

KFM 11: Crystal Structure Defects / Real Structure / Microstructure

Chair: Prof. Dr. Theo A. Scherer (KIT Karlsruhe)

Time: Thursday 14:00–17:55

Location: POT 51

KFM 11.1 Thu 14:00 POT 51

eutectic: a game changer — ●SANDHYA SHARMA¹, HAFIZ MUHAMMAD ZEESHAN¹, ELENA VOLOSHINA^{1,2}, and YURIY DEDKOV^{1,2} — ¹Centre of Excellence ENSEMBLE3 Sp. z o. o., Wolczynska Str. 133, 01-919 Warsaw, Poland — ²Department of Physics, Shanghai University, 99 Shangda Road, 200444 Shanghai, P.R. China

The world of semiconductors has drastically improved the lifestyle due to its versatile applications. The demand for new efficient semiconductors is increasing day by day, giving birth to the idea of new synthesis methods. Many synthesis techniques have been utilized to engineer band gap of semiconductors to achieve higher efficiency. Here, a perspective on the importance of semiconductor eutectic materials has been presented as one of the future potential candidates, along with the micro (μ) pulling method (as a synthesis method for semiconductor eutectic materials) that not only control factors effecting the devices but also provides variety of options for band gap modification. The efficiency of the present devices in comparison with the eutectic composites has been made, showing the semiconductor eutectic materials as a better candidate for future devices.

KFM 11.2 Thu 14:20 POT 51

Determining the Crystallization Mechanism in Optical Switching Experiments with Electron Backscatter Diffraction — ●MAXIMILIAN MÜLLER and MATTHIAS WUTTIG — I. Institute of Physics (IA), Aachen, Germany

To tailor phase-change materials for computing and data storage applications unraveling the contribution of nucleation and crystal growth to crystallization is essential. Usually, these processes are studied at low temperatures. Subsequently, from the temperature dependence of both processes at low temperature, the role of these processes at high temperatures is extrapolated. This is inherently dangerous if the underlying processes do not follow Boltzmann kinetics.

In this study, crystallization was achieved by short laser pulses with pulse lengths between a few ns to several μ s. Afterwards, the resulting grain structure was analyzed by different techniques, including atomic force microscopy and Electron Backscatter Diffraction (EBSD). The grain size distribution is determined by these experiments which helps disentangling the processes of nucleation and growth. Significant differences are observed concerning the nucleation of different compounds. Trends for the nucleation and growth rate as a function of stoichiometry are analyzed and explained based upon systematic changes in bonding.

KFM 11.3 Thu 14:40 POT 51

Vacancies in Prussian White Cathode Materials employing Positron Annihilation Spectroscopy — ●DOMINIK BORAS¹, IDA NIELSEN², ALEXANDER BUCKEL³, TORE ERICSSON², LENNART HÄGGSTRÖM², TORSTEN E.M. STAAB¹, and WILLIAM R. BRANT² — ¹Institute for Functional Materials and Biofabrication, Julius-Maximilians Universität Würzburg, 97070 Würzburg, Röntgenring 11 — ²Department of Chemistry - Ångström Laboratory, Uppsala University, Box 538, SE-751 21 Uppsala, Sweden — ³Altris AB, Kungsgatan 70b, SE-753 18 Uppsala, Sweden

We are presenting a novel attempt to characterise Prussian blue analogues. Prussian White samples have been synthesized with different sodium content and, then, characterized by common methods (ICP-OES, TG, SEM) but also by Mössbauer spectroscopy. We prepared three different sample states: fully and half-sodiated as well as desodiated. As a new method positron annihilation lifetime spectroscopy (PALS) has been applied to characterize the different samples states. We can state that the methods of PALS gives reasonable results for Prussian White with varying sodium and water content. The relative intensity of the longer positron lifetime component (405ps) is increasing with decreasing sodium content, which is an indication that the positron "sees" less of the open crystal channels filled by movable ions, since those become more and more occupied by intercalated Na-atoms. This first attempt aims to present the potential of PALS to characterise Prussian Blue analogue materials with respect to defects and occupation of its crystal channels by movable ions.

