KFM 3: Crystal Structure, Defects, Real Structure and Microstructure in Materials

Chair: Enrico Langer - Technische Universität Dresden

Time: Monday 9:30–13:10 Location: E 124

KFM 3.1 Mon 9:30 E 124

Higher-Order Topological Insulators — •Frank Schindler[1], Ashley Cook[1], Maia Vergniory[2], Zhijun Wang[3], Stuart Parkin[4], Andrei Bernevig[3], and Titus Neupert[1] — [1]University of Zurich, Switzerland — [2]University of the Basque Country, Spain — [3]Princeton University, USA — [4]Max Planck Institute of Microstructure Physics, Germany

Three-dimensional topological (crystalline) insulators are materials with an insulating bulk, but conducting surface states which are topologically protected by time-reversal (or spatial) symmetries.

Here, we extend the notion of three-dimensional topological insulators to systems that host no gapless surface states, but exhibit topologically protected gapless hinge states. Their topological character is protected by spatio-temporal symmetries, of which we present two cases: (1) Chiral higher-order topological insulators protected by the combination of time-reversal and a four-fold rotation symmetry. Their hinge states are chiral modes and the bulk topology is Z2-classified. (2) Helical higher-order topological insulators protected by time-reversal and mirror symmetries. Their hinge states come in Kramers pairs and the bulk topology is Z-classified.

We provide the topological invariants for both cases. Furthermore, we discuss current developments concerning material realizations of these novel phases of matter.

KFM 3.2 Mon 9:50 E 124

Stability of carbon clathrates: a theoretical investigation — •Conrad Steigemann and Miguel Marques — Martin-Luther-Universität Halle- Wittenberg

Due to their structure, clathrates naturally offer a good possibility to be doped by a variety of atoms to change the properties of the scaffold element drastically. Besides germanium and silicon showing clathrate structures, no stable clathrates of carbon could be found yet. Studies [Zeng et al. 2015] suggest a substitution of single carbon atoms with boron to stabilise the structure.

In this contribution, we perform extensive calculations of the energy landscape of carbon clathrates in order to understand if these can indeed be synthesized. This will be done by using a combination of high-throughput density-functional theory and global structural prediction methods.

KFM 3.3 Mon 10:10 E 124

Band gap engineered multicomponent equitatomic rare earth oxides synthesized by nebulized spray pyrolysis — •Leonardo Velasco Estrada[1], Abhishek Sarkar[1,2], and Horst Hahn[1,2,3] — [1]1Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Joint Research Laboratory Nanomaterials, Technische Universität Darmstadt and Karlsruhe Institute of Technology, Alarich-Weiss-Str. 2, 64287 Darmstadt, Germany — [3]Helmholtz Institute Ulm, Electrochemical Energy Storage, Helmholtzstr. 11, 89081 Ulm, Germany

Several multicomponent equitatomic rare earth oxides (ME-REOs) systems containing up to 7 elements (Ce, Gd, La, Nd, Pr, Sm and Y) were synthesized by nebulized spray pyrolysis. The systems showed narrow direct and indirect band gaps in the range of 1.95 * 2.14 eV, respectively. X-ray diffraction as well as transmission electron microscopy confirmed that all the systems crystallized as phase pure fluorite type (fm3m) structure. X-ray photoelectron spectroscopy revealed that Ce and Pr are in a 4+ and in a mixed oxidation state (3+/4+), respectively, while the other constituent elements are in a 3+ oxidation state. In this study the observed narrow band gap is closely related to the presence of multivalent Pr, since the phase pure fluorite type systems that were synthesized without Pr exhibited a band gap $>$ 3eV. Interestingly, the narrow band gaps were not highly affected by the high chemical complexity of the systems. Therefore, this category of materials offers flexibility for band gap engineering and tunability.

