck Institute for Chemical Energy Conversion (grant sum: 4 Mio € in total). Another project is on structure-degradation relationships for electrocatalysts. This project will last till 2017 and has a grant sum of 240.000 €.



Coupling of an electrochemical scanning flow cell (SFC) to an online electrochemical mass spectrometer (OLEMS). A tip (white part) is introduced from the top of the cell and a PTFE membrane (20 nm pore size) is placed at its bottom. When the cell is approached to the working electrode, the distance between membrane and electrode is only 50-100 µm. Volatile products evolving on the electrode evaporate through the membrane and are analysed time respectively potential/current resolved by the mass spectrometer.
Photo: J. P. Grote

Selected Publications

Computational Materials Design:

T. Hickel, R. Nazarov, E.J. McEniry, G. Leyson, B. Grabowski, J. Neugebauer: *Ab Initio Based Understanding of the Segregation and Diffusion Mechanisms of Hydrogen in Steels*. JOM, 66, 8, 1399-1405 (2014)

F. Körmann, B. Grabowski, B. Dutta, T. Hickel, L. Mauger, B. Fultz, J. Neugebauer: *Temperature Dependent Magnon-Phonon Coupling in bcc Fe from Theory and Experiment*. Phys. Rev. Lett., 113, 165503 (2014)

Interface Chemistry and Surface Engineering:

D. Iqbal, J. Rechmann, A. Sarfraz, A. Altin, G. Genchev, A. Erbe: *Synthesis of ultrathin poly(methyl methacrylate) model coatings bound via organosilanes to zinc and investigation of their delamination kinetics*. ACS Applied Materials and Interfaces, 6, 18112-18121 (2014)

S. Raman, T. Utzig, T. Baimpos, B.R. Shrestha, M. Valtiner: *Deciphering the scaling of single-molecule interactions using Jarzynski's equality*. Nature Communication, 5, 5539 (2014)

Microstructure Physics and Alloy Design:

W. Guo, E. A. Jägle, P.-P. Choi, J. Yao, A. Kostka, J. M. Schneider, D. Raabe: *Shear-Induced Mixing Governs Codeformation of Crystalline-Amorphous Nanolaminates*. Phys. Rev. Lett., 113, 035501 (2014)

Y.H. Wen, H.B. Peng, D. Raabe, I. Gutierrez-Urrutia, J. Chen, Y.Y. Du: *Large recovery strain in Fe-Mn-Si-based shape memory steels obtained by engineering annealing twin boundaries*. Nature Communications, 5, 4964 (2014)

Structure and Nano-/Micromechanics of Materials:

P. Imrich, C. Kirchlechner, C. Motz, G. Dehm: *Differences in deformation behavior of bicrystalline Cu micropillars containing a twin boundary or a large-angle grain boundary*. Act. Mat., 73, 240–250 (2014)

S. Brinckmann, B. Völker, G. Dehm: *Crack deflection in multi-layer four-point bending samples*. Int. Jour. of Fract., 190, 167–176 (2014)

Selected Talks

Computational Materials Design:

J. Neugebauer: *Materials design based on predictive ab initio thermodynamics*. CMD25 JMC, Paris, France, 24 - 29 Aug 2014

J. Neugebauer: *Identifying H induced failure mechanisms in structural materials: A multiscale approach*. MRS Fall Meeting, Boston, USA, 30 Nov - 5 Dec 2014

Interface Chemistry and Surface Engineering:

A. Erbe: *Introduction to Metallurgical Joining*. 6th International Conference on Tribology in Manufacturing Processes & Joining by Plastic Deformation. Darmstadt, Germany, 23 Jun 2014

S. Raman, T. Utzig, H.-W. Cheng, T. Baimpos, B.R.Shrestha, M. Valtiner: *AFM and SFA – two complementary techniques: Recent advances and exciting synergies*. Surface Forces Apparatus Conference. Cancún, Mexico, 24 – 29 Aug 2014

Microstructure Physics and Alloy Design:

D. Raabe, M. Herbig, Y. Li, L. Morsdorf, S. Goto, P. Choi, R. Kirchheim: *Bulk Nanostructured Steels*. Institute of Materials (IMX), Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne , Switzerland, 17 Nov 2014

