KFM 9: Microscopy and Tomography with X-ray Photons, Electrons, Ions and Positron

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

Time: Wednesday 9:00–13:15 Location: POT 106

KFM 9.1 Wed 9:00 POT 106

$FePX_3$ (X: S, Se): A stable new 2D material for water splitting — •Hafiz Muhammad Zeeshan[1], Sandhya Sharma[1], Elena Voloshina[1,2], and Yuriy Dedkov[1,2] — [1]Centre of Excellence ENSEMBLE3 Sp. z o.o., Wolczynska Str. 133, 01-919 Warsaw, Poland. — [2]Department of Physics, Shanghai University, 99 Shangda Road, 200444 Shanghai, P. R. China.

The interaction of high-quality transition metal trichalcogenides (TMTs) single crystals $FePX_3$ (X: S, Se) with water molecules is studied using NEXAFS and XPS in a wide range of temperature and partial pressure of H_2O. The physisorption nature of interaction between H_2O and $FePX_3$ is found at low temperatures and relatively small concentrations of water molecules, that is supported by the DFT results. When temperature of the $FePX_3$ samples and partial pressure of H_2O are increased, the interaction at the interface is defined by two competing processes - adsorption of molecules at high partial pressure of H_2O and desorption of molecules due to the increased surface mobility and physisorption nature of interaction. Our intensive XPS/NEXAFS experiments accompanied by DFT calculations bring new understanding on the interaction of H_2O with surface of a new class of 2D materials, TMTs, pointing to their stability and reactivity, that is important for further applications in different areas, like sensing and catalysis.

KFM 9.2 Wed 9:20 POT 106

Solving complex nanostructures with ptychographic atomic electron tomography — •Philipp Pelz — Institute for Micro- and Nanostructure Research, Friedrich-Alexander Universitaet Erlangen, Cauerstr. 3, 91058 Erlangen

Knowledge of the three-dimensional atomic structure of natural and manufactured materials allows us to calculate their physical properties and deduce their function from first principles. Phase-contrast electron microscopy methods like ptychography are ideally suited to solve the 3D atomic structure of nanomaterials containing light and heavy elements. We perform mixed-state electron ptychography from 34.5 million diffraction patterns to reconstruct a high-resolution tilt series of a double wall-carbon nanotube (DW-CNT), encapsulating a complex ZrTe sandwich structure. Class averaging of the resulting reconstructions and subpixel localization of the atomic peaks in the reconstructed volume reveals the complex three-dimensional atomic structure of the core-shell heterostructure with 17 picometer precision.

KFM 9.3 Wed 9:40 POT 106

Status and Upgrades of the Beam Facility at the High-Intensity Positron Source NEPOMUC — •Christoph Hugenschmidt — Forschungs-Neutronenquelle Heinz Maier-Leibnitz (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The bright low-energy positron beam provided by the neutron induced positron source in Munich (NEPOMUC) at FRM II is used in a large variety of experiments in materials science, condensed matter and surface physics as well as in fundamental research, e.g., for the creation of a positron-electron pair plasma. Within this contribution, an overview of the current status and developments of the positron beam facility with its instrumentation is given. Plans for the installation of a buffer gas trap for the creation of high-density positron pulses as well as ideas for increasing the performance of the remoderated positron bam are elucidated. The upgrades of the positron beam instruments (i) Coincident Doppler-Broadening Spectrometer (CDBS) using a scanning positron micro beam, (ii) instrument for the 2D measurement of the Angular Correlation of Annihilation Radiation (2D-ACAR), and (iii) the surface spectrometer are highlighted. Finally, the planned extension of the positron beam facility and the future operation of positron beam experiments in the experimental hall East are presented.