KFM 3.4 Mon 10:30 E 124

Zinc-blende and wurtzite phase formation in indium phosphide nanowires grown by template-assisted selective epitaxy — •Philipp Staudinger[1], Stephan Wirths[1], Marta D. Rossell[1,2], Marilyne Sousa[1], Kirsten E. Moselund[1], and Heinz Schmid[1] — [1]IBM Research Zuerich, 8803 Rueschlikon, Switzerland — [2]Electron Microscopy Center, EMPA, 8600 Duebendorf, Switzerland

Group III-V semiconductor nanowires (NWs) are expected to provide a platform for a wide range of future applications such as high-performance field effect transistors and optoelectronic devices. Nanostructures offer a new type of band structure engineering based on the formation of zinc-blende (ZB) - wurtzite (WZ) polytypism. These crystal phases are distinctively different in terms of physical properties facilitating applications such as direct bandgap materials in the 495-570 nm wavelength regime. However, the crystallographic quality of NWs remains difficult to control, resulting typically in the formation of a high number of planar defects. So far, using Template-Assisted Selective Epitaxy (TASE), the growth of WZ phase has not been observed.

We demonstrate that both WZ and ZB crystal phases can be obtained using TASE. InP NWs were selectively grown using metal organic vapor phase epitaxy at temperatures of 625 °C and a V/III ratio of 50 inside predefined hollow oxide templates of varying dimensions. The crystal phase was determined by micro photoluminescence spectroscopy along with scanning transmission electron microscopy. Both ZB and WZ phases were found in nearly pure form, giving promise for novel device applications such as high efficient green LEDs.

KFM 3.5 Mon 10:50 E 124

Local properties of PPKTP waveguide structures probed by Raman spectroscopy — •Julian Brockmeier[1], Michael Rüsing[1], Christof Eigner[1], Laura Padberg[1], Peter Mackwitz[1], Christine Silberhorn[1,2], Gerhard Berth[1,2], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany

Periodically poled waveguides in Potassium Titanyl Phosphate (PPKTP) have promising capabilities for integrated quantum optical applications [1]. However a fundamental understanding of the underlying physics for a defined domain patterning of waveguides, especially in the submicron region, is important. In this context we report on our systematic analysis of periodically poled Rb-exchanged waveguides in KTP in the framework of various fabrication-parameters e.g. melt-composition, exchange-temperature and fabrication order performed by confocal Raman spectroscopy. The vibrational properties of the periodically poled waveguides were determined for different scattering geometries in three dimensions. We found specific phonon modes linked to the stoichiometric/crystallographic structure and to the induced stress.

[1] Marco Fiorentino et al., 'Spontaneous parametric down-conversion in periodically poled KTP waveguides and bulk crystals', OPTICS EXPRESS, 15 (12) 7479 (2007)

20 min. break

KFM 3.6 Mon 11:30 E 124

Phase identification in spark plasma sintered (SPS) Fe-Al-Si powders — •Jaromír Kopeček[1], Jarmila Remiášová[1], Ladislav Klimša[1], Petr Haušild[2], Miroslav Karlík[2], František Laufek[3], Kateřina Nová[4], Jakub Šesták[4], Boris Severa[4], Filip Průša[4], and Pavel Novák[4] — [1]Department of Functional Materials, Institute of Physics of the CAS, Prague, Czech Republic. — [2]Department of Materials, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Czech Republic. — [3]Czech Geological Survey, Prague, Czech Republic. — [4]Department of Metals and Corrosion Engineering, University of Chemistry and Technology Prague, Prague, Czech Republic.

Fe-Al-Si alloys are interesting materials with promising corrosion properties. The components of such alloys are cheap, nevertheless the way of preparation is complicated and increasing the price of the product. Our group investigated properties of Fe - 20 wt. % Al - 20 wt. % Si alloy prepared by mechanical alloying followed by spark plasma sintering under various conditions. The element powders were used for

mechanical alloying. The microstructure and phase composition were investigated with optical and electron microscopies (including EDS and EBSD) and X-ray diffraction. It was found that mechanically alloyed powders contain mainly of-stoichiometric binary phases, whereas sintered samples contain significant amount of ternary phase. The phase description is complicated as the phases dimensions are small and composition is off-stoichiometric both in powders or compacted alloys.

KFM 3.7 Mon 11:50 E 124

Size Calibration of IR-Laser Scattering Tomography by using Tailored Oxygen Precipitates in Cz-Si — •Robert Kretschmer[1,3], Andreas Sattler[1], Dawid Kot[2], Gudrun Kissinger[2], and Martin Stutzmann[3] — [1]Siltronic AG, Johannes-Hess-Strasse 24, 84489 Burghausen — [2]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder) — [3]Walter Schottky Institut, Am Coulombwall 3, 85748 Garching

Infrared Light Scattering Tomography (LST) is the standard method for detection of bulk micro defects in silicon. It is mainly used to determine the density of oxygen precipitates, which can act as internal getter for metal impurities during device manufacturing process. Since gettering efficiency depends on precipitate dimensions, bulk defect size is an important parameter to be measured.