D. Raabe, C. Tasan, M. Diehl, D. Yan, C. Zambaldi, M. Koyama, P. Shanthraj, F. Roters: *Experimental and simulation analysis of dual phase steel micromechanics*. Department of Engineering and Materials, Oxford University, United Kingdom, 10 Nov 2014

Structure and Nano-/Micromechanics of Materials:

C. Kirchlechner: *From Idealized Single Crystals Towards Applied Polycrystals: Insights into Plastic Deformation Provided by X-Ray µLaue Diffraction*. Gordon Research Conference - Thin Film & Small Scale Mechanical Behavior, Waltham, USA, 13 - 18 Jul 2014

G. Dehm: *Differences in deformation behavior of Cu structures containing individual grain boundaries*. MRS Fall Meeting, Boston, USA, 30 Nov – 5 Dec 2014

News and Events

Past Events

May – September 2014: MS Wissenschaft – a mobile Science Fair

The MPIE presented its computer simulations on suitable alloys for improved hip implants during the science fair "MS Wissenschaft" – an altered cargo ship which cruised through Germany and Austria and attracted about 90 000 visitors.

25 June 2014: Workshop on Tribology and Wear

The workshop covered various aspects of tribology and wear such as the high-resolution friction force microscopy of metallic surfaces, combinatorial metallurgy for rapid maturation of high performance alloys and the stability and failure of frictional interfaces. The workshop belongs to a series of one-day meetings at the MPIE.

30 June – 2 July 2014: Macan Meeting on Metal-Oxide Systems

The topic of this meeting was the merging of atomistic and continuum analysis of nanometer length-scale metal-oxide systems for energy and catalysis applications.

27 – 28 January 2015: Workshop on Hydrogen Embrittlement and Sour Gas Corrosion

This workshop covered a broad variety of topics concerning hydrogen embrittlement and sour gas corrosion in oil and gas industry, with a focus on corrosion resistant alloys. Presented talks were for example about hydrogen flux, sulphide stress cracking and spatially resolved measurement of hydrogen uptake during corrosion.

Upcoming Events

14 April 2015: KopfSalat

"KopfSalat" is a new regular event taking place at the MPIE and addressing a broad public interested in science. The institute invites twice a year a leading expert to give a presentation about their recent research. The next "KopfSalat" will take place on 14 April where Prof. Hans Hatt, University of Bochum, will give an insight about his research on smelling and tasting.
http://kopfsalat.mpie.de

21 – 24 June 2015: Workshop on Grain Boundary Migration - Theory meets Experiment

The general scope of this international workshop is to bring together the worldwide leading experts in the field of grain boundary migration. The workshop will cover various aspects of grain boundary physics from a theoretical and experimental perspective: structure, energetics, and migration kinetics with a specific focus on the atomic mechanisms causing grain boundary mobility.
http://gb2015.mpie.de/

28 September – 2 October: Conference on Intermetallics

This conference combines a good balance between research and application. Topics such as γ-TiAl, iron aluminides and silicides will be discussed. There will also be a session about synergies between theory and experiment in thermodynamic assessments of intermetallics.
http://www.intermetallics-conference.de/

Imprint

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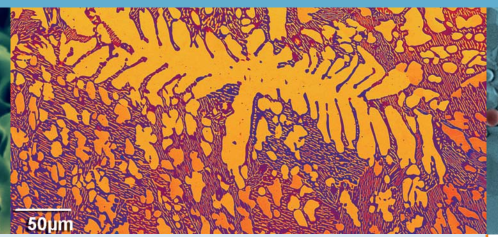
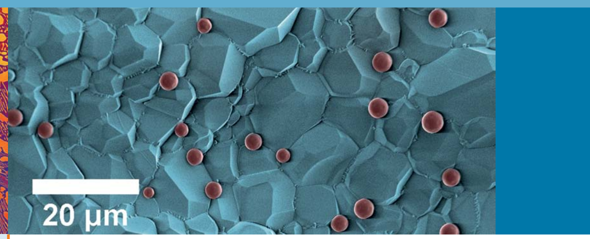
Max-Planck-Institut für Eisenforschung GmbH





Nanostructured solar cells: Tailored semiconducting nano-composites as optimized light absorbers

Semiconducting nano-composites — consisting of nanoparticles embedded in a host matrix — offer exciting prospects for solar energy conversion, light emission and electronic applications. Such composites allow for the targeted synthesis of functional materials with tailored electronic and optical properties. For device applications a detailed understanding of the link between atomistic structure and the composite properties is required.

