

## KFM 3: Focus Session: (Multi-)Ferroic States I

The focus session is dedicated to (multi)ferroic states at interfaces and in heterostructures. The design of (emergent) properties at interfaces, modelling methods and advanced characterization tools will be of interest. Typical examples may include electrostatic and strain boundary conditions at interfaces, domains and domain walls in (multi)ferroics and applications in nano-electronic device

Chair: Johanna Nordlander (Paul Drude Institute)

Time: Monday 9:30–11:30

Location: EMH 225

KFM 3.1 Mon 9:30 EMH 225

**Domain Size Engineering by Grain Scaling in Polycrystalline Hexagonal DyMnO<sub>3</sub>** — ●RUBEN DRAGLAND, KATHARINA WOLK, ELVIA CHAVEZ PANDURO, KASPER AAS HUNNESTAD, JAN SCHULTHEISS, and DENNIS MEIER — Norwegian University of Science and Technology (NTNU), Trondheim, Norway

Controlling the density and distribution of ferroelectric domain walls is essential for the development of domain wall electronics, giving intriguing opportunities for continued downscaling of active electronic components. The microstructure is a vital parameter for domain engineering, and a proportional relation between grain and domain size is established. However, inversely proportional domain scaling has been observed in ErMnO<sub>3</sub>, while domain-microstructure relations in other polycrystalline systems of the hexagonal manganite family remains to be explored.

Here, the domain structure in a hexagonal DyMnO<sub>3</sub> polycrystal is investigated, exhibiting a non-uniform grain size distribution which is attributed to the material's propensity to crystallize in the orthorhombic phase. By systematically quantifying the domain sizes during post-processing, inverted scaling of domain size with grain size is observed, identifying the inverse scaling as an intrinsic phenomenon, effectively ruling out processing and heat treatment as the main origin. The observed impact of non-uniform grain sizes on the domain structure is of interest to understand the complex nanoscale domain physics in ferroelectric polycrystals, and reveals new opportunities for tuning their macroscopic response towards broader time scales.

KFM 3.2 Mon 9:50 EMH 225

**The three-dimensional multiferroic domain structure of hexagonal manganites** — LUKAS HECKENDORN, ●AARON MERLIN MÜLLER, MANFRED FIEBIG, and THOMAS LOTTERMOSER — Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

We simulate and visualize the three-dimensional domain structure and associated topological features of multiferroic hexagonal manganites. Due to the improper nature of their ferroelectric order, hexagonal manganites exhibit unconventional six-fold vortices in their ferroelectric domain patterns. In 3D, these domain patterns are characterized by vortex lines, which are 1D topological defects that form loops in bulk materials. Below the Néel temperature, an additional antiferromagnetic order rigidly coupled with the ferroelectric order emerges, forming vortex domain patterns of its own. In our simulations, we observe new types of antiferromagnetic three-fold, four-fold and six-fold vortex lines in addition to ferroelectric six-fold vortex lines. We relate the existence of these vortex lines to the rigid coupling between orders. Our numerical investigation is performed with a phase-field model to simulate the domain structure in three dimensions using a Landau-free-energy expansion.

KFM 3.3 Mon 10:10 EMH 225

**Suppression of ferroelectric transition in hexagonal manganites** — ●SOUJANYA MADASU and ARKADIY SIMONOV — Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Hexagonal manganites are an interesting class of multiferroics where the improper nature of ferroelectricity induces a structural crosstalk between high temperature polarization and low temperature frustrated antiferromagnetic.

In this talk, we will be addressing methods to suppress ferroelectric transition caused by the \*up-up-down\* cation displacement of hexagonal manganites through doping on the A site. This suppression of ferroelectric states destroys the template for low temperature antiferromagnetic ordering of Mn spins and thus frustrates the magnetic transition. We study this structural evolution by subjecting the doped manganites to various annealing conditions and then measure their low temperature magnetic behaviour. Finally, we compare experimental observations with theoretical considerations to analyze the magnetic

properties and structure of these hexagonal manganites.

KFM 3.4 Mon 10:30 EMH 225

**Reversible domain wall displacement in ferroelectric ErMnO<sub>3</sub>** — ●MANUEL ZAHN<sup>1,2</sup>, KYLE KELLEY<sup>3</sup>, AARON M. MÜLLER<sup>4</sup>, SABINE M. NEUMEYER<sup>3</sup>, THOMAS LOTTERMOSER<sup>4</sup>, SERGEI V. KALININ<sup>5</sup>, NEUS DOMINGO<sup>3</sup>, ISTVÁN KÉZSMÁRKI<sup>1</sup>, DENNIS MEIER<sup>2</sup>, and JAN SCHULTHEISS<sup>2</sup> — <sup>1</sup>University of Augsburg, Augsburg, Germany — <sup>2</sup>Norwegian University of Science and Technology (NTNU), Trondheim, Norway — <sup>3</sup>Oak Ridge National Laboratory, Oak Ridge, USA — <sup>4</sup>ETH Zurich, Zurich, Switzerland — <sup>5</sup>University of Tennessee, Knoxville, USA