KFM 11.4 Thu 15:00 POT 51

Disorder engineering for symmetry lowering in Prussian Blue analogues (PBAs) — ●YEVHENIIA KHOLINA, THOMAS WEBER, and ARKADIY SIMONOV — ETH Zürich, Switzerland, Department of Materials, Laboratory for Multifunctional Ferroic Materials

A simple consequence of Neumann's principle is that certain properties can exist in crystals with a certain symmetry. As a result, a lot of materials engineering is focused on designing particular symmetries, which allow the properties of interest. In oxide perovskites as well as their molecular analogues, control of crystal symmetry is achieved by octahedral tilts and cation ordering. In this work we show an alternative way of symmetry lowering, using disorder. We focus on Mn[Co]PBA with the chemical composition $\text{Mn}[\text{Co}(\text{CN})_6]_{2/3}$. These crystals have 1/3 of $\text{Co}(\text{CN})_6$ sites vacant. The structure of such PBAs is believed to be cubic with space group $\text{Fm}\bar{3}\text{m}$. However, the optical measurements indicate that the crystal is twinned and an actual structure has tetragonal symmetry or lower. We collect single-crystal x-ray diffuse scattering from untwinned crystal to probe the local structure and quantitatively characterise defect distribution, using 3D- Δ PDF analysis. The symmetry of the local structure is reduced to tetragonal by local vacancies ordering. The vacancies have stronger correlation along c direction. Such asymmetry is formed because the crystal is growing in this direction. This means the symmetry can be lowered by choosing a specific direction of the crystal growth. We believe this result can be applied to other disordered crystalline materials and be an effective way to lower the symmetry for properties design.

KFM 11.5 Thu 15:20 POT 51

Single crystal growth of the Mott insulator BaCoS₂: structure and hole doping — ●HANEEN ABUSHAMMALA, TESLIN THOMAS, ANDREAS KRYSSIG, and ANNA BOEHMER — Experimentalphysik IV, Ruhr-Universität Bochum, Universitätsstrasse 150, 44801 Bochum, Germany

The quasi-2D BaCoS₂ is a Mott insulator with a stripe-like antiferromagnetic ordering at $T_N=290$ K. Both chemical doping or hydrostatic pressure drive the system into a paramagnetic metallic phase. Interestingly, there is no structural transition at the metal-insulator transition of this phase, which offers ideal conditions to investigate the Mott transition in a model multiband system [1].

Nevertheless, BaCoS₂ remains little studied, and the interplay of electronic and structural features is still unclear. High-quality single crystals are needed to elucidate this issue. The synthesis of single-crystalline BaCoS₂ is challenging owing to its metastability, with a decomposition into Ba₂CoS₃, CoS and S below 850°C. The BaCoS₂ phase can only be obtained via quenching from high temperature. Moreover, BaCoS₂ melts incongruently, which calls for a flux growth method necessitating separation of the crystals from the flux by the end of the growth. We have successfully grown single crystals of pure and the hole-doped BaCoS₂ using a self-flux method with high-temperature flux separation and quench. The structural and anisotropic electrical transport properties are determined and discussed.

[1] Abushammala, Lenz, Baptiste, Casula, Klein and Gauzzi, in preparation (2022).