We propose to use a size calibration for LST method based on reference wafers with bulk defects of well-defined size, shape and density. These defects have been fabricated through thermal growth of oxygen precipitates. A simulation applying a diffusion-limited model was performed to optimize thermal cycles for reaching pre-defined target defect sizes. The comparison of LST results with TEM shows that precipitate size can be controlled in the relevant calibration range from 20-100 nanometers.

KFM 3.8 Mon 12:10 E 124

Coarsening and growth of metastable γ'' precipitates in Ni-based superalloys — •Felix Schleifer, Markus Holzinger, Yueh-Yu Lin, Michael Fleck, and Uwe Glatzel — Metals and Alloys, University of Bayreuth, Germany

We develop a phase field model for the simulation of diffusion-limited precipitation in Ni-based superalloys with industry-relevant chemical complexity. In the wrought alloy Inconel 718 superior performance at high temperatures is achieved by coherent γ'' precipitations in the fcc matrix. Under non-equilibrium conditions the metastable Ni_3Nb intermetallic compound γ'' with tetragonal structure is the main strengthening phase in the alloy. During heat treatment and aging the formation and coarsening of such precipitates is controlled by Nb-diffusion in the matrix.

The thermodynamic formulation of the model will be validated by comparison to respective CALPHAD equilibrium calculations using the commercial software ThermoCalc. Furthermore, an elastic term is included in the model to account for external loads, anisotropic lattice mismatch stresses as well as elastic inhomogeneities between the considered phases.

This project was recently started as part of the second phase of the DFG priority program 1713. We aim to study steady state growth and coarsening of the precipitated particles as a function of the basic two heat treatment parameters i. e. temperature and time. Phase field studies concerning multiple particles and microstructure evolution under mechanical loading will be carried out subsequently.

KFM 3.9 Mon 12:30 E 124

On the microstructure of the shape memory alloy Co-Ni-Al using complementary diffraction techniques — •Leonid Potapov[1], Enrico Langer[1,2], Katerina Krátká[1], Jaromir Kopeček[3], and Siegfried Däbritz[1] — [1]TU Dresden, IFMP, Dresden, Germany — [2]TU Dresden, IHM, Dresden, Germany — [3]Institute of Physics of the CAS, Prague, Czech Republic

Shape memory alloys can have a quite complex microstructure, making the investigation of their properties very challenging. This work deals with the characterization of austenitic samples of $Co_{38}Ni_{33}Al_{29}$, grown by the Bridgeman method at different pulling rates. In this alloy, a mixture of ordered bcc crystal β matrix and a secondary dendritic fcc γ phase enriched with Co was observed by the combination of X-ray Kossel microdiffraction, EBSD and EDX methods. Thereby the Kossel technique reveals the presence of anisotropic superstructure reflections of the {100} type in the β phase. EBSD linescans into heavily strained β matrix areas suggest a superposition of diffraction patterns of bcc and fcc even at great distances from the phase boundaries. This makes the evaluation of patterns very intricate and may cause problems for automated EBSD. Furthermore, the fcc pattern appears to dominate deeply inside the matrix. This might be caused by Co-rich γ-like micro/nano precipitates, embedded in the matrix and inducing internal strains. In analogy to our previous Kossel measurements, pairs of parallel Kikuchi bands from both patterns can be used to retrieve the orientation relationship between β matrix and γ precipitates, which appears to be close to the Nishiyama-Wasserman relationship.

KFM 3.10 Mon 12:50 E 124

In-situ imaging techniques for the study of magnetocaloric materials — •Anja Waske, Alexander Funk, and Rudolf Schäfer — IFW Dresden

In-situ temperature-dependent magneto-optical imaging is applied to study the thermal hysteresis of magnetocaloric MnFePSi spherical powder-packed beds across their magneto-elastic transition. Cooling and heating imaging series are used to analyze the transition of such a complex powder ensemble. The magnetization versus temperature behavior reconstructed from these local measurements shows very good agreement with integral measurements of the magnetization of the whole packed bed. Hence, local magneto-optical imaging measurements represent the ensemble behavior well if the number of measurements is large enough.