KFM 2: Focus Session: Defects and Interfaces in Multiferroics 1

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. Marion Höfling (DTU Copenhagen)

Time: Monday 9:30–12:25 Location: H5

Invited Talk KFM 2.1 Mon 9:30 H5

Domain-wall engineering in multiferroic materials — •Guillaume Nataf — GREMAN UMR7347, CNRS, University of Tours, INSA Centre Val de Loire, 37000 Tours, France

Ferroelectric and ferroelastic domain walls are two-dimensional topological defects with thicknesses approaching the unit cell level that can move in response to an electric-field or an applied stress. They exhibit emergent functional properties, such as polarity in non-polar systems or electrical conductivity in otherwise insulating materials, and due their complex strain profiles they interact with phonons as 'defects' would.

In this talk I will: (1) Show how to characterize domain walls with optical techniques (polarized light optical microscopy, liquid crystal decoration, Raman spectroscopy); (2) Discuss how domain walls move in response to an electric field or an applied stress, through discrete impulsive jumps, indicators of avalanches on a broad range of scales; (3) Show that domain walls can be used to induce large thermal conductivity variations in materials.

KFM 2.2 Mon 10:00 H5

Engineering of improper ferroelectric vortex- and stripe-like domains in polycrystalline $ErMnO_3$ — •Max Haas, Jan Schultheiss, and Dennis Meier — Norwegian University of Science and Technology (NTNU), 7034 Trondheim, Norway

The functionality and physical properties of ferroelectric materials are intimately coupled to their domain structure. An exciting recent discovery are topologically protected vortex domains in hexagonal manganites, which are of interest for different fields ranging from nanoelectronics to cosmology-related questions. A key characteristic of the domain structure is the vortex density, that can readily be tuned via the cooling rate across the ferroelectric phase transition.
Here, we explore the effect of cooling rate variations in combination with three-dimensional spatial confinement in high-quality $ErMnO_3$ polycrystals. Utilizing piezoresponse force microscopy, we demonstrate a propensity for the formation of stripe-like domains. Analogous to the vortex-like domains observed in $ErMnO_3$ single crystals, we find that the periodicity of the stripe-like domains depends on the cooling rate through the Curie temperature. For cooling rates in the range of 10^{-2} to 10^{1} K/min, the periodicity of the stripe-domains increases logarithmically. This scaling behavior is explained based on the interplay between cooling rate and long-ranging strain fields, offering new possibilities for the engineering of domains and domain walls in polycrystalline improper ferroelectrics.

KFM 2.3 Mon 10:20 H5

Tuning multiferroic properties in hexagonal $YMnO_3$ by manipulation of the structural order — •M. Giraldo[1], H. Sim[2], A. Simonov[1], M. Lilienblum[1], A. Samir[1], E. Gradauskaite[1], Y. Heo[1], M. Rossell[3], M. Trassin[1], J.-G. Park[2], Th. Lottermoser[1], and M. Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]Department of Physics and Astronomy, Seoul National University — [3]Electron Microscopy Center, EMPA

We investigate the enhancement and suppression of the structural distortion (Q) in hexagonal $YMnO_3$ upon substituting Mn by Al and Ga. We demonstrate its consequences on the electric and magnetic long-range order. We deploy various techniques for a systematic investigation. We observe a progressive decrease in the structural order. This behaviour is caused by the chemical pressure induced by the ionic size of Al and Mn. On the level of the ferroelectric domains, the suppression of the structural order manifests in a progressive size decrease upon increased Al concentration. We do not observe a domain size variation upon Ga substitution. Our experiments suggest that, surprisingly, the progressive reduction on the structural distortion is not directly proportional to a decrease in ferroelectric polarization. On the magnetic level, we find a progressive decrease of the ordering temperatures. This is due to the direct perturbation of the magnetic sublattices formed by the Mn^{3+} moments and the progressive dilution of the magnetic long-range order. By tracing changes in the inherent properties of these systems, we aim to broaden the understanding for new routes in the manipulation of ferroic properties in these compounds.

KFM 2.4 Mon 10:40 H5

Strain-induced multiferroic ribbons in non-multiferroic phase of $MnWO_4$ — •Lea Forster[1], Shingo Toyoda[2], Manfred Fiebig[1,2], Taka-hisa Arima[2,3], Yoshinori Tokura[2,4,5], and Naoki Ogawa[2,5,6] — [1]Deptartment of Materials, ETH Zurich, Switzerland — [2]RIKEN CEMS, Saitama, Japan — [3]Department of Advanced Materials Science, University of Tokyo, Kashiwa, Japan — [4]Tokyo College, University of Tokyo, Tokyo, Japan — [5]Department of Applied Physics, University of Tokyo, Tokyo, Japan — [6]PRESTO, JST, Kawaguchi, Japan

Local structures, such as structural defects, interfaces, and domain walls have the potential to exhibit different physical properties than the bulk. The occurrence of magnetic and electric orders in a confined area may be of particular interest for technological applications, for example, to electrically control the magnetization in memory devices. However, probing local multiferroic structures is challenging caused by a lack of experimental techniques. In this study, we demonstrate a ribbon-shaped, spatially confined multiferroic phase in a non-multiferroic environment in $MnWO_4$. We use optical second harmonic generation imaging to show that a multiferroic phase can be generated by local strain within a non-multiferroic bulk structure. Furthermore, we reveal within the confined multiferroic regions domains with different electric polarization directions and demonstrate deterministic writing of a multiferroic state by the application of strain.

