KFM 15: Crystal Structure Defects / Real Structure / Microstructure

Chair: Theo Scherer (Karlsruhe Institute of Technology)

Time: Thursday 9:30–13:15 Location: H9

Invited Talk KFM 15.1 Thu 9:30 H9

Is CVD diamond now ready to become an electronic material? — •Philippe Bergonzo — University College London UK — Seki Diamond System, San Jose CA, USA

CVD Diamond is an exceptional material combining superlative properties like electronic properties, thermal conductivity, biocompatibility, radiation resistance, and optical properties. These advantages make diamond an excellent material for a broad range of applications, including radiation detectors, high transparency windows, electronic devices, quantum devices, sensors, etc. Remarkable devices have been fabricated and are still respected as a reference. But still, can diamond come out of the lab to become a competitive device material? Although diamond synthesis is a pretty well-established technique, there are still more than 80% of the machines growing diamond on the planet that grow it to make gemstones. And this has always inhibited the progress this material deserved. Only very recently, and with the recent huge downturn that affects the gem business, one can consider that we may have reached an inflection point where CVD diamond may soon benefit from being something else than a gemstone. Potentially, innovative developments for physics may not be kept secret because they could be more valuable for the gem market, if this latter one is collapsing. In this context, how can we facilitate this progress? Drawing from typical cases where diamond-based devices are used for specific applications, examples will be used to illustrate material opportunities and challenges towards diamond to become a standard for device applications.

KFM 15.2 Thu 10:00 H9

Numerical analyses and loss tangent measurements for the W7-X ECRH gyrotron diamond output windows — •Gaetano Aiello[1], Andreas Meier[1], Heinrich Peter Laqua[2], Theo Scherer[1], Sabine Schreck[1], and Dirk Strauss[1] — [1]KIT, Karlsruhe, Germany — [2]IPP, Greifswald, Germany

The 140 GHz 1 MW gyrotron for the electron cyclotron resonance heating (ECRH) system at the stellarator Wendelstein 7-X (W7-X) is being upgraded to 1.5 MW continuous wave operation to increase the total heating power for achieving operating regimes with high plasma beta and low collisionality. The gyrotron features a chemical vapor deposition (CVD) polycrystalline diamond window with an aperture of 88 mm and a disk of 1.8 mm thickness and 106 mm diameter. In this work, numerical analyses of the window are shown with loss tangent values provided by experimental measurements on 25 bare diamond disks. Computational fluid dynamics (CFD) conjugated heat transfer and structural analyses were carried out to check the window performance at 1.5 MW operation, when cooled by water and silicon oil Dow Corning 200(R) 5cSt.

KFM 15.3 Thu 10:15 H9

Single- and polycrystalline diamond characterization with superconducting microresonators — •Francesco Mazzocchi[1], Martin Neidig[2], Sebastian Kempf[2], Dirk Strauss[1], and Theo Scherer[1] — [1]Karlsruhe Institute Of Technology IAM-AWP — [2]Karlsruhe Institute Of Technology IMS

The development of high optical quality, ultra-low-loss single-crystal diamond windows is essential for the realization of future nuclear fusion facilities, such as DEMO, due to the anticipated increase in power for microwave ECRH systems. So far, accurate measurement of the dielectric properties (ϵr and $\tan\delta$) of these materials has primarily relied on Fabry-Perot microwave resonators in different setups, with a resolution limit around 1E-5 in the determination of the loss tangent. Superconducting thin-film resonators, capable of reach Q factors in excess of 1E6, have the potential to assess the dielectric characteristics of ultra-low-loss materials like single- and polycrystalline diamond while offering a significant boost in resolution when compared to the state-of-the-art Fabry-Perot resonance cavities. We hereby report measurements performed at low (4 - 9 K) an ultra-low (10 - 700 mK) temperatures of several samples including single and poly-crystalline diamond. The samples have been grown with different techniques, including CVD, cloning and HPHT processes.