By precisely controlling the size and shape of nanoparticles (NPs), their surface chemistry, arrangement into superlattices and insertion into a suitable host matrix, one can create semiconducting nano-composites with specifically tailored electronic, optical and mechanical properties. Bulk silicon for example has a band gap of 1.1 eV and is an indirect semiconductor, effectively preventing its application as a light emitter. Silicon nanoparticles on the other hand exhibit radically different properties, featuring efficient photoluminescence. The band gap becomes a function of the NP diameter, allowing for light emission over a wide range of colours. Such NPs can be inserted into a host matrix to achieve efficient charge transport and create durable nano-composites.

Nano-composites also allow integrating complex functional properties into a single material. The Coulomb interaction is strongly enhanced, due to the quantum confinement of the electrons into the small space of the NPs. With respect to solar energy conversion, this enhanced Coulomb interaction can drive a process called multi-exciton generation (MEG), where one incoming solar photon creates several electron-hole pairs instead of just one. Utilizing MEG enables in principle to build single junction solar cells that exceed the Shockley-Queisser limit in solar energy conversion efficiency of 31%.

Recent advances in wet chemical techniques allow for the synthesis of NPs, their assembly into superlattices and embedding into a host matrix using only inexpensive solution processing. However, the atomistic and structural details of such composites are poorly understood, due to the complexity of the synthesis conditions and the unavailability of robust experimental techniques to probe nanointerfaces at the microscopic level. For device applications a detailed understanding of the atomistic structure and its link to the resulting composite properties is required.

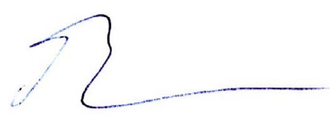
Starting January 2014, the Atomistic Modelling Group has been awarded a "NanoMatFutur" grant

EDITORIAL

Dear Colleagues and Friends of the MPIE,

Renewable energies and the role of materials and the associated harsh environmental exposure for these systems are currently a hot topic in industry and basic research. In this newsletter edition we demonstrate how our researchers contribute to this field, both in terms of theoretical and experimental approaches such as employed for the improvement of solar and fuel cells, and new wet chemical synthesis techniques. Moreover, a new independent Max Planck Research Group on 'Nanoanalytics and Interfaces' was established. Please also have a look at the upcoming events and workshops.

Enjoy reading and best regards,



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

Awards and Achievements

Dr. Poulumi Dey, postdoc in the group 'Computational Phase Studies', won the Best Poster Award at the "Asia Sweden Meeting on Understanding Functional Materials from Lattice Dynamics" in Assam, India.

Prof. Michael Finnis from the Imperial College London has received a Humboldt Research Award and is currently working at the MPIE and the ICAMS (Bochum).

Dr. Raheleh Hadian, postdoc in the group 'Adaptive Structural Materials', has been granted a scholarship from the Alexander von Humboldt Foundation.

Dr. Rong Hu, postdoc in the group 'Atom Probe Tomography, has received a scholarship of the Alexander von Humboldt Foundation.

Mehmet Ikbal Isik, PhD student in the group 'High-Temperature Materials', has won the Best Electron Micrograph Award at the "17th International Metallurgy and Materials Congress" in Istanbul, Turkey.

Prof. Surya Kalidindi from the George W. Woodruff School of Mechanical Engineering (Atlanta, USA) has received a Humboldt Research Award and is currently working at the MPIE.

