KFM 32: Crystal Structure Defects / Real Structure / Microstructure II

Chair: Theo Scherer (KIT Karlsruhe)

Time: Friday 9:30–11:40 Location: E 124

KFM 32.1 Fri 9:30 E 124

Novel class of rubrene single crystals with enhanced stability — •Moha Naeimi, Katharina Engster, Regina Lange, Tim Völzer, Stefan Lochbrunner, Ingo Barke, and Sylvia Speller — University of Rostock, Institute of physics, Rostock, Germany

Rubrene is an organic semiconductor recognized for its favorable properties, including high charge carrier mobility and excellent thermal stability. Its conjugated structure makes it a promising material for use in organic electronic devices. The precise control of rubrene crystallization, evolving from an amorphous to the stable orthorhombic phases enables comprehensive study of optical and electronic properties [1], as well as the investigation of exciton distribution and dynamics [2]. Through precise control of amorphous rubrene deposition on the substrate, high-rate heating and enhanced partial pressure [3], we introduce a novel class of rubrene single crystals in orthorhombic phase with different crystal orientations. Distinguished by ultra-flat and smooth surfaces with an hourglass shaped signature exhibiting four different zones of two types (i.e., diamond and triangle shaped), we characterize their optical properties and investigate their surface potential.

[1] Kathryn A. McGarry et al., Chem.Mater.2013, 25, 2254-2263

[2] Pavel Irkhin and Ivan Biaggio, Phys. Rev. Lett. 2011, 107, 017402

[3] Xin Ye et al. Chem. Mater. 2018, 30, 2, 412-420

KFM 32.2 Fri 9:50 E 124

Hidden structural transition upon dehydration of Prussian Blue analogues (PBAs) — •Yevheniia Kholina and Arkadiy Simonov — ETH Zurich, Switzerland, Department of Materials, Laboratory for Disordered Materials

Prussian blue analogues (PBAs) are a diverse family of transition metal cyanide materials with chemical formula $M[M'(CN)_6]_{1-x}\cdot\square_y\cdot nH_2O$, which we abbreviate here as M[M'] (M and M'=transition metal ions, □=vacancy). These materials are known for their highly connected porous network, enabled by structural vacancies of $M'(CN)_6$ with sufficiently large channels to transport or store small molecules and ions. Currently, these systems are actively investigated for application as hydrogen storage media, humidity sensors, and alkali ion sieves. One step that is often overlooked in the research is drying. PBAs are typically grown from water solutions and water has to be removed by heating the sample either in a vacuum or in a dry atmosphere. Since drying doesn't change the average structure, it is generally assumed that this step doesn't alter the porous network of PBAs. We demonstrate that the dehydration step in fact causes a hidden structural transition that involves irreversible rearrangements of vacancies. Such rearrangements modify the pore-network characteristic, like the fraction of accessible volume and conductance of matter through the channels. We collect diffuse scattering from Mn[Co] single crystals and use 3D-ΔPDF analysis to characterize their local structure and monitor structural changes upon water removal.

KFM 32.3 Fri 10:10 E 124

EXAFS study of exfoliated MoS2 nanoflakes in ALBA Synchrotron — •Najme Taghavi — Independent Researcher

Using an ultrasonic probe in a water-ethanol solution, MoS2 2D nanoflakes were prepared with varying ultrasonic powers and sonication times. The resulting samples were analyzed using EXAFS spectroscopy, which revealed that the oxidation-state of the Mo atom remained unchanged. However, increasing the power of the ultrasonic probe and sonication time led to changes in the Mo-S1 and Mo-Mo bond distances, with a decrease in the Mo-S2 bond distance. Additionally, longer sonication times resulted in a higher Deby-waller parameter. While increasing the sonication probe power significantly reduced the amplitude reduction parameter (S02), a slight increase was observed with longer sonication times.

10 min. break

KFM 32.4 Fri 10:40 E 124

FInding models of disorder using Inverse Ising methods — •Arkadiy Simonov — ETH Zürich, Zürich, Switzerland

Many functional materials, such as thermoelectrics or superconductors, exhibit disorder. Consequently, their properties depend crucially not only on their average structure but also on the details of their real structure. Experimentally, the real structure can be probed using single-crystal diffuse scattering; however, the analysis of this data currently relies on modeling methods like Monte Carlo and their subsequent refinement, which is very time-consuming. In this talk, we will present faster methods for constructing trial models consistent with experimental diffuse scattering based on the family of approximate solutions to the Inverse Ising problem, including susceptibility propagation and density consistency techniques. The methods naturally work well for structures with a high amount of disorder. Interestingly, they also perform well for certain cases with strong disorder correlations

KFM 32.5 Fri 11:00 E 124

Amplitude phase-field quasicrystal — •Marcello De Donno[1], Marco Salvalaglio[1,2], Luiza Angheluta[3], and Ken Elder[4] — [1]Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany — [3]Njord Centre, Department of Physics, University of Oslo, 0371 Oslo, Norway — [4]Department of Physics, Oakland University, Rochester, Michigan 48309, USA

Quasicrystals challenge classical crystallography with their atypical atomic arrangements, characterized by a lack of periodicity while retaining long-range order. They represent a unique state of matter, lying between crystalline and amorphous structures. Since their discovery in 1982, quasicrystals have been shown to be capable of improving the mechanical properties of alloys, offering heightened strength, hardness, and resistance to wear. Additionally, their propensity for low friction makes them excellent candidates for coatings aimed at diminishing wear in moving parts.

The study of quasicrystals requires understanding the interaction between the exotic microscopic arrangement and the macroscopic properties of the material. We propose a novel mesoscale theory for quasicrystals, taking advantage of an extension we designed to the amplitude phase-field crystal model. We characterize the topological defects forming in the structure, and we discuss their kinematics. Finally, we derive self-consistent laws for linear elasticity in the quasicrystal.

KFM 32.6 Fri 11:20 E 124

Quantum sensing for materials testing — •Simon Philipp[1], Niklas Mathes[2], Marvin Feuerhelm[1], Ali Riza Durmaz[1], Xavier Vidal[3], Rudolf Schäfer[4], Thomas Straub[1], and Christian Elsässer[1] — [1]Fraunhofer IWM, Wöhlerstrasse 11, 79108 Freiburg — [2]Fraunhofer IAF, Tullastraße 72, 79108 Freiburg — [3]Tecnalia, Parque Científico y Tecnológico de Gipuzkoa Mikeletegi Pasealekua, 2, E-20009 Donostia-San Sebastián (Gipuzkoa) — [4]Leibniz-Institut für Festkörper- und Werkstoffforschung, Helmholtzstraße 20, 01069 Dresden

Micromagnetic materials testing has been utilized for the measurement of a variety of relevant properties for material sciences and engineering, some of which being residual stress, micro-structure, or hardness. Recently, it has been shown [1] that the inverse magneto-strictive, or Villari effect [2] can potentially be exploited to retrieve a magnetic signature of fatigue and early-stage crack initiation in micro-mechanical specimens.

In this work, we demonstrate magneto-mechanical testing of ferromagnetic materials as a novel use case for quantum magnetometry at the interface of basic research and industry. As an example, we show recent data on magneto-mechanical testing of Fe and FeSi microspecimen under ambient conditions, using a combination of different quantum sensors.

[1] P. A. Koss et al., Applied Sciences 12, 1329 (2022). [2] G. Riesgo et al., Materials (Basel, Switzerland) 13 (2020). [3] S. C. Scholten et al., Journal of Applied Physics 130, 150902 (2021).