Many of the intriguing characteristics of ferroelectric materials arise from the physical responses at the level of the domains. In conventional ferroelectric systems, such as like Pb(Zr,Ti)O<sub>3</sub>, BaTiO<sub>3</sub>, and LiNbO<sub>3</sub>, polarization reversal between monodomain states takes place through a nucleation and growth process. Different from these systems, hexagonal manganites (RMnO<sub>3</sub>, R = Sc, Y, In, and Dy-Lu) host topological meeting points of domain walls that cannot be erased, giving rise to a fundamentally different switching behavior. Here, we explore the confined switching dynamics of ferroelectric domains in ErMnO<sub>3</sub>, using band-excitation piezoresponse force microscopy (BE-PFM). Our measurements reveal reversible local displacement of ferroelectric walls induced by the electric field. Interestingly, we observe a continuous breathing-like mode of the domains when cycling the electric field. Our study provides new insights into the dynamics of the topologically protected domains and expands previous switching studies towards the domain level.

KFM 3.5 Mon 10:50 EMH 225

**Current distribution in simple ferroelectric domain-wall-based devices** — ●LEONIE RICHARZ<sup>1</sup>, JIALI HE<sup>1</sup>, KONSTANTIN SHAPOVALOV<sup>2</sup>, EDITH BOURRET<sup>3</sup>, ZEWU YAN<sup>3,4</sup>, ANTONIUS T.J. VAN HELVOORT<sup>1</sup>, and DENNIS MEIER<sup>1</sup> — <sup>1</sup>NTNU Norwegian University of Science and Technology, Trondheim, Norway — <sup>2</sup>University of Liège, Liège, Belgium — <sup>3</sup>Lawrence Berkeley National Laboratory, Berkeley, CA, USA — <sup>4</sup>ETH Zurich, Zurich, Switzerland

Ferroelectric domain walls can exhibit fundamentally different electronic properties than the surrounding bulk material, making them interesting for the application in next-generation electronic devices. After comprehensive studies of the fundamental physics of domain walls, the community is now more and more shifting the focus towards their integration and performance in different device architectures.

Here, we investigate the distribution of electrical currents in domain wall networks in ErMnO<sub>3</sub>, considering basic two-terminal architectures. We deposit static metal electrodes on the domain walls and use a conductive atomic force microscopy tip as an additional movable monitoring contact. In this way, we can investigate the influence of the metal-semiconductor interface between the electrode and the sample, as well as the influence of the domain walls on the current distribution in the ferroelectric material.

Our results provide insight into the current evolution in ferroelectric domain wall systems, facilitating the design of ferroelectric domain wall-based devices.

KFM 3.6 Mon 11:10 EMH 225

**Influence of ferroelectric domain structures on thermal conductivity in ErMnO<sub>3</sub> ceramics** — RACHID BELRHITI NEJJAR<sup>1</sup>, MANUEL ZAHN<sup>2</sup>, FABIEN GIOVANNELLI<sup>1</sup>, MAX HAAS<sup>2</sup>, JAN SCHULTHEISS<sup>2</sup>, DENNIS MEIER<sup>2</sup>, and ●GUILLAUME F. NATAF<sup>1</sup> — <sup>1</sup>GREMAN UMR7347, CNRS, University of Tours, INSA Centre Val de Loire, 37000 Tours, France — <sup>2</sup>NTNU Norwegian University of Science and Technology, Høgskoleringen 1, Trondheim 7034, Norway

Domain walls in ferroelectric and ferroelastic materials interact with phonons conducting heat and are thus interesting tools to tune ther-

mal conductivity [1]. Recent results show that ferroelectric domain walls in single crystals of ErMnO<sub>3</sub> reduce thermal conductivity [2]. To reveal the full potential of domain walls for thermal applications, it is required to demonstrate their influence on thermal conductivity in ceramics, where grain sizes and grain boundaries can also play a role. Here, we investigated the thermal conductivity of several ceramics of ErMnO<sub>3</sub> with different grain sizes and different densities of domain walls. Different domain sizes were obtained by crossing the Curie tem-

perature with different cooling rates. Different grain sizes result from different sintering temperatures [3]. Our measurements performed with a laser flash system between 160 K and 360 K demonstrate a correlation between the thermal conductivity and the domain structure in ceramics of ErMnO<sub>3</sub>, including at and above room temperature.

[1] Limelette et al. *Phys. Rev. B* 108, 144104 (2023) [2] Pang et al. *Mater. Today Phys.* 307, 100972 (2023) [3] Schultheiß et al. *Adv. Mater.* 34, 2203449 (2022)