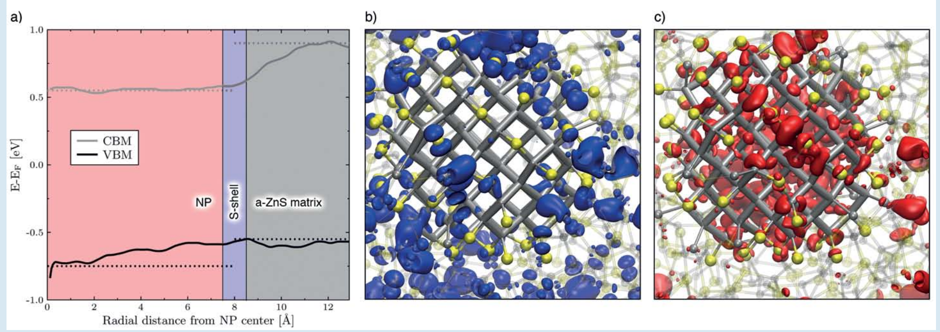
from the German Federal Ministry for Education and Research (BMBF). Over the course of 4 years, we systematically investigate technologically relevant nano-composites to build a detailed understanding of their structure and explore new ways to tune their properties.

A major roadblock to utilizing MEG in device applications is the band gap problem: the same quantum confinement which enables efficient MEG enlarges the band gap, shifting the onset of MEG beyond the solar spectrum. One needs simultaneously strong quantum confinement and small band gaps on the order of 0.5 eV. Silicon and Germanium both feature metastable high pressure phases called BC8 and ST12, respectively, much like diamond is a high pressure phase of carbon. We demonstrated from ab initio many-body perturbation theory calculations that NPs with such high pressure core structures exhibit simultaneously low band gaps and strongly increased MEG rates. The concept of creating NPs with core structures made from allotropes of elemental semiconductors is introduced as a new way of tuning the properties of nano-composites. Recent experiments demonstrate the successful synthesis of NPs with BC8 and ST12 core structures from chemical solution processing.

To allow for efficient charge transport the NPs are embedded in a host matrix. First principles molecular dynamics and simulated annealing were used to obtain structural models of Si NPs embedded in amorphous zinc sulfide. By using large-scale many-body perturbation theory calculations we demonstrate that this system features a so-called type II band alignment, which is highly desirable: the conduction states are localized within the NPs, whereas the valence states are delocalized throughout the matrix. Such an alignment between the NP and matrix states is a prerequisite to obtain efficient band-like charge transport.

Presently, we are calculating phase diagrams for solution processed nano-composites, where both NP synthesis and matrix embedding has been performed by wet chemistry. A multitude of structures possibly realized at the NP surface is considered, such as surface termination, reconstructions, passivation, oxidation, substitution of subsurface atoms, ligand dissociation, core-shell formation and the adsorption of the ligands on NPs with different structures. This study provides guidance about the experimental conditions which lead to specific structural motifs and is expected to lead to a detailed understanding of the structural properties of nano-composites.

Author: Dr. Stefan Wippermann



Silicon nanoparticles (NPs) embedded in amorphous zinc sulfide feature charge separated transport channels:

a) shows the valence and conduction band edges inside the NP, in the interface region (S-shell) and inside the matrix.

b/c) structural model of a Si NP with a diameter of 1.6 nm. Blue/red isosurfaces denote the spatial distribution of valence/conduction band edge states, respectively. The valence band is delocalized throughout the matrix, whereas the conduction states are localized within the NPs.

Nanostructured Materials for Renewable Energies Independent Research Group established

In consequence of the growing energy needs of our society and the increasing environmental pollution due to fossil fuels alternative energy-producing, cost-efficient and environmental friendly concepts are needed. Diverse nanostructured materials are suitable for application in this field. The correlation between atomic arrangement, chemical composition and properties of the nanostructures and occurring interfaces is one of the main research activities of the new Independent Research Group "Nanoanalytics and Interfaces" at the MPIE.

Yasmin Ahmed Salem (YAS): Your group's name is 'Nanoanalytics and Interfaces' – which goals do you have?

