MM 42: Topical Session: In Situ and Multimodal Microscopy in Materials Physics I (joint session MM/KFM)

Time: Wednesday 15:30–18:00 Location: C 130

Topical Talk MM 42.1 Wed 15:30 C 130

Charges, Structure, Properties - Concepts and Applications of four-dimensional electron microscopy — •Knut Müller-Caspary[1,3], Benedikt Diederichs[1,2], Ziria Herdegen[1], Tizian Lorenzen[1], Felix Dushimineza[1,3], Max Leo Leidl[1,3], Achim Strauch[3], and Frank Filbir[2] — [1]Ludwig-Maximilians-Universität München, Dept. of Chemistry, Butenandtstr. 11, 81377 München — [2]Institute of Biological and Medical Imaging, Helmholtz Zentrum München, 85764 Neuherberg, Germany — [3]Forschungszentrum Jülich, Wilhelm Johnen Str., 52425 Jülich

Scanning an electron probe across a specimen and recording a diffraction pattern at each scan point established 4D-STEM as a versatile concept to characterise materials. We start with a very brief introduction of mapping electric fields and electrostatic potentials by using direct methods such as centre-of-mass imaging and analytical ptychographic solutions to the inverse single-scattering problem. Applications to large-scale electric field mapping and 2D materials will be shown. For thicker specimens, structure retrieval needs to invert multiple scattering. In this respect, we report a parametric inverse multislice concept in which both partial coherence of the probe and multiple frozen phonon states are taken into account. In particular, we investigate the impact of thermal diffuse scattering on different inverse multislice approaches. The concept is demonstrated via simulations first, and then applied to measure ionic displacements in ferroelectrics with picometre precision.

MM 42.2 Wed 16:00 C 130

TEM investigations of local structure and dynamics in PdNiP bulk metallic glass — •Olivia Vaerst[1], Martin Peterlechner[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Karlsruhe Institute of Technology, Laboratory for Electron Microscopy (LEM), Karlsruhe, Germany

The bulk metallic glass PdNiP is kinetically highly stable against crystallisation and therefore often used as a model system for investigations of the glassy state. Such investigations include experiments to further explore the glass formation and the structure-property relations of metallic glasses. In this work, the focus lies on understanding the atomic structure and local mobility of PdNiP in various thermomechanical states. For this purpose, multimodal transmission electron microscopy (TEM) measurements are performed using advanced techniques. The main method used is electron correlation microscopy (ECM), where diffracted intensities of a time series of dark-field images are correlated to deduce structural dynamics parameters with nanometer spatial resolution. A systematic analysis of the effect of varying electron beam parameters on the dynamics is conducted and optimal measuring parameters for PdNiP are determined. 4D-STEM fluctuation electron microscopy (FEM) is used for complementary structural investigations concerning the medium-range order of the different thermo-mechanical material states. The results on local dynamics and structural properties are discussed with respect to properties measured by macroscopically averaging methods.

MM 42.3 Wed 16:15 C 130

Strain mapping of a sigma 5(310) grain boundary in a Cu bi-crystal using scanning transmission electron microscopy — •Anoosheh Akbari[1], Harald Rösner[1], Esakkiraja Neelamegan[1], Hui Ding[2], Christian.H Liebscher[2], Sergiy Divinskiy[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Grain boundaries play an important role in determining the physical properties of materials. With respect to diffusion, extended strain fields localized at GBs can modify atomic transport along GBs. In order to understand the effect of strain on GB diffusion in more detail, the evolution of strain along GBs under mechanical treatment is investigated. For this purpose, a Cu bi-crystal containing a sigma 5(310) GB was fabricated by a modified Bridgman technique, followed by annealing at 800 °C. The surface was mirror-liked polished subsequently followed by FIB lamella target preparation of the GB in cross-sectional view. The elastic strain along and around the GB was measured on a nanometer scale, using nano-beam diffraction patterns (NBDPs) acquired using a 1 nm STEM probe with grains oriented in zone axis conditions. A custom written code was employed to extract the strain maps. On the atomic scale, the strain was characterized using geometrical phase analysis applied to high resolution STEM images confirming the results obtained by NBDP. The analysis was finally extended to deformed samples.

MM 42.4 Wed 16:30 C 130

Unfolding structural features of NaNbO3 using atomic resolution 4D-STEM — •Hui Ding[1], Yu Huang[2], Mao-Hua Zhang[3], Jing-Feng Li[2], and Christian H. Liebscher[1] — [1]Structure and Nano- / Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]School of Materials Science and Engineering, Tsinghua University, Beijing, China — [3]Department of Materials Science and Engineering, Penn State University, University Park, USA

As one of the most promising lead-free antiferroelectrics, $NaNbO_3$ suffers from irreversibility of the phase transition, limiting further application in electronic devices. Understanding the structural complexity and establishing a well-defined structure-property relationship of $NaNbO_3$ is of great importance for targeted tailoring of its functionality.

