DF 24: Crystallography in Materials Science (Joint Session with KR)

Time: Thursday 15:00–17:30 Location: CHE 184

Invited Talk DF 24.1 Thu 15:00 CHE 184

Crystals: Structure, Properties and Heart of Energy Conversion Devices — •Tilmann Leisegang[1], Juliane Hanzig[2], Erik Mehner[2], Matthias Zschornak[2], Falk Meutzner[2], Tina Nestler[2], Bianca Störr[2], Charaf Cherkouk[2], Ulrike Wunderwald[1], and Dirk C. Meyer[2] — [1]Fraunhofer-THM, Am-St.-Niclas-Schacht 13, 09599 Freiberg — [2]TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Str. 23, 09596 Freiberg

Crystalline materials are wide spread in our today's life. More than 98 % of the solid fraction of the earth comprises crystalline matter, most of which are oxides. Single-crystals in particular are the basis for many applications - lasers, LEDs, sensors, etc. - and play an important role in fundamental research for instance in superconductivity or magnetic properties. The discipline that elucidates the impact of the crystal structure on the physical properties of particularly crystalline materials - crystallography - is of specific importance for the design of new materials. X-ray and other diffraction methods are of great relevance for the investigation of crystal structures and their peculiarities. Moreover, crystallography can be utilized to establish new concepts and thus may contribute solving today's challenges in science and technology. In this context, the work presented highlights several examples. First, it is demonstrated how composition variations can be used to change the three dimensional crystal structure - including commensurate or incommensurate modulated phases - in order to tune the materials properties. Second, applications of crystals for energy conversion devices are presented.

DF 24.2 Thu 15:30 CHE 184

Clusters in intermetallic compounds: fullerenes and more — •Julia Dshemuchadse and Walter Steurer — Laboratory of Crystallography, Department of Materials, ETH Zurich, Switzerland

The study of the structure of metals has kept crystallographers busy for the past century: starting with the simplest of structures – sphere packings, such as found in aluminium or copper – up to some of the most complex inorganic structures known to date with more than 20 000 atoms per unit cell [1]. But knowing all the atomic positions does not yet provide us with a deeper understanding of the design of the structure.

Different cluster interpretations of the atomic arrangement in an intermetallic can provide us with recurring motifs in the form of atomic environments, *i.e.* coordination polyhedra, or larger, endohedral clusters, such as dual Frank-Kasper polyhedra and fullerene-like shells (*e.g.*, [2]). These cluster descriptions illustrate common features in structures either within the same intermetallic system or of related structures with entirely different constituents. However, they do not necessarily represent chemical entities and their meaningfulness is usually derived from their repeated occurrence in diverse compounds.

We will present possible ways of structure description for complex intermetallic phases and clues toward their significance.

[1] T. Weber, J. Dshemuchadse, M. Kobas, M. Conrad, B. Harbrecht and W. Steurer, *Acta Cryst. B* 65, 308–317 (2009).

[2] J. Dshemuchadse, S. Bigler, A. Simonov, T. Weber, W. Steurer, *Acta Cryst. B* 69, 238–248 (2013).

DF 24.3 Thu 15:45 CHE 184

Theoretical investigation of the high pressure structure of CaTe — •Oliver Potzel and Gerhard Taubmann — Institute of Theoretical Chemistry, University of Ulm, D-89069 Ulm, Germany

The majority of the alkaline halides and the alkaline earth chalcogenides undergoes a structural phase transition from the B1 (rock-salt) structure to the B2 (CsCl) structure at elevated pressures [1].

The x-ray diffraction data of CaTe at high pressures (320 - 400 kbar) fit to a simple cubic indexing (B2) except for two reflections near the (110) peak [2]. This indicates the possible existence of an intermediate structure within the transition from the B1 to the B2 structure.

We are currently using the evolutionary algorithms of the USPEX code [3] with the periodic DFT code VASP [4] in order to predict the structure of CaTe at a pressure of 350 kbar.

Preliminary DFT studies without genetic algorithms pointed to an AgO structure. In these calculations, all known (binary) AB structures were taken into account.

The results are to be verified by the comparison of the calculated data to the experimental diffraction data.

[1] O. Potzel, G. Taubmann, J. Solid State Chem. 184, 1079 (2011)
[2] H.G. Zimmer, H. Winzen, K. Syassen, PRB 32, 4066 (1985)
[3] A.R. Oganov , C.W. Glass, J. Chem. Phys. 124, 244704 (2006)
[4] G. Kresse, J. Furthmüller, PRB 54, 11169 (1996)

DF 24.4 Thu 16:00 CHE 184

In-situ ion beam irradiation: X-ray scattering & diffraction experiments — Olga Roshchupkina, Carsten Baehtz, Stefan Facsko, Lothar Bischoff, Matthias Posselt, and •Joerg Grenzer — Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden

Ion beam techniques are widely used in semiconductor industry e.g. for introducing dopant atoms into materials. Ion implantation is characterized by fast dynamic processes associated with the evolution of collision cascades resulting in formation of defects such as vacancies, interstitials, etc. As a consequence, typically a strained layer that expands in the direction normal to the substrate surface is formed. This is due to the fact that the bulk material prevents any lateral macroscopic expansion and as a result the thin irradiated layer is subjected to an in-plane biaxial compressive stress. Ion irradiation is a very fast process and it is almost impossible to monitor it in-situ with the present x-ray sources. However, the accumulation of damage and the diffusion of defects are much slower processes and can be studied in-situ by X-rays. An in-situ ion beam implantation experiment was set up at ROBL/MRH at ESRF. Samples were irradiated using 20 keV He^+ ions at room temperature. Reciprocal space maps to investigate the evolution of the strain depending on the accumulation of defects, as well as the conversion of the strained layer into a completely (X-ray) amorphous layer on single crystal Si and Al_2O_3 substrates were measured and discussed.