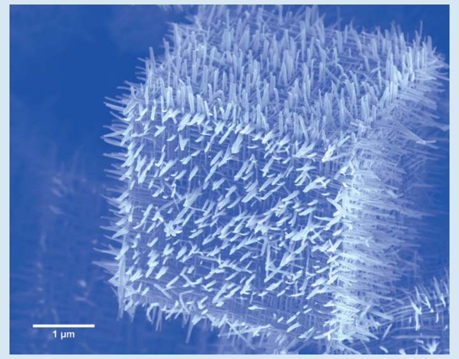
Prof. Dr. Christina Scheu (CS): Well, my group deals with the development of competitive and environmental friendly nanostructured materials for renewable energy applications. These materials have a high reactivity through a high surface area and – in combination with another material – a high interface density where e.g. charge carrier separation can take place. We synthesize and characterize these materials for photovoltaics, fuel cells and photocatalysis and clarify their structure property relation.

YAS: And on which materials do you focus?

CS: We mostly focus on nanostructured semiconducting materials and thin metallic films. Hereby we examine the material respectively the material combination as well as its morphology and structure related properties. Our main focus lies on material systems of oxides, carbides and sulphides as well as polymers and composites.

YAS: Which characterization methods do you use for the analysis of these nanostructured materials?

CS: We use various electron microscopy based techniques and focussed ion beam sectioning to investigate the morphology of the nanostructures. However, as interfaces and grain boundaries influence structural, optical and functional properties of the materials, we need also characterization methods which allow a resolution down to the atomic scale.



SEM micrograph of a Nb_3O_7 (OH) cube. This material can be used in photocatalysis to produce hydrogen and in hybrid solar cells as a electrode material. Copyright: S. Betzler

Therefore, we especially use modern (ex-situ and in-situ) transmission electron microscopy (TEM) to examine the atomic structure, chemical composition and bonding characteristics. The latter features are explored with electron energy-loss spectroscopy (EELS) measurements. We are also interested to explain the growth mechanisms of nanostructures with the aim of producing customised systems with high chemical stability and a low amount of defects. Thus, we use different synthesising strategies such as wet-chemical routes or physical methods like vapour phase deposition. In addition, we have strong cooperation with different groups which synthesize nanostructured materials with various chemical approaches.

YAS: Do you have external collaboration partners?

CS: We have several cooperation partners like the universities in Munich and Constance (Germany), the Israel Institute of Technology, the National Center for Scientific Research in Marseille (France), the Massachusetts Institute of Technology and the National Center for Electron Microscopy both in the USA and also the Niels Bohr Institute in Denmark.

YAS: Your group is structured as an Independent Research Group – what are the differences compared to the other research groups at the institute?

CS: The main difference is that we have an independent status within the MPIE and do not belong to one department. This allows me to continue with the research direction, which I have started as a Professor at the Ludwig-Maximilian-University in Munich. My group benefits from the excellent infrastructure and support from the administration of the MPIE and on the same time we are building on close cooperation with all the departments of the MPIE.

Short CV

Prof. Christina Scheu did her doctorate 1996 at the Max Planck Institute for Metals Research in Stuttgart (Germany) in the field of analytical TEM and interfaces. She continued her work there 1999 after being a Minerva Fellow at the Technion - Israel Institute of Technology – in Haifa, Israel. In 2003 she continued her research as head of the group 'Electron Microscopy and Metallography' at the university of Stuttgart. From 2005 to 2008 she was head of the group 'Nano- and Microanalytics' at the University of Leoben (Austria). 2008 she was appointed as a full Professor at the Ludwig-Maximilian-University (Munich). Since April 2014 she holds a joint position as an independent group leader at the MPIE and as a Professor at the RWTH Aachen.

Author: Yasmin Ahmed Salem, M.A.

Designing novel interfaces for better solar cells

Nowadays, big efforts are invested to invent new ways to extract the energy from renewable sources. Photovoltaic materials, which convert the light (photons) to electricity (voltage), are very promising for alternative energy. Important photovoltaic technologies are multi-crystalline Si solar cells and Cu(In,Ga)Se_2 or $Cu_2ZnSnSe_4$ thin-film solar cells. But to further establish these technologies, both the reduction of production costs and the increase of solar cell efficiency are essential. The latter is reported to be strongly dependent on the internal interfaces as they can affect the transport of the photogenerated charge carriers.

