KFM 7: Focus Session: Defects and Interfaces in Multiferroics 2

The focus session is dedicated to advanced nano scale-characterization, property-engineering, and modelling methods of multiferroic materials focusing on defects and interfaces. Typical examples may include ferroic domain walls, microstructural levers, or strain effects. Further, applications in novel nanoelectronic devices and nano-related engineering concepts of macroscopic properties of multiferroics are of interest.

Organizers: Dr. Jan Schultheiß (Augsburg University, NTNU Trondheim) and Dr. Marion Höfling (DTU Copenhagen)

Chair: Dr. Jan Schultheiß (Augsburg University, NTNU Trondheim)

Time: Monday 15:00–17:25 Location: H5

Invited Talk KFM 7.1 Mon 15:00 H5

Multiferroic coupling on the level of domain walls — •Mads C. Weber[1,2], Yannik Zemp[1], Marcela Giraldo[1], Ehsan Hassanpour[1,3], Quintin Meier[1], Yusuke Tokunaga[4], Yoshinori Tokura[4,5], Sang-Wook Cheong[6], Nicola N. Spaldin[1], Thomas Lottermoser[1], and Manfred Fiebig[1] — [1]ETH Zurich — [2]Le Mans University — [3]University of Bern — [4]University of Tokyo — [5]RIKEN — [6]Rutgers University

Multiferroic materials are of interest for the coupling of different ferroic properties on the level of the domains. However, this coupling is not only limited to the bulk but concerns the domain walls too. Here, we show on the example of three different multiferroic systems, that the multi order-parameter coupling on the domain wall level leads to a wide variety of intrinsic domain wall phenomena. In (Dy,Tb)FeO_3, we demonstrate that the interaction of two independent magnetic sublattices gives rise to a polar, multiferroic domain wall in a non-multiferroic environment. The crosstalk of ferroelectricity, structural distortions and magnetic order in hex-$ReMnO_3$ leads to spin rotations of 60°, 120° or 180° about the magnetic domain walls. Depending on the position of the magnetic domain walls with respect of the ferroelectric domain walls, these walls can exchange their rotational character. In the last example, we show that the interplay of two structural distortions in hybrid improper ferroelectrics induces head-to-head and tail-to-tail orientations of the polarization of adjacent ferroelectric domains. These examples illustrate the wide variety of domain wall phenomena thanks to (multi)ferroic coupling effects on the nanoscale.

KFM 7.2 Mon 15:30 H5

3D imaging of multiferroic $(LuFeO_3)_9/(LuFe_2O_4)_1$ superlattices by atom probe tomography — •Kasper Hunnestad[1], Hena Das[2], Constantinos Hatzoglou[1], Megan Holtz[3], Charles Brooks[3], Antonius T. J. Helvoort[1], Darrell Schlom[3,4], Julia Mundy[5], and Dennis Meier[1] — [1]Norwegian University of Science and Technology, Norway — [2]Tokyo Institute of Technology, Japan — [3]Cornell University, USA — [4]Kavli Institute at Cornell for Nanoscale Science, USA — [5]Harvard University, USA

Oxide interfaces are a rich source for novel physical phenomena, ranging from interfacial superconductivity to unusual (multi-)ferroic effects. Over the last decade, significant progress has been made in both the understanding and engineering of oxide interfaces, propelled by the ongoing progress in the development of atomic-scale characterization techniques.

Here, we introduce atom probe tomography (APT) as versatile tool for studying oxide interfaces, investigating the 3D atomic-scale structure and chemical composition of multiferroic $(LuFeO_3)_9/(LuFe_2O_4)_1$ superlattices. Our APT measurements reveal a substantial accumulation of oxygen vacancies at the $LuFe_2O_4$ layers. Based on the data, we quantify the vacancy concentration and discuss their accumulation in relation to calculated defect formation energies and the multiferroic domain structure. In general, this research establishes a new pathway for studying the interaction of interfaces and point defects in oxides, expanding related atomic-scale investigations into 3D.

KFM 7.3 Mon 15:50 H5

Electric-field control of oxygen defects and local transport properties in $ErMnO_3$ — •Jiali He[1], Ursula Ludacka[1], Donald M. Evans[1], Theodor S. Holstad[1], Erik D. Roede[1], Kasper A. Hunnestad[1], Konstantin Shapovalov[2], Zewu Yan[3,4], Edith Bourret[4], Antonius T. J. van Helvoort[1], Sverre M. Selbach[1], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Norway — [2]Institute of Materials Science of Barcelona, Spain — [3]ETH Zurich, Switzerland — [4]Lawrence Berkeley National Laboratory, USA

The electronic properties of complex oxides can be tuned via oxygen defects, offering intriguing opportunities for controlling conductivity. Recently, anti-Frenkel defects moved into focus for minimally invasive property engineering, and their creation makes it possible to adjust the electronic properties without long-range ionic migration or stoichiometry changes. Here, we present a detailed analysis of the electric-field-driven formation and time-voltage-dependent evolution of anti-Frenkel defects in hexagonal $ErMnO_3$. By combining atomic force microscopy and scanning electron microscopy, we investigate the local electronic transport properties associated with the written defects, complemented by numerical simulations. The study reveals that oxygen interstitial - vacancy pairs can be split under an applied electric field. This splitting leads to spatially separated and well-defined vacancy- and interstitial-rich regions, forming a bipolar nanoscale junction. The results provide new insight into the electric-field-driven ionic migration in $ErMnO_3$ and defects physics in functional oxides.

