KFM 11: (Multi)ferroic States: From Fundamentals to Applications (V)

This focus session explores the intricate properties of (multi)ferroic states, spanning from fundamental understanding to cutting-edge applications. Topics include the design and control of (multi)ferroic states and domain structures at interfaces, domain walls, and in heterostructures. Emphasis will be placed on theoretical models, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices.

Chair: Manuel Zahn (University of Augsburg)

Time: Wednesday 9:30–10:45 Location: H9

Invited Talk KFM 11.1 Wed 9:30 H9

Towards 3D nanoscale chemical mapping with atom probe tomography — •Kasper Hunnestad, Constantinos Hatzoglou, Antonius van Helvoort, and Dennis Meier — Norwegian University of Science and Technology, Trondheim, Norway

The discovery of new physical phenomena in materials is closely linked to the progress in characterization, and is propelled by the ability to observe and study physical processes occurring at the atomic level. Nanoscale structural characterization has been a cornerstone for many discoveries related to ferroic phenomena. Chemical characterization at the atomic level, however, remains a major challenge.

In the first part of this talk, I will present how atom probe tomography (APT) can be incorporated into the toolkit of nanoscale research to study ferroic oxide materials. In the second part of this talk, a special emphasis will be put on various ferroic phenomena, such as ferroelectric domain walls and interface effects. The focus will be on understanding their chemical state and the role of defects in controlling their physical properties.

The presentation will demonstrate that correlations between defect chemistry and ferroic phenomena can be experimentally probed with nanoscale spatial resolution using APT, opening an avenue to obtain a deeper understanding of ferroic materials.

KFM 11.2 Wed 10:00 H9

Tuning of ferroelectric polarization by lattice chemistry — •Ipek Efe[1], Alexander Vogel[2], William S. Huxter[1], Elzbieta Gradauskaite[1], Christian L. Degen[1], Marta D. Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]ETH Zurich — [2]Empa, Switzerland

Engineering the lattice chemistry in oxide thin film systems opens up new possibilities for tuning electrostatic boundary conditions beyond the depolarizing-field tuning approaches. Controlling the formation of polarizing charged layers may stabilize highly desired polar textures such as charged domain walls and charge planes, offering great promises for future ultralow-energy-consuming oxide electronics. Here, we demonstrate lattice-chemistry engineering of perovskite oxide ferroelectrics in a heterostructure utilizing Aurivillius-type layering. We insert functional perovskite oxides, including $BiFeO_3$ and $BaTiO_3$, into the layered framework of the Aurivillius phase. By exploiting the characteristic charged interfaces present in the Aurivillius crystal structure and varying the perovskite constituent, we fine-tune the electric-dipole configurations within our composite heterostructures. Using in-situ optical second harmonic generation, we directly resolve the influence of controlled atomic-scale poling of the Aurivillius charged layers on the perovskite constituent. As a result, we achieve new properties while preserving the functionalities of the parent compounds.

KFM 11.3 Wed 10:15 H9

Vector Scanning Electron Microscopy for Domain Imaging in Ferroelectric Polycrystals — •Ellinor Benedikte Anjali Lindström, Ruben Skjelstad Dragland, Jonas Åmli Ingdal, Jan Schultheiss, Jiali He, and Dennis Meier — NTNU Norwegian University of Science and Technology, Norway

Domain imaging in polycrystalline ferroelectrics is challenging due to the non-uniform crystallographic orientation of grains. To gain the full information including the domain polarization and orientational information, imaging techniques such as piezoresponse force microscopy (PFM) and scanning electron microscopy (SEM) are often complimented by electron backscatter diffraction (EBSD) experiments.

Here, we introduce a new SEM-based approach that allows simultaneous mapping of domains and grain orientation information. By performing systematic SEM measurements as a function of the stage rotation angle on the model system $ErMnO_3$, we observe distinct contrast intensity changes within the same grain. Notably, the domain contrasts invert when the stage is rotated by 180°. Complementary PFM and EBSD data confirm that these changes in contrast correlate with both the domain state and the orientation of the polar axis relative to the surface. Our approach offers a contact-free alternative to vector PFM and partially reduces the need for EBSD, giving new opportunities for domain imaging in ferroelectrics.

KFM 11.4 Wed 10:30 H9

Ranges and limits of p-doping in Y:HfO_2 - an electronic structure study by HAXPES — •Oliver Rehm[1], Lutz Baumgarten[2], Florian Wunderwald[3], Andrei Gloskovskii[4], Christoph Schlueter[4], Thomas Mikolajick[3,5], Uwe Schroeder[3], and Martina Müller[4] — [1]Universität Konstanz — [2]Forschungszentrum Jülich — [3]NaMLab, Dresden — [4]DESY, Hamburg — [5]TU Dresden

Ferroelectric HfO_2-based thin films exhibit huge potential for the next generation of nonvolatile memory applications, such as FeRAM or FeFET. However, the application of HfO_2-based thin films as active ferroelectrics (FE) in devices still faces reliability issues like wake-up, imprint, and fatigue. A critical concentration of oxygen vacancies (OVs) determines both the stabilization of a FE phase as well as the breakdown during electrical cycling. For p-doped HfO_2, the electronic limits of OV formation remain an experimentally open question.

We investigated Y:HfO_2 samples synthesized via atomic layer deposition (ALD) with Y doping concentrations from 2.1% to 8.6%. TiN/Y:HfO_2 interfaces are investigated regarding the local chemistry and electronic properties by hard X-ray photoelectron spectroscopy (HAXPES). The Hf 4f core level is analyzed to identify Hf^{3+} components and rigid binding energy (BE) shifts, both of which serve as indicators for OVs. We determine the (unexpected) formation of OVs as a function of Y doping, with the conclusion that Y doping above a threshold limit has a detrimental effect on interface stability, thereby promoting increased OV formation at the interface that finally speeds up fatigue and breakdown.