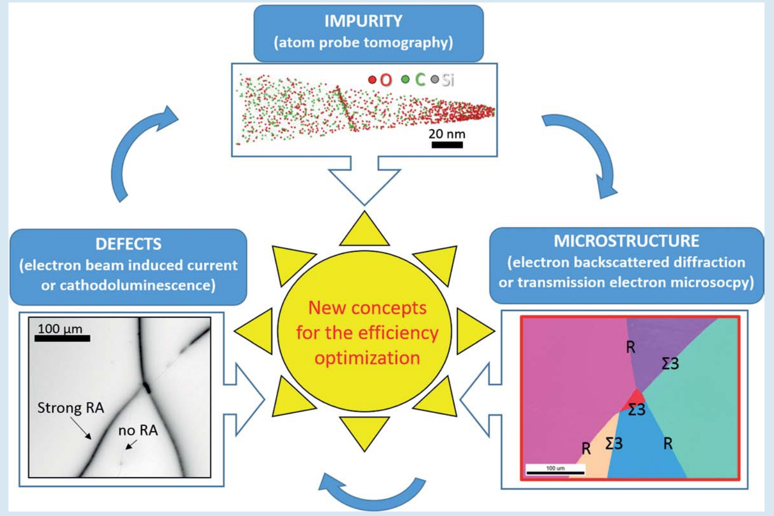
In the last decade, designing new and better internal interfaces in such photovoltaic material becomes very crucial for controlling the quality of the cell. But to propose new development strategies, the mechanisms of the efficiency improvement at the atomic scale need to be first well understood. This can be done only by using advanced nanotechnology approaches, such as atom probe tomography, in order to track the atoms redistribution and their related phenomena (impurity segregation at grain boundaries or p-n Junction, clustering, diffusion).

Atom probe tomography is a very new technique, which was invented only couple of decades ago and therefore very attractive. The advantage of this powerful tool is that it shows both the structure and the composition of materials at atomic-scale. The resolution limit of this technique is 0.2 nm for the lateral resolution and 0.1 nm for the depth resolution, therefore it is considered as a high-resolution technique. The impurity level is as low as 20 ppm (0.002 at.%).

Therefore, the aim of Oana Cojocaru-Mirédin and her group "Interface design in solar cells" is to perform chemical, structural, electrical, and optical characterization of the internal interfaces in solar cells by using nanotechnology approaches, such as atom probe tomography, in conjunction with complementary techniques (electron backscatter diffraction, transmission electron microscopy, cathodoluminescence, and electron beam-induced current).

The overarching goal is then to synthesize novel and improved multi-crystalline Si and Cu(In,Ga)Se_2 or $Cu_2ZnSnSe_4$ thin-film solar cells in direct work with several institutes specialized on solar research.

Author: Dr. Oana Cojocaru-Mirédin



Research strategy: designing solar materials with higher efficiency can be done only by a full understanding of the correlation between impurity, defect and microstructure.

Awards and Achievements

Dr. Karl Mayrhofer, head of the group 'Electrocatalysis', has won the DECHEMA Prize 2014 of the Max-Buchner-Forschungsstiftung.

George Polymeros, PhD student in the group 'Electrocatalysis', has won the Ballard CSC Poster Prize at the Surface Electrochemistry Session of CSC in Vancouver, Canada.

Torsten Schwarz, PhD student in the group 'Interface Design of Solar Cells, won the "E-MRS Graduate Student Award" at the European Materials Research Society Spring Meeting in Lille, France.

Halil Ibrahim Sözen, PhD student in the group 'Computational Phase Studies', received a Merkle scholarship of the Deutsches Stiftungszentrum.

Thomas Utzig, PhD student in the group 'Interaction Forces and Functional Materials, won the ACS-Langmuir Poster Award at the "CAI-STEM SFA 2014 Conference" in Cancún, Mexico.

Ashokanand Vimalanandan, PhD student in the group 'Molecular Structures and Surface Design', won the "Young Author's EFC Poster Prize" at the EUROCORR 2014 in Pisa, Italy.