Here, we employ atomic resolution HAADF-STEM and 4D-STEM to probe the local atomic structure of $NaNbO_3$ thin films resolving the Nb, Na and O sublattices simultaneously. Reconstructed differential phase contrast STEM images indicate either the coexistence of P4bm (tetragonal) and $P2_1ma$ (orthorombic) phases, instead of the intrinsic Pbcm phase, or the formation of a new hybrid phase. In particular, the O columns form a zig-zag pattern along the Nb columns in the (001) plane due to O octahedral tilting, which is the characteristic of the $P2_1ma$ phase. However, an alternating contrast of the Na columns, characteristic for the P4bm phase, is observed and confirmed by 4D-STEM image simulations.

MM 42.5 Wed 16:45 C 130

Machine learning-enabled tomographic imaging of chemical short-range order in Fe-based alloys — •Yue Li and Baptiste Gault — Max-Planck Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Chemical short-range order (CSRO), describing preferential local ordering of elements within the disordered matrix, can change the mechanical and functional properties of materials. CSRO is typically characterized indirectly, using volume-averaged (e.g. X-ray/neutron scattering) or through projection microscopy techniques that fail to capture the complex, three-dimensional atomistic architectures. Quantitative assessment of CSRO and concrete structure-property relationships have remained so far unachievable. Here, we present a machine-learning enhanced approach to break the inherent resolution limits of atom probe tomography to reveal three-dimensional analytical imaging of the size and morphology of multiple CSRO. We showcase our approach by addressing a long-standing question encountered in a body-centred-cubic Fe-18Al and Fe-19Ga (at.%) alloy that sees anomalous property changes upon heat treatment, supported by electron diffraction and synchrotron X-ray scattering techniques. The proposed strategy can be generally employed to investigate short/medium/long-range ordering phenomena in a vast array of materials and help design future high-performance materials.

MM 42.6 Wed 17:00 C 130

TESCAN 4D-STEM for Multimodal Characterization of Challenging and Interesting Specimens — Lars-Oliver Kautschor[1] and •Robert Stroud[2] — [1]TESCAN GmbH. Zum Lonnenhohl 46, Dortmund — [2]TESCAN USA, 765 Commonwealth Dr #101, Warrendale, PA 15086, USA

The all-new TESCAN TEM solution: TESCAN TENSOR - the world*s first Integrated, Precession-assisted, Analytical 4D-STEM will be presented. Designed from the ground up TESCAN TENSOR*s quality throughput, and robustness of 4D-STEM acquisition, analysis, and processing has been optimized with state-of-the-art technologies, such as Precession Electron Diffraction (PED), 4D-STEM computing and visualization, electrostatic beam blanking, and ultra-high vacuum at the specimen area. Additionally, TESCAN TENSOR features real-time, automated data analysis and processing, which empowers an unprecedented level of system accessibility, utilization, and productivity. The methodology behind this advanced (electron diffraction) microscope will be explained as the solution of choice for a range of nanoscale applications.

MM 42.7 Wed 17:15 C 130

Micro-CT goes multimodal - 3D elemental analysis with new the SPECTRAL CT, — •Lars-Oliver Kautschor — TESCAN GmbH. Zum Lonnenhohl 46, Dortmund

X-ray micro-computed tomography (micro-CT) has opened new avenues of research and understanding. It is now recognized as an essential technique for non-destructive 3D imaging. Extending the technique to the temporal regime, through time-resolved 3D imaging (or 4D imaging), provides a new route to better and more complete understanding of materials evolution, facilitating in situ investigations ranging from mechanical deformation to fluid flow in porous materials. With the new SPECTRAL CT, TESCAN offers the possibility to perform elemental analysis inside your sample none-destructively. In this talk we explore the general technique of micro-CT as well as the advantages of the new SPECTRAL.

Topical Talk MM 42.8 Wed 17:30 C 130

Unsupervised Machine Learning Analysis for Electron Microscopy Datasets — •Mary Scott — Department of Materials Science and Engineering, University of California, Berkeley, Berkeley, CA 94720, USA — National Center for Electron Microscopy, Molecular Foundry, Lawrence Berkeley National Lab, Berkeley, CA 94720, USA

Electron microscopy is the characterization method of choice to observe local atomic-scale and microstructural features within materials that play a critical role in material performance. Recently developed high frame rate electron detectors acquire diffraction patterns from nanoscale regions at frame rates of 100 kHz, an approach that enables multimodal analysis from the same dataset to create maps of crystal orientation, strain, and more. This method, termed 4D-STEM, creates datasets can contain tens of thousands of diffraction patterns from heterogeneous structural regions. The large datasets cannot be analyzed manually, and lack of prior knowledge of the crystal structure of diverse samples limits the application of supervised automated approaches, motivating the development of unsupervised analysis. Here I will overview implementation of an automated, unsupervised clustering pipeline for 4D-STEM data, emphasizing the importance of input data representation. Futhermore, I will describe an ensemble approach to generate more stable clustering results. This type of unsupervised data analysis pipeline is an important step towards incorporating rapid 4D-STEM analysis into material discovery and design efforts, particularly when evaluating defect-rich and disordered materials.