KFM 3: Microscopy and Tomography with X-ray, Photons, Electrons, Ions and Positrons

Time: Monday 9:30–10:50 Location: H7

KFM 3.1 Mon 9:30 H7

Small-Angle X-ray Scattering: Characterization of arbitrarily shaped nanoparticles using the Debye equation — •Jérôme Deumer[1], Brian Richard Pauw[2], Sylvie Marguet[3], Dieter Skroblin[1], Olivier Taché[3], Michael Krumrey[1] und Christian Gollwitzer[1] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin — [2]Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin — [3]Université Paris-Saclay, CEA, CNRS, NIMBE, 91191 Gif-sur-Yvette, France

We propose a versatile software package in the form of a Python extension, named CDEF (Computing Debye's scattering formula for Extraordinary Formfactors), to approximately calculate scattering profiles of arbitrarily shaped nanoparticles for small-angle X-ray scattering (SAXS). CDEF generates a quasi-randomly distributed point cloud in the desired particle shape and then applies the open source software DEBYER for efficient evaluation of Debye's scattering formula to calculate the SAXS pattern. The usage of the software is demonstrated for the evaluation of scattering data of Au nanocubes with rounded edges, which were measured at the four-crystal monochromator beamline of PTB at the synchrotron radiation facility BESSY II in Berlin. Our implementation is fast enough to run on a single desktop computer and perform model fits within minutes. The accuracy of the method was analyzed by comparison with analytically known form factors.

KFM 3.2 Mon 9:50 H7

Flat-field correction of highly-dynamic processes — •Thea Engler[1], Johannes Hagemann[1], Christian Schroer[1], and Mathias Trabs[2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Karlsruhe Institue of Technology KIT, Germany

Using hard coherent x-rays, as produced in PETRA III at DESY and in the European XFEL, objects with a size of μm to nm can be imaged with full-field phase-contrast imaging. With single-pulse imaging, specifically dynamic processes on the nanosecond-timescales can be investigated. A recorded single-pulse hologram of the object under investigation in a lens-less imaging setup is disturbed by illumination artifacts. The origin of these artifacts are aberrations in the optics, such as figure errors and surface roughness. For further analysis, the illumination artifacts have to be removed, which is achieved by a flat-field correction. Therefore, the x-ray image of the object of interest is divided by an empty-beam image. This approach assumes temporal stability of both illumination and object. In the case of XFEL experiments, the pulse-to-pulse fluctuations stemming from the SASE process violate this assumption. For the imaging conducted at PETRA III, in addition to vibrations in the beamline's optical components, the object itself incorporates dynamic movements. The common case of the flat-field correction can be improved by recording an empty-beam image-series. With principal component analysis (PCA) of the image series and a careful selection of the principal components, a synthetic flat-field can be reconstructed for each object-image.

KFM 3.3 Mon 10:10 H7

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 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.

KFM 3.4 Mon 10:30 H7

Stereo X-Ray Microscopy: Seeing the nanocosm in 3D — •Sina Röper[1,2], Karolina Stachnik[2], Lukas Grote[2], Mattias Åstrand[3], Hanna Ohlin[3], Martin Seyrich[1], Sarah-Alexandra Hussak[2], Thomas Frisk[3], Andreas Schropp[1], Ulrich Vogt[3], Dorota Koziej[2], and Christian Schroer[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]University of Hamburg, Hamburg, Germany — [3]KTH Royal Institute of Technology, Stockholm, Sweden

Understanding the nucleation and growth mechanisms involved in the synthesis of nanomaterials is a key factor in determining their performance and functionality. In many cases, these processes are still not well understood in particular, due to the difficulty of observing them *in situ* or *operando*. Scanning hard X-ray microscopy offers the potential for *in situ* nanoimaging of complex chemical systems under relevant environmental conditions. However, standard X-ray tomography relies on the rotation of the sample with respect to the X-ray beam. This is typically not possible for the synthesis of nanoparticles in solution, which requires an extended reaction cell.

We have developed a new stereoscopic X-ray imaging technique with improved depth resolution to overcome these challenges. By simultaneously illuminating the sample with two nanofocused X-rays at different angles, we increased the effective numerical aperture and improved the spatial resolution along the X-ray beam path. This provides a significant gain in depth-sensitivity in ptychography with multi-slicing and allows us to obtain 3D structural information from 2D scans.