KFM 11.6 Thu 15:40 POT 51

Monitoring the S-phase formation in an high-purity Al-Cu-Mg alloy by truncation during heating-up — ●TORSTEN E.M. STAAB, DOMINIK BORAS, SEBASTIAN BREITFELDER, and TIMO STROBL — IFB, Julius-Maximilians Universität Würzburg, 97070 Würzburg, Röntgenring 11

We are presenting a novel attempt to combine in-situ and ex-situ measurements for aluminum alloys. As a model alloy we have chosen an Al-1.7Cu-1.3Mg (at.%) alloy, which has been cast from high purity elements (5N Al, 4N Cu and 4N Mg). As basic method DSC (heating ramp: 5 K/min) has been employed to determine different states during S-phase formation: onset, maximum of the exothermal peak, end of exothermal reaction. Sample states were frozen-in by an abrupt truncation of the heating ramp (5 K/min), i.e. cooling quickly to room temperature. So, the current sample state is frozen-in. After truncation all samples have been measured without further preparation by X-

ray diffraction (XRD) and positron annihilation lifetime spectroscopy (PALS). Thus we could correlate exactly different sample states, which is impossible by conventional experiments, i.e. heating to a certain temperature and then holding a certain time. This paves the way to investigate defined and comparable sample states by methods, which require an extensive sample preparation, like TEM or 3DAP, and in-situ methods like DSC or XRD at synchrotron beamlines.

15 min. break

KFM 11.7 Thu 16:15 POT 51

Local structure of titanite CaTiSiO_5 — ●ARKADIY SIMONOV — ETH Zürich, Zürich, Switzerland

Titanite, CaTiSiO_5 , is a multifunctional nesosilicate mineral which recently received attention as a material for building tunable capacitors and oscillators. Near 500K titanite shows a nonlinear dielectric response with positive dielectric tunability and thus its dielectric susceptibility can be efficiently controlled using a voltage bias, moreover capacitors made of this material have unusually low dielectric losses and thus high quality factor [1]. The origin of such a good performance is not currently understood, but one hypothesis is that it is related to an unusual locally antipolar disordered structure which is observed in titanite above 500K in the paraelectric $A2/a$ phase.

In this work we present the analysis of the local structure of titanite in the $A2/a$ phase. We use single crystal diffuse scattering as our probe and analyze it using a non-parametric method based on three dimensional difference pair distribution function ($3D-\Delta PDF$) refinement. We show that despite the $A2/a$ structure is on average paraelectric, locally it is antipolar. It shows Ti^{4+} displacements which have strong ferro correlations along the b direction and weak locally anti-ferro correlations in a and c directions. Such locally antipolar structure can provide a crossover path for the low temperature $P2_1/a$ structure under applied electric field and thus explain the low dielectric losses observed in this material.

[1] Murata, T., Asaka, T., Hirose, S. (2021). J. Am. Cer. Soc. 104(11), 5794-5802.

KFM 11.8 Thu 16:35 POT 51

Pfaffian invariant identifies magnetic obstructed atomic insulators — ●DANIEL VARJAS^{1,2,3,4}, ISIDORA ARAYA DAY^{3,4}, ANASTASIA VARENTCOVA³, and ANTON R. AKHMEROV³ — ¹Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — ²Department of Physics, Stockholm University, AlbaNova University Center, 106 91 Stockholm, Sweden — ³QuTech, Delft University of Technology, Delft 2600 GA, The Netherlands — ⁴Kavli Institute of Nanoscience, Delft University of Technology, P.O. Box 4056, 2600 GA Delft, The Netherlands

We derive a Z_4 topological invariant that extends beyond symmetry eigenvalues and Wilson loops and classifies two-dimensional insulators with a C_4T symmetry. To formulate this invariant, we consider an irreducible Brillouin zone and constrain the spectrum of the open Wilson lines that compose its boundary. We fix the gauge ambiguity of the Wilson lines by using the Pfaffian at high symmetry momenta. As a result, we distinguish the four C_4T -protected atomic insulators, each of which is adiabatically connected to a different atomic limit. We establish the correspondence between the invariant and the obstructed phases by constructing both the atomic limit Hamiltonians and a C_4T -symmetric model that interpolates between them. The phase diagram shows that C_4T insulators allow ± 1 and 2 changes of the invariant, where the latter is overlooked by symmetry indicators.