15 min. break

Invited Talk KFM 2.5 Mon 11:15 H5

Charged Higher Order Topologies in Room Temperature Magnetoelectric Multiferroic Thin Films — •Shelly Conroy[1,2], Kalani Moore[2], Sinead Griffin[3], Lynette Keeney[4], and Eoghan O'Connell[2] — [1]Imperial College London, London, United Kingdom — [2]University of Limerick, Limerick, Ireland — [3]Lawrence Berkeley National Laboratory, Berkeley, USA — [4]Tyndall National Institute, Cork, Ireland

Multiferroic topologies are an emerging solution for future low-power magnetic nanoelectronics due to their combined tuneable functionality and mobility. Here, we show that in addition to being magnetoelectric multiferroic at room temperature, thin film Aurivillius phase Bi6TixFeyMnzO18 is an ideal material platform for both domain wall and vortex topology based nanoelectronic devices. Utilising atomic resolution electron microscopy and atom probe tomography, we reveal the presence and structure of 180 type charged head-to-head and tail-to-tail domain walls passing throughout the thin film. Theoretical calculations confirm the sub-unit cell cation site preference and charged domain wall energetics for Bi6TixFeyMnzO18. Finally, we show that polar vortex type topologies also form at out-of-phase boundaries of stacking faults when internal strain and electrostatic energy gradients are altered. This study could pave the way for controlled polar vortex topology formation via strain engineering in other multiferroic thin films. Moreover, these results confirm the sub-unit-cell topological fea-

tures play an important role in controlling the charge and spin state of Aurivillius phase films and other multiferroic heterostructures.

KFM 2.6 Mon 11:45 H5

X-ray investigation of a multiferroic $YBaCuFeO_5$ single crystal — •Arkadiy Simonov[1], Marisa Medarde[2], and Ruggero Frison[3] — [1]ETH Zürich, Zürich, Switzerland — [2]Paul Scherrer Institut (PSI), Willigen, Switzerland — [3]University of Zürich, Zürich, Switzerland

Recent reports have shown that type-II multiferroic materials can be created using chemical disorder. Disorder frustrates magnetic interaction and induces a magnetic spiral state which breaks the inversion symmetry of the crystal [1]. Such a mechanism is robust since it involves only nearest-neighbor magnetic exchanges and can stabilize the spiral state almost up to room temperature in materials like $YBaCuFeO_5$. However, due to the complexity of characterizing and controlling chemical disorder, this mechanism is rarely used in practice to design novel multiferroic materials.

In this work we propose single-crystal x-ray diffuse scattering as a method for characterizing disorder. Using YBaCuFeO5 as our model system, we show that diffuse scattering can efficiently probe the local structure induced by chemical disorder. Moreover, when measured at sufficiently high resolution, diffuse scattering is also sensitive to the magnetic phase transition from antiferromagnetic to spiral state of the $YBaCuFeO_5$. This is unusual, and likely indicates that atomic relaxations induced by this transition are larger than the values observed in typical type-II multiferroics.

[1] M. Morin et al. Nat. Comms. 7, (2016): 133758.

KFM 2.7 Mon 12:05 H5

A phase-field model for ferroelectrics with local chemical defects — •Dilshod Durdiev[1], Frank Wendler[1], Takahiro Tsuzuki[2], Shuji Ogata[2], Ryo Kobayashi[2], Masayuki Uranagase[2], and Hikaru Azuma[2] — [1]Friedrich-Alexander University Nuremberg-Erlangen, Fürth, Germany — [2]Nagoya Institute of Technology, Nagoya, Japan

In this work, an electromechanical fully coupled phase-field model (PFM) is developed, based upon the approach [1], to study domain evolution and polarization switching under the combined influence of the mechanical and electrical loads and local chemical defects in a $BaTiO_3$ single crystal. The free energy density of the system includes the Landau potential, gradient, mechanical, piezoelectric and electrical energy, respectively. We apply a Fourier spectral method to solve the coupled constitutive equations. Molecular dynamics simulations with core-shell potentials are conducted to capture the domain wall dynamics including vacancies and cation-anion vacancy dipoles [2]. We develop procedures to obtain kinetic and energetic parameters of the PFM from these simulations. Scaling relations are applied to transfer local fields (of vacancies and aliovalent dopants) as well as local bond effects (from vacancies) from the micro- to the continuum scale.

[1] D. Schrade, et al., Arch. Appl. Mech., 83,1393–1413 (2013).
[2] T. Tsuzuki, et al., Appl. Phys. 131, 194101 (2022).