Coffee break

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Focused Ion Beam implantation of Erbium into Y2SiO5 crystals — •Nadezhda Kukharchyk[1], Jasper Rödiger[2], Arne Ludwig[1], Alexey Ustinov[3], Pavel Bushev[4], and Andreas D. Wieck[1] — [1]Ruhr University Bochum, Bochum — [2]RUBION, Bochum — [3]Karlsruhe University, Karlsruhe — [4]University of Saarland, Saarbrücken

In the context of research on quantum computation and information, different systems have been developed and investigated recently. Particular interest is focused on the systems based on the rare earth (RE) elements, which feature semi-shielded 4f-electrons from external crystal fields and therefore possess long optical and microwave coherence time. Among all the REs, exclusively erbium has the transition which falls into Telecom C-Band at 1540 nm. In the present work, we perform Focused Ion Beam (FIB) implantation of Erbium ions into Y2SiO5 substrates. The FIB allows us to have a high control over the implanted pattern and area, as well as the depth and even the choice of the isotopes - which gives high flexibility in the system preparation. Luminescence of the implanted crystals appears to be an effective way to characterize the system. The measurements were performed in the confocal regime with an excitation at 488 nm and detection in the range of 450 nm to 900 nm at room temperature. A marked intensity-to-fluence dependence is observed and compared to the spectra from the grown doped crystals. Additionally the influence of defects and annealing was studied.

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White beam synchrotron x-ray topography of sapphire single crystals — •Atefeh Jafari[1,2], Angelica Cecilia[3], Jürgen Härtwig[4], Andreas Danilewsky[5], Dimitrios Bessas[4], Viktor Asadchikov[6], Boris Roschin[6], Denis Zolotov[6], Alexander Deryabin[6], Ilya Sergeev[7], Svetoslav Stankov[3], Tilo Baumbach[3], Pavel Alexeev[1,7], Hans-Christian Wille[7], and Raphaël Hermann[1,2] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institute PGI, JARA-FIT, Forschungszentrum Jülich, Germany — [2]Faculté des Sciences, Université de Liège, Liège, Belgium — [3]Institute for Photon Science and Synchrotron Radiation, KIT, Germany — [4]European Synchrotron Radiation Facil-

ity, Grenoble, France — [5]Crystallographic institute, University of Freiburg,Germany — [6]Shubnikov Institute of Crystallography, RAS, Moscow, Russia — [7]Deutsches Elektronen-Synchrotron, Hamburg, Germany

Sapphire single crystals grown by different techniques have been assessed with white beam and meV-resolution synchrotron x-ray topography at ANKA, KIT and PETRA III, DESY, and ESRF, respectively. Excellent crystal quality is required for the use in backscattering x-ray monochromators for nuclear resonance scattering with resonance energies above 30 keV. X-ray topography reveals defects and dislocations and hints at their origin. Crystals grown by the Kyropoulos method show the lowest dislocation density. Support of the Helmholtz-Russia joint research group HRJRG-402, ANKA, PETRA III and ESRF is acknowledged.

DF 24.7 Thu 17:00 CHE 184

Improving Nanomagnetometry Based on Nitrogen-Vacancy Centers by Coupling to Superparamagnetic Iron Oxide Nanoparticles — •Nikola Sadzak, Janik Wolters, Andreas W. Schell, Sten Wenzel, and Oliver Benson — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, Berlin, Germany

The single negatively charged nitrogen-vacancy (NV) defect center in diamond is known to be a stable solid-state single photon source [1], with an electronic spin showing long coherence times even at room temperature. Furthermore, the optical readout of the spin state and its microwave-assisted manipulation allow this defect to be used either as a qubit register [2] or as a magnetic field sensor [3]. Here, we perform the coupling of individual NV centers in nanodiamond with single-domain superparamagnetic iron oxide nanoparticles. By showing huge magnetic susceptibilities and no hysteresis, the latter can be used as local microwave amplifiers, allowing the achievement of faster Rabi oscillations between the NV center electronic spin sublevels. Moreover, we investigate the effects on the NV- electronic spin dynamics and coherence times and discuss some applications in NV-based nanomagnetometry.

[1] I. Aharonovich et al., Rep. Prog. Phys. 74, 076501 (2011).
[2] L. Robledo et al., Nature 477, 574-578 (2011).
[3] J. R. Maze et al., Nature 455, 644-648 (2008).

DF 24.8 Thu 17:15 CHE 184

Selective preparation of single-crystalline alpha- & beta-phase perylene platelets — •André Pick and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, 35032 Marburg

Though polarization resolved optical absorption spectroscopy in transmission geometry is a simple method to characterize optoelectronic properties of pi-conjugated molecular crystals their large absorption requires rather thin crystals. Moreover such studies are complicated by the presence of polymorphism and structural defects like twinning. For the case of the polycyclic aromatic hydrocarbon perylene two crystalline phases (alpha and beta) are known which comprise different molecules per unit cell. Both crystalline phases exhibit also characteristic differences in the habitus of single crystals which allows their differentiation. Here, we present a method to selectively prepare thin platelets of both polymorphisms, which are suitable for optical studies of single crystals. In order to get full morphological information, the crystallites were characterized by means of optical microscopy, X-ray diffraction and atomic force microscopy.