KFM 9.4 Wed 10:00 POT 106

Optimising the scintillator geometry for positron annihilation spectroscopy - A GEANT4 Simulation — •Dominik Boras — Chair of chemical technology and material synthesis, Würzburg, Germany

To better understand the efficiency and the role of backscattering events of a Positron annihilation lifetime spectrometer, a GEANT4 simulation of the atomic processes is conducted. The gamma quanta from the radioactive decay of 22-Na and from the annihilation positron are detected by a scintillator-photomultiplier combination. In the basic setup of the simulation, as scintillation material plastic BC422Q-0.5wt.% was used due to its good energy resolution. Different geometries of the scintillator (box, cone, pyramid and tube) were simulated and their influence on the detection efficiency and the instrument resolution function was investigated. Furthermore, the influence of the measured sample material (density, atomic number) on the scattering of gamma quanta was considered.

KFM 9.5 Wed 10:20 POT 106

Formation and time dynamics of hydrogen-induced vacancies in nickel — •Maik Butterling[1], Luca Chiari[2], Masanori Fujinami[2], Maciej Oskar Liedke[1], Eric Hirschmann[1], Ahmed Gamal Attallah[1], and Andreas Wagner[1] — [1]Institute for Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Applied Chemistry and Biotechnology, Chiba University, 1-33 Yayoi, Inage, Chiba 263-8522, Japan

The formation of hydrogen-induced defects in nickel was investigated by positron annihilation lifetime spectroscopy and the time dynamics of those defects during room temperature aging was tracked with an unprecedented time resolution of the order of minutes using an ultrahigh-flux slow positron beam. Those measurements showed the formation of a large number of atomic vacancies simply by hydrogen addition at room temperature. It could be proved that they were monovacancy-level defects and that hydrogen was trapped and bound to those vacancies during the hydrogen charge. Room temperature aging, i.e. below the stage III temperature in Ni, and the concomitant hydrogen desorption induced the agglomeration of those monovacancies into large vacancy clusters which remained even after all the hydrogen had desorbed and hydrides had disappeared.

These results [1] constitute the first empirical evidence that vacancy-hydrogen complexes are induced in Ni only by hydrogen charging and demonstrate that hydrogen has a primary role in the formation and stabilization of vacancies even at room temperature.

[1] L. Chiari, et al., Acta Materialia 219(2021), 117264

KFM 9.6 Wed 10:40 POT 106

Electron tomography analysis of Ge/SiGe asymmetrically coupled quantum wells — •Ekaterina Paysen[1], Giovanni Capellini[2,3], and Achim Trampert[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]IHP - Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany — [3]Dipartimento di Scienze, Università degli Studi Roma Tre, Roma, Italy

We present a method for the three-dimensional (3D) characterisation of the morphology and chemical intermixing of buried interfaces in a Ge/SiGe asymmetrically coupled quantum well structure applying electron tomography method based on high-angle annular dark-field (HAADF) scanning transmission electron microscopy. For this purpose, a needle-shaped specimen with a diameter of a few 100 nanometres is prepared with a focused ion beam, from which a tilt series of HAADF projections is recorded. Subsequently, the series is used to calculate a complete 3D image or tomogram of the specimen with the simultaneous iterative reconstruction technique. The analysis of iso-concentration surfaces enables a quantitative determination of morphological quantities such as the root mean square roughness and lateral correlation length individually for each interface. Subnanometre-thin cross-sections from the tomogram are used to measure the chemical interface width with the highest spatial resolution. An advantage of this method is thus the investigation of the interfaces as 3D entities in their buried state on a length scale of a few 100 nanometres without the projection problem.