KFM 15.4 Thu 10:30 H9

Simulated nano-extrusion of graphene hyperbolic pseudosphere surfaces — •Peter Klaver[1], Alfredo Iorio[2], Ruggero Gabbrielli[3], and Dominik Legut[1] — [1]VSB Technical University of Ostrava, Ostrava, Czech Republic — [2]Charles University, Prague, Czech Republic — [3]Independent researcher

We produce curved graphene hyperbolic pseudosphere surfaces in molecular dynamics (MD) simulation of a nano-scale extrusion process. During the extrusion process the carbon atoms form pentagons, hexagons and heptagons and such a mixture is unrealistically less stable than pure graphite or diamond. During relaxation and lengthy high temperature annealing after the extrusion process, polycrystalline curved graphene with a limited number of point defects is formed. The point defects cause bending of the graphene and the pseudosphere edges even more. When these free edges are removed from the simulations by attaching periodic flat graphene sheets to the pseudosphere edges, the carbon atoms assume positions with a root mean square deviation of some tenths of Å from the mathematical hyperbolic pseudosphere surface. The hyperbolic pseudospheres proved to be mechanically stable against large shearing and elongation deformations as well as against annealing at 1500 K. Our methodology is easy to use, employing the REBO2 carbon interaction potential within the open source MD code LAMMPS. Our method offers a practical way to create simulated stable, curved graphene surfaces with a wide variety of desired shapes. It allows for the testing in advance of the stability of graphene shapes that are to be produced experimentally.

KFM 15.5 Thu 10:45 H9

Inverted Designs of Dielectric Metasurfaces Based on TiO_2.: A Study on Quasi-Bound States in Continuum (qBIC) — •Justin Schulz[1], Jack Dobie[1,2], Oisin McCormack[1,2], Yongliang Zhang[1], Hodjat Hajian[1], Owen Moynihan[2], Brian Corbett[2], and A. Louise Bradley[1,2] — [1]School of Physics, Trinity College Dublin, Dublin 2, Ireland — [2]IPIC, Tyndall, University College Cork, Cork, Ireland

Dielectric metasurfaces, engineered to manipulate light primarily by controlling the phase and amplitude of the scattered light, have garnered significant interest in recent years, particularly due to their ability to support quasi-Bound States in Continuum (qBIC).
Building upon previous work on slotted disk metasurfaces fabricated in Si_3N_4, we investigate inverted TiO_2-based designs. TiO_2, with its high refractive index, offers distinct advantages in enhancing the resonance properties of dielectric metasurfaces, enabling more efficient light-matter interactions. A key objective of this work is to perform a comparative analysis between slotted disk structures and their inverted counterparts, with a focus on their respective lattice and qBIC modes. Future prospects of TiO_2-based dielectric metasurfaces and the potential applications in low-energy switching and polariton lasing are discussed, with a particular focus on their integration with transition-metal dichalcogenide (TMDC) monolayers or quantum dots. This project is funded through; Taighde Éireann/Research Ireland Frontiers for the Future Award - SFI-21/FFP-P/10187, 12/RC/2278_2, and 12/RC/2276_P2.

15 Minutes Break

KFM 15.6 Thu 11:15 H9

Phase modifications in Beta-Gallium Oxide via Focus ion beam irradiations — •Umutcan Bektas, Nico Klingner, Paul Chekhonin, Fabian Ganss, Rene Hübner, Maciej Oskar Liedke, and Gregor Hlawacek — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Gallium oxide (Ga2O3) is a highly versatile material with power electronics, optoelectronics, and battery technologies applications. Among its polymorphs, monoclinic β-Ga2O3 is the most chemically and thermally stable phase. However, managing the metastable polymorph phases remains challenging, and the fabrication technology for nanoscale structures is still under development. We aim better to understand the polymorph conversion mechanisms under ion irradiation. In this study, we investigate the β-Ga2O3 samples irradiated with different ions and fluences, together with α- and κ-Ga2O3 thin films.

Focused ion beam (FIB) irradiation was used to locally modify the samples under controlled conditions by varying the ion beam current, size, spacing, scan type, and ion species. The irradiated regions were characterized using electron backscatter diffraction and transmission electron microscopy to analyze structural changes. Broad beam irradiation experiments were complemented by positron annihilation spectroscopy methods to determine defect types and concentrations. Initial results indicate that spatially resolved polymorph transitions can be achieved using FIB irradiation. In addition, the defect size and concentration were found to depend on the polymorph and the implanted ion species, providing critical into defect engineering in Ga2O3.

