KFM 5: Instrumentation, Microscopy and Tomography with X-ray Photons, Electrons, Ions and Positrons

Chair: Theo Scherer (Karlsruhe Institute of Technology)

Time: Monday 15:00–17:00 Location: H9

KFM 5.1 Mon 15:00 H9

Simulation study of beam splitting of vortex electron beams inside crystals — •Christian Bick and Dorothee Hüser — Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

Electron vortex beams have long been of interest for applications such as electron magnetic circular dichroism (EMCD), beam shaping and nanoparticle manipulation. They have attracted new attention with the recent development of an orbital angular momentum (OAM) sorter, theoretical developments in analysis of momentum transfer and as a quantum logic gate.

When propagating through a crystal, the vortex electron wave interacts with the asymmetric crystal potential, causing the wave to split into intensity centres around atomic columns, called channelling. This behaviour gives rise to a total OAM that can no longer be described by an integer vortex quantum number. In this simulation-based study we track the behaviour of electron beams inside different crystals. We show an in-depth analysis of the wave phase propagating through the crystal for different materials, focussing our research on beam splitting into intensity centres with their own OAM. This study was carried out using multislice simulations of the electron beam propagation through the crystal potential together with vector analysis to identify the local vortex centres.

KFM 5.2 Mon 15:15 H9

Single-phase valence band structure of a $Ge_{0.85}Si_{0.15}$ Crystal - Insights by momentum microscopy — •Andreas Fuhrberg[1], Pia M. Düring[1], Kevin Gradwohl[2], Olena Fedchenko[3], Yaryna Lytvynenko[3], Olena Tkach[3], Sergii Chernov[4], Christoph Schlueter[4], Gerd Schönhense[3], Hans-Joachim Elmers[3], and Martina Müller[1] — [1]Universität Konstanz — [2]IKZ, Berlin — [3]Universität Mainz — [4]DESY, Hamburg

Spin qubits are the fundamental components of quantum computing devices. Planar $Ge/Ge_{1-x}Si_x$ heterostructure qubits have proven to be advantageous for upscaling and fabrication. The Si concentration of the $Ge_{1-x}Si_x$ buffer has been shown to be an important parameter for tuning the valence band (VB) electronic structure of $Ge/Ge_{1-x}Si_x$ qubits by homoepitaxial strain, which is difficult to realize experimentally without phase separation.
Synchrotron-based hard X-ray momentum microscopy (MM) is used to study the VB electronic structure of a $Ge_{0.85}Si_{0.15}$ single crystal grown to provide well-defined small strain. Our MM experiments reveal an individual VB structure of $Ge_{0.85}Si_{0.15}$, that is clearly distinct from Si and Ge references. The shape of the heavy/light hole band and split-off band follows that of Ge, but with lower binding energies at Γ, X and L points and a reduced split-off band gap, hence no evidence for phase separation. Additional diffraction experiments, supported by Bloch wave calculations, show that the Si atoms occupy Ge lattice positions within the crystal. This result is very promising for the future experimental realization of single-phase GeSi-based spin qubits.

KFM 5.3 Mon 15:30 H9

Miniature device for in situ application of strain inside Scanning Tunnelling Microscope — •Uladzislau Mikhailau, Rashed Alhamli, and Peter Wahl — University of St Andrews, St Andrews, United Kingdom

Recent studies [1] have demonstrated that uniaxial strain significantly affects the macroscopic properties of strongly correlated electron systems. Scanning Tunneling Microscopy (STM) is a powerful technique for investigating changes in the electronic structure induced by such lattice deformation. Controlled application of strain adds an additional degree of freedom to tune, e.g., Van Hove singularities in quantum materials [2] and thereby control their ground state. To perform such studies, we have developed a specialized STM sample holder capable of applying strain at cryogenic temperatures and in high magnetic fields. Strain is applied by bending a plate beneath the sample, with stress adjustable up to the crystal's buckling limit. The device allows for the application of uniaxial or biaxial strain, depending on the configuration of the bending plate. With these capabilities, the system provides a versatile platform for exploring strain-induced phenomena through a powerful combination of atomic scale imaging in strain tuning.

[1] Clifford W. Hicks et al., Strong Increase of T_c of Sr_2RuO_4, Under Both Tensile and Compressive Strain. Science 344, 283 (2014).

[2] Chandrasekaran, A., Rhodes, L.C., Morales, E.A. et al. On the engineering of higher-order Van Hove singularities in two dimensions. Nat Commun 15, 9521 (2024).