15 min. break

KFM 7.4 Mon 16:25 H5

Deep learning evaluation of conductive atomic force microscopy data — Lorenz Glück[1,2], •Manuel Zahn[1,3], Lukas Puntigam[1], Donald M. Evans[1], Somnath Ghara[1], Michael Heider[2], and Stephan Krohns[1] — [1]Experimental Physics V, University of Augsburg, 86159 Augsburg — [2]Organic Computing Group, University of Augsburg, 86159 Augsburg — [3]Institut für Angewandte Physik, Technische Universität Dresden, 01069 Dresden

Machine learning has gained an enormous interest in the past decade to boost data evaluation in many fields of applied physics. For example, feature recognition in high dimensional datasets in scanning probe microscopy (SPM) can be improved and hidden effects resolved. However, the physical relevance of resolved features is normally still determined by humans.

In this work, we investigate if the regularization of a deep learning (DL) neuronal network, composed of long-short term memory and temporal convolutional network based layers inside an autoencoder architecture, can be utilized to characterize physical significance. We do this on a conductive atomic force microscopy dataset, collected on ferroelectric GaV4S8, as the general properties have already been identified and there are emergent traits at the domain walls. The resolved features from the DL approach are compared to those derived from classical clustering algorithms and classically resolved local material properties. This set up is the first steps to automatic evaluation of physically significant properties in GaV4S8, and is expected to be applicable to other ferroelectric systems.

KFM 7.5 Mon 16:45 H5

Oxygen off-stoichiometry and domain wall conductance in $ErMnO_3$ — •Leonie Richarz[1], Jan Schultheiss[1], Edith Bourret[2,3], Zewu Yan[3], Antonius T.J. van Helvoort[1], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]ETH Zurich, Switzerland — [3]Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Ferroelectric domain walls are natural interfaces, separating volumes with different orientation of the spontaneous polarization. Due to their symmetry, electrostatics, and strain, the walls can develop completely different electronic properties than the surrounding domains. In ferroelectric oxides, oxygen off-stoichiometry is an additional versatile control parameter. This is reflected by the neutral ferroelectric domain

walls in hexagonal manganites: Depending on the oxygen content, their conduction behavior varies from insulating to highly conducting.

In this work, we monitor the electronic transport properties at the domain walls as a function of temperature and oxygen partial pressure with nanoscale spatial resolution. Conductive atomic force microscopy measurements on high-quality $ErMnO_3$ single crystals show anomalous conductance at the domain walls within the whole temperature range of 25 to 300°C. Furthermore, we find that by annealing the sample in nitrogen, the domain wall conductance can be enhanced. Our results provide new insight into the impact of environmental parameters on the electronic domain wall properties. This is of interest for the development of atmospheric sensors, adding a new direction to the field of domain wall nanotechnology.

KFM 7.6 Mon 17:05 H5

Manipulation of improper ferroelectric domains in $Gd_2(MoO_4)_3$ using temperature, electric fields, and mechanical stress — •Ivan Ushakov[1], Theodor Holstad[1], Didier Perrodin[2], Edith Bourret[2], Thomas Tybell[1], and Dennis Meier[1] — [1]Norwegian University of Science and Technology (NTNU), Norway — [2]Lawrence Berkeley National Laboratory, USA

In improper ferroelectrics, the spontaneous polarization arises as a biproduct of magnetic or structural order, promoting the formation of domains and domain walls with unusual electronic transport phenomena and scaling behavior. $Gd_2(MoO_4)_3$ is a classical example of an improper ferroelectric material where a structural instability leads to the formation of a polar axis.

Here, we expand previous mesoscale microscopy studies of the domain structure to the nanoscale. By using piezoresponse force microscopy, we image the patterns of ferroelectric and structural antiphase domains in $Gd_2(MoO_4)_3$. In addition to the established domain patterns, we resolve so far unexplored stripe-like nanodomains with a periodicity of about 60 nm. Temperature-dependent measurements show that the nanodomains are stable up to 70°C. Furthermore, we demonstrate reversible switching of these nanodomains by local electric fields and their control via mechanical stress. Our findings provide new insight into the nanoscale domain-physics of $Gd_2(MoO_4)_3$ and introduce novel opportunities for domain engineering in improper ferroelectrics.