15 min. break

KFM 9.7 Wed 11:15 POT 106

Weak-signal extraction enabled by deep-neural-network de-

noising of diffraction data — •Jens Oppliger[1], Michael Marco Denner[1], Julia Küspert[1], Qisi Wang[1], Oleh Ivashko[2], Ann-Christin Dippel[2], Martin von Zimmermann[2], Fabian Donat Natterer[1], Mark Hannes Fischer[1], Titus Neupert[1], and Johan Chang[1] — [1]Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland — [2]Deutsches Elektronen-Synchrotron DESY, Notkerstrasse 85, 22607 Hamburg, Germany

Removal or cancellation of noise has wide-spread applications for imaging and acoustics. In every-day-life applications, denoising may even include generative aspects which are unfaithful to the ground truth. For scientific applications, however, denoising must reproduce the ground truth accurately. We show how data can be denoised via a deep convolutional neural network such that weak signals appear with quantitative accuracy. In particular, we study X-ray diffraction on crystalline materials. We demonstrate that weak signals stemming from charge ordering, insignificant in the noisy data, become visible and accurate in the denoised data. This success is enabled by supervised training of a deep neural network with pairs of measured low- and high-noise data. This way, the neural network learns about the statistical properties of the noise. We demonstrate that using artificial noise (such as Poisson and Gaussian) does not yield such quantitatively accurate results. Our approach thus illustrates a practical strategy for noise filtering that can be applied to challenging acquisition problems.

KFM 9.8 Wed 11:35 POT 106

Positron beams for materials research — •Andreas Wagner[1], Maik Butterling[1], Ahmed Gamal Elsherif[1], Eric Hirschmann[1], Maciej Oskar Liedke[1], and Reinhard Krause-Rehberg[2] — [1]Institute for Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Dept.of Physics, 06099 Halle/Saale, Germany

The Helmholtz-Center Dresden - Rossendorf operates several user beamlines for materials research using positron-annihilation energy and lifetime spectroscopy. The superconducting electron linear accelerator ELBE drives several secondary beams including hard X-ray production from electron-bremsstrahlung, which serves as an intense source of positrons by means of pair production. The Mono-energetic Positron Source MePS [1] utilizes positrons with variable kinetic energies ranging from 0.5 to 18 keV for depth profiling of atomic defects and porosities on nm-scales in thin films. High timing resolutions (σt *100 ps) at high average rates (105 s-1) and adjustable beam repetition rates allow performing high-throughput experiments. The MePS facility has partly been funded by the Federal Ministry of Education and Research (BMBF) with the grant PosiAnalyse (05K2013). AIDA was funded by the Impulse- und Networking fund of the Helmholtz-Association (FKZ VH-VI-442 Memriox) and by the Helmholtz Energy Materials Characterization Platform. [1] A. Wagner, et al., AIP Conference Proceedings, 1970, 040003 (2018).

KFM 9.9 Wed 11:55 POT 106

Strain Distribution in Au/ZnO Microstructures for biomagnetic sensing utilizing Scanning X-Ray Nano Diffraction and Coherent X-Ray Diffraction Imaging — •Philipp Jordt[1], Niklas Wolff[1], Stjepan Hrkac[2], Jorit Gröttrup[1], Sindu Shree[1], Di Wang[3], Anton Davydok[4], Christina Krywka[4,1], Ross Harder[5], Christian Kübel[3], Oleg Shpyrko[2], Rainer Adelung[1], Olaf Magnussen[1], Lorenz Kienle[1], and Bridget Murphy[1] — [1]Kiel University, Germany — [2]UCSD, USA — [3]KNMF, KIT, Germany — [4]Hereon, Germany — [5]XSD, ANL, USA

Magnetic field sensors based on piezoelectric and magnetostrictive materials are a possible path to a new generation of sensors, capable of detecting bio-magnetic fields from human physiology at room temperature in an unshielded environment. A huge hurdle are the very low field strengths of these signals. One approach to further enhance the sensitivity is employing the piezotronic effect, which arises from the combination of a piezoelectric material and a Schottky contact. Here, a study on the strain distribution in ZnO nano and microrods coated with gold is presented. Scanning X-ray nano diffraction mapped the 2 dimensional strain distribution across 30-50 μm rods together with insitu current-voltage curves. It is demonstrated that the gold coating and the resulting Schottky contact has a direct impact on the lattice parameters in vicinity of the Au/ZnO interface and further, that the crystal quality of the ZnO is immensely influential on the properties of the Schottky contact. The full 3D strain distribution inside a 1 μm rod was characterized by coherent X-ray diffraction imaging.