KFM 15.7 Thu 11:30 H9

An EXAFS analysis of the laser-driven tetragonal to cubic phase-transition in $BaTiO_3$ — •Janosch Tasto[1], Rajdwip Bhar[1], Simon Rauls[1], Marco Reinhard[2], Dimosthenis Sokaras[2], Uwe Bovensiepen[1], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]SLAC National Accelerator Laboratory, Stanford University

This work aims to establish time-resolved Extended X-ray Absorption Fine Structure (tr-EXAFS) spectroscopy as a methodology for solids where the structural information of the EXAFS is combined with a pump-probe setup to study local dynamic lattice processes in the time domain. As a first step along this road, the information contained in a difference-EXAFS scan between the pumped and unpumped state is analyzed.

As proof of concept, the structural cubic to tetragonal phase transition in ferroelectric $BaTiO_3$ is analyzed. The coexistence of displacive and order-disorder phenomena accompanying this transition is debated in the literature of this widely investigated material. Difference-EXAFS scans at the Ti-K and Ba-L_3 edge between the tetragonal and cubic phase provide a direct way to investigate changes in structure and thermal induced disorder in the vicinity of the absorbing atom. We correlate our spectroscopic findings with *ab initio* multiple-scattering calculations using the FEFF10 code to quantify thermal and structural contributions.

We thank the Deutsche Forschungsgemeinschaft (in the framework of the Collaborative Research Center 1242) for financial support.

KFM 15.8 Thu 11:45 H9

Dislocation correlations in GaN epitaxial films revealed by EBSD and XRD — •Domenik Spallek, Vladimir M. Kaganer, Philipp John, Oliver Brandt, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Threading dislocations in group-III nitrides are omnipresent and are a challenge especially in heteroepitaxial growth for device applications. However, the correlation of individual dislocations with each other and the resulting screening of the strain is often disregarded although it is a necessity to describe elastic energies in an extended crystal.

In this study, two GaN epitaxial layers with threading dislocation densities (TDD) of 5×10^8 cm^{-2} and 1.8×10^{10} cm^{-2} are investigated by x-ray diffraction (XRD) and high-resolution electron backscatter diffraction (HR-EBSD), complemented by Monte Carlo simulations to model and interpret the experimental results.

While the XRD measurement directly gives quantitative results about the average strain in the illuminated area, a cross-correlation analysis of Kikuchi patterns results in spatially-resolved maps for the components of the strain and rotation tensors. Through an analysis of the strain-strain correlation functions for the measured and simulated maps, it is found that the spatial resolution in the HR-EBSD maps is highly anisotropic. Furthermore, we discover that the strain is significantly underestimated for higher dislocation densities. As main result, the screening distances for dislocations were determined as 2 μm and 0.3 μm for the sample with the lower and higher TDD, respectively.

KFM 15.9 Thu 12:00 H9

Multiscale modeling of intergranular corrosion in iron — •Vahid Jamebozorgi[1], Karsten Rasim[2], and Christian Schröder[3] — [1]Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences and Arts, Interaktion 1, 33619 Bielefeld, Germany — [2]Faculty of Physics, Bielefeld University, Universitätsstraße 4, 33615 Bielefeld, Germany — [3]Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences and Arts, Interaktion 1, 33619 Bielefeld, Germany

Localized corrosion, particularly intergranular corrosion, causes a significant economical and structural challenge across various industries. An accurate predictive intergranular corrosion modeling should incorporate atomic scale details, including crystallographic aspects of grain boundaries, and their evolution by time increment. However, the size and scale limitations imposed by atomistic methods hinder the development of realistic models. To overcome these limitations, we propose a novel multiscale modeling approach that combines the detailed atomistic insights provided by reactive molecular dynamics with the computationally tractable finite element method. This multiscale strategy not only ensures the preservation of crucial atomistic details but also enables the simulation of larger spatial and temporal scales, thereby offering a comprehensive view on the microstructure*s evolution during the intergranular corrosion process.