KFM 11.9 Thu 16:55 POT 51

Probing Centrosymmetry of Emergent Materials by Convergent Beam Electron Diffraction — ●S. SUBAKTI^{1,2}, Y.

WANG³, A. CHAKRABORTY⁴, A.K. SRIVASTAVA⁴, D. WOLF¹, T. DOERT³, M. RUCK³, S.S.P. PARKIN⁴, B. BÜCHNER^{1,2}, and A. LUBK¹ — ¹Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — ²Institut für Festkörperphysik, TU Dresden, D-01062 Dresden, Germany — ³Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062 Dresden, Germany — ⁴Department for Nano-Systems from Ions, Spins, and Electrons (NISE), Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle(Saale), Germany

Many exotic physics present in materials, such as chiral magnetic textures, hinges on the (non)existence of centrosymmetry. Consequently unambiguous structural determination beyond x-ray diffraction (XRD), which is to a certain extent blind to centrosymmetry, is indispensable. Here, we present structural investigation of two emergent quantum materials, namely Fe_3GeTe_2 and Rh_2NiSb , by means of convergent beam electron diffraction (CBED). Analyzing the diffraction group symmetries of the CBED patterns in combination with extinction rules and results from XRD analysis, we conclude the space group of these materials. Importantly, both phases are non-centrosymmetric, suggesting possible presence of chiral magnetic textures and multiferroicity.

KFM 11.10 Thu 17:15 POT 51

Nonsymmorphic chiral symmetry and solitons in the Rice-Mele model — ●EDWARD MCCANN — Lancaster University, Lancaster, United Kingdom

The charge-density-wave (CDW) phase of the Rice-Mele model in one dimension has alternating onsite energies and constant nearest-neighbor hopping parameters. The chiral symmetry of the CDW wave phase is nonsymmorphic, resulting in a breaking of the bulk topology by an end or a texture in the alternating energies. We consider the presence of solitons (textures in position space separating two degenerate ground states) in finite systems with open boundary conditions. We identify the parameter range under which an atomically-sharp soliton in the CDW phase supports a localized state which lies within the band gap, and we calculate the expectation value of the nonsymmorphic chiral operator for this state, and the soliton electric charge [1]. Finally, we discuss other models with similar, nonsymmorphic nonspatial symmetries.

[1] R. E. J. Allen et al, Phys. Rev. B 106, 165409 (2022).

KFM 11.11 Thu 17:35 POT 51

The Initial Molecular Interactions in the Course of Enthalpy Relaxation and Nucleation in Polyethylene terephthalate (PET) as Monitored by Combined Nanocalorimetry and FTIR Spectroscopy — ●WYCLIFFE KIPNUSU¹, EVGENY ZHURAVLEV², CHRISTOPH SCHICK^{2,3}, and FRIEDRICH KREMER¹ — ¹Peter Debye Institute for Soft Matter Physics, Leipzig University, Linnestr. 5, 04103, Leipzig, Germany — ²Universität Rostock Institute of Physics, Albert-Einstein_str. 23-24, Rostock, DE 18051, Germany — ³Kazan, Russia

Fast scanning calorimetry (FSC) and Fourier transform infrared (FTIR) spectroscopy are combined to trace for the same sample the evolution of the calorimetric properties and of the intra- and inter-molecular interactions in polyethylene terephthalate (PET). FSC enables to rapidly quench the sample to amorphous state and to monitor nucleation and crystal growth at isothermal conditions. By Determining the difference IR spectra between a quenched and an annealed sample unravels the the intra- and inter-molecular interactions in detail; (i) as first response already during enthalpy relaxation, the far reaching Coulomb interactions between the polar C=O moieties are active; (ii) in contrast, the ethylene unit and the aromatic ring show a response only, if homogeneous nucleation sets in, while the COC moiety remains uninfluenced; (iii) a hierarchy is observed in the sequence of the response of the different molecular moieties.