KFM 9.10 Wed 12:15 POT 106

Correlation of Mechanical Stress and the Positron Lifetime in Aluminum Alloys — •Lucian Mathes[1], Vassily Vadimovitch Burwitz[1], Adrian Langrehr[1], Maik Butterling[2], Maciej Oskar Liedke[2], Eric Hirschmann[2], Andreas Wagner[2], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum, TU München — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics

Positron annihilation lifetime spectroscopy (PALS) is a sensitive technique to analyze the type and concentration of lattice defects on an atomic level. We applied ex-situ and in-situ PALS to plastically deformed technical Al and Al alloys. Thereby we are able to observe the creation and evolution of stress-induced defects in the region beyond the elastic Hook regime of the specimen. The in-situ bulk measurements were performed using a β^+ emitter in a new experimental setup combining tensile tests and PALS at TUM that also allows for investigation of the reversible elastic deformation of samples. The depth-dependent positron lifetime was measured ex-situ at the accelerator-based positron source MEPS at ELBE. For each sample we recorded the tensile stress, and the corresponding stress-strain curves. This allows us to determine the relation between applied stress, strain and mean positron lifetime. Within this contribution, we also discuss the evolution of the defect population with increasing deformation by examining the intensity change of the different positron lifetime components found in the PALS spectra.

KFM 9.11 Wed 12:35 POT 106

Start-to-end simulations of partially coherent X-ray imaging experiments at synchrotron beamlines — •Martin Seyrich — Deutsches Elektronen-Synchrotron DESY, Centre for X-ray and Nano Sciece CXNS, Hamburg, Germany

In the last decade, coherent X-ray imaging techniques, such as ptychography and holography, have grown a large user base at third and fourth generation X-ray light sources. In contrast to conventional microscopy techniques, coherent imaging techniques do not directly project an image on a detector. Instead, the image of the object is retrieved algorithmically from interference patterns, usually under the assumption of a fully coherent illumination.

Real X-ray sources are not perfectly coherent, they can be simulated as stochastic sources emitting an ensemble of waves. These waves can be propagated from the source through the entire beamline ending at the detector. The simulated interference patterns can then be treated with the same phase retrieval algorithms as experimental data.

Here, we present our extensions to existing established simulation software (OASYS / SRW) that permit the user to perform such start-to-end simulations with relative ease. We will present simulated data sets of ptychographic and holographic experiments, and discuss the computational demands of such simulations.

KFM 9.12 Wed 12:55 POT 106

Illumination corrected X-ray near-field microscopy — •Thea Engler[1,2], Johannes Hagemann[1], Christian G. Schroer[1,2], and Mathias Trabs[3] — [1]Deutsches Elektronen-Synchrotron, DESY, Germany — [2]Universität Hamburg, Germany — [3]Karlsruhe Institut of Technology, KIT, Germany

At synchrotron facilities, such as Petra III at DESY, small objects (μm) can be imaged with X-ray propagation-based phase-contrast imaging, i.e. near-field holography (NFH).

Reaching high resolution involves the use of nano-focusing optics. The imperfections of these optics cause aberrations in the illumination of the object and also upon further propagation in the measured hologram of the object. To correct the hologram for these artifacts, a flat-field correction must be applied. Considering a temporally stable beam, the hologram is divided by an empty-beam image, i.e. an image of the illumination without the object. With the common flat-field correction, the hologram is not fully corrected for the illumination function since the division is performed only in intensities in the detector plane.

Instead, the division of illumination and object should be performed in terms of complex wavefields in the sample plane, where the object transmission function physically interacts with the illumination function. Using a simulated dataset, we develop an algorithmic scheme using the recently proposed refractive formulation to take the illumination during the phase retrieval process properly into account.