15 Minutes Break

KFM 15.10 Thu 12:30 H9

Landau Theory for Quasicrystals at the Mesoscale — •Marcello De Donno[1], Luiza Angheluta[2], Ken R. Elder[3], and Marco Salvalaglio[1,4] — [1]Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany — [2]Njord Centre, Department of Physics, University of Oslo, 0371 Oslo, Norway — [3]Department of Physics, Oakland University, Rochester, Michigan 48309, USA — [4]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany

Quasicrystals challenge traditional concepts of crystallinity by exhibiting ordered yet aperiodic atomic structures. Their peculiar atomic arrangements give rise to exceptional physical properties, including high hardness, low friction, and remarkable wear resistance, making them worth exploring for high-performance engineering applications. Additionally, their slow dislocation creep leads to high-temperature strength and stability in plastic regimes. We present a mesoscale field theory that unifies the modeling of growth, elasticity, and dislocations in quasicrystals. Using the amplitude formulation of the density-wave representation, our approach models the dynamics of quasicrystals through a free energy functional for complex amplitudes, with non-conserved dissipative dynamics describing their evolution. By specifying only the lattice structure in reciprocal space, our theory self-consistently captures elasticity-including phononic and phasonic deformations-along with defect nucleation and motion. Predictions include the kinematics of dislocations and the formation of semi-coherent interfaces, offering new insights into the mechanics of quasicrystals.

KFM 15.11 Thu 12:45 H9

An all-order phonon approach to thermal diffuse scattering — •Benjamin Fahl and Arkadiy Simonov — ETH,Zurich,Switzerland

Phonons play a role in various phenomena, from superconductivity through phonon-electron coupling and spintronics via phonon-spin interactions, to dynamical stability of solids, and are fundamental to elastic properties. They can be probed by measuring Thermal Diffuse Scattering (TDS) from single crystals. However, modelling of the TDS, is a computational challenge due to the number of intensities in the experiment. With existing software, like AB2TDS, the full experiment can be calculated only in one- or two-phonon approximations. Approximations of higher order are possible, but are computationally expensive and can be performed only on small portions of reciprocal space. In this work, we propose a new method for modeling and fitting TDS signals using joint atomic displacement parameters in YELL. This approach uses the crystal's dynamical matrix as input, which is derived by various methods including universal potentials, DFT, or approximated from elastic constants. By using a Fast-Fourier Transform, our method can quickly calculate large volumes of TDS in infinite phonon approximation. This development will enhance the 3D-ΔPDF suite, enabling extraction of elastic constants from various materials and extending to the analysis of high-amplitude soft phonons, which are relevant in negative thermal expansion materials like ScF_3. The softwares capability to handle higher-order phonon contributions makes it particularly valuable for systems where these effects are significant, addressing a current gap in available tools.

KFM 15.12 Thu 13:00 H9

Solving the phase problem: retrieving complex structure factors using Large-Angle Rocking-Beam Electron Diffraction — •Sam Fairman[1], Grigory Kornilov[2], Benedikt Haas[2], Zbignew Galazka[3], Adnan Hammud[4], Niklas Delby[5], and Christoph T. Koch[2] — [1]Physikalisch Technische Bundesanstalt, Berlin, Germany — [2]Humboldt Universität zu Berlin, Berlin, Germany — [3]Leibniz-Institut für Kristallzüchtung, Berlin, Germany — [4]Fritz-Haber-Institut, Berlin, Germany — [5]Nion Company, Kirkland, WA,

USA

X-ray crystallography phasing methods have previously been successfully applied to electron diffraction experiments. However, dynamical scattering, caused by the electron's much larger scattering cross section, is normally viewed as a hindrance to structural determination and is mitigated, e.g. by continuous rotation or precession. Presented here is an ab-initio method that makes use of dynamical scattering to solve the phase problem directly from experimental data. A custom weighting scheme is combined with the ADAM optimizer to directly fit the complex structure factors in the Bloch-wave formalism to Large-Angle Rocking-Beam Electron Diffraction data. Our method allows for an approximate $5-$fold increase in spatial resolution compared to the largest spatial frequency directly measured. This recovery of resolution is ideal for beam sensitive materials where high order diffraction data is impossible to measure. Simulated and experimental results are presented for non-centrosymmetric GaN and centrosymmetric $\beta-Ga_2O_3$.