KFM 5.4 Mon 15:45 H9

Defects in Materials: Limitations of the Trapping Model - the Influence of Corrupt Components in Positron Lifetime Spectra — •Torsten Staab, Dominik Boras, and Danny Petschke — LCTM / IFB, Department of Chemistry, University of Wuerzburg, Roentgenring 11, D-97070 Wuerzburg, Germany

Since the early days of positron lifetime spectroscopy, the meaningful decomposition of lifetime spectra into two or more components has been highly disputed. This procedure is extremely important to extract correct defect densities. Since the procedure of fitting several exponential decays folded by a mimicked instrumental resolution function to extract positron lifetimes and intensities is an "ill-posed problem", the goodness of the fit relies heavily on the quality of the recorded data. In the past there have been several simulation attempts to create and decompose spectra into two or three components (lifetimes and intensities). However, those attempts always assumed "ideal", random number Monte Carlo simulated data. Hence, the following data analysis has been fairly straight forward. By our recently developed digital twin of a positron lifetime spectrometer we could clearly see the strong influence of back scattered and corrupted coincidences on the lifetime spectrum. Unfortunately, those events cannot be removed by physically filtering digitised pulses. Changes in the geometry of the set-up lead to much more realistic bulk positron lifetimes of light materials (Mg, Al, Si) in accordance with calculations and correct decompositions in accordance with the trapping model, while the efficiency is reduced by 95%.

15 min. break

KFM 5.5 Mon 16:15 H9

Investigating Mechanical Properties of Porous Materials with Brillouin Light Scattering and Machine-Learned Force Fields — •Florian Lindner[1], Nina Strasser[1], Sandro Wieser[2], Egbert Zojer[1], and Caterina Czibula[3] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institute of Materials Chemistry, TU Wien, Austria — [3]Institute of Bioproducts and Paper Technology, Graz University of Technology, Austria

Brillouin light scattering (BLS) is based on the inelastic scattering of light from thermally activated gigahertz acoustic phonons. As the later are correlated with a material's elastic tensor via the Christoffel dispersion the elastic constants can be determined in a non-destructive and contactless manner. From these, practically relevant mechanical properties like the Young's modulus can be derived. In this contribution we show, how BLS can be used to study the mechanical properties of metal organic frameworks (MOFs), a class of porous crystalline materials with a plethora of possible applications. The measured mechanical properties are then compared to state-of-the-art dispersion corrected DFT calculations and simulations based on machine learned interatomic potentials [1], which speed up simulations by many orders of magnitude [2]. This allows to additionally determine thermoelastic properties of MOFs at elevated temperatures, which in combination with suitable experiments will portray the full potential of the used methodology.

[1] arXiv:2409.07039 (submitted to JPCL, currently under review); [2] npj Comput Mater 10, 18 (2024);

KFM 5.6 Mon 16:30 H9

TwinPALS: A Digital Twin for Laboratory-Based Positron Annihilation Lifetime Spectroscopy — •Dominik Boras — Julius-Maximilians University, Würzburg, Germany

In this work, we present a comprehensive digital twin of a laboratory-based Positron Annihilation Lifetime Spectroscopy (PALS) system.

This digital twin is capable of simulating entire spectra while incorporating all effects of the hardware used in the PALS system, as well as varying source strengths. For the first time, it is possible to visualize unwanted components within the lifetime spectrum and assess their impact on the interpretability of these spectra. The digital twin enables the identification of issues within one's own setup and allows for digital testing of potential optimizations before physical implementation. The TwinPALS system is designed in a modular structure. The first module is responsible for constructing the digital world, taking into account the influences of position, dimension, and the materials used. The second module combines a customized version of the DLTPulsgenerator with software to process the information from the first module, incorporating considerations of radioactivity, positron lifetime, and PMT blurring. The third and final module serves to visualize the output stream from the second module, utilizing the DDRS4PALS software. In summary, this system is a modular digital twin that can be adapted to the requirements of the system being simulated.

KFM 5.7 Mon 16:45 H9

TwinPALS: A digital Twin for laboratory-based Positron Annihilation Lifetime Spectroscopy — •Dominik Boras, Danny Petschke, and Torsten Staab — LCTM / IFB, Department of Chemistry, University of Wuerzburg, Roentgenring 11, D-97070 Wuerzburg, Germany

In this work, we present a comprehensive digital twin of a laboratory-based Positron Annihilation Lifetime Spectroscopy (PALS) system. This digital twin is capable of simulating entire spectra while incorporating all effects of the hardware used in the PALS system, as well as varying source strengths. For the first time, it is possible to visualize unwanted components within the lifetime spectrum and assess their impact on the interpretability of these spectra. The digital twin enables the identification of issues within one's own setup and allows for digital testing of potential optimizations before physical implementation. Additionally, this approach facilitates the validation of software-based physical filters and provides a unique opportunity to visualize their effects on unwanted components in the spectra. The digital twin represents a comprehensive simulation framework that allows for a multitude of hardware investigations in the digital realm, effectively functioning as a digital mirror of the complete hardware setup. This enables researchers to conduct extensive, risk free experiments and optimize system configurations, ultimately improving the quality and reliability of PALS data.