KFM 13: Focus Session: (Multi-)Ferroic States III

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: Morgan Trassin (ETH Zürich)

Time: Wednesday 9:30–12:30 Location: EMH 225

KFM 13.1 Wed 9:30 EMH 225

What can we expect from multiferroic antiskyrmions? — •Jiri Hlinka — Institute of Physics, Czech Acad. Sci., Prague, Czechia

The prediction and experimental confirmation of magnetic skyrmions - the objects with nontrivial swirling spins patterns - revolutionized the physics of nanoscale magnetism and opened new horizons for spintronics. In spite of the inherently shorter and faster correlations of the electric polarization, the recent developments in electric skyrmionics follow these innovations. Our recent work with M. Goncalves and M. Pasciak[arXiv:2303.07389] reveals that classical ferroelectric perovskite - barium titanate - can host 2-3 nm wide polar columns spontaneously surrounded by a unique noncollinear polarization pattern that has never been described before. Based on the reference-frame-invariant topological charge of this topological defect, we name it *ferroelectric antiskyrmion*. In this contribution we shall address the question about the existence and properties od whether similar topological defects can exist in multiferroic materials like bismuth ferrite.

KFM 13.2 Wed 10:00 EMH 225

Topological aspects of switching in ferroic materials — Francesco Foggetti[2,1], Margherita Parodi[1,3], Naoto Nagaosa[4], and •Sergey Artyukhin[1] — [1]Italian Institute of Technology, Genova, Italy — [2]Dept. of Physics and Astronomy, Uppsala University, Sweden — [3]Department of Physics, University of Genova, Italy — [4]CEMS RIKEN, Tokyo, Japan

Topology has played a prominent role in condensed matter physics in the recent years. In magnetism, topological properties of domain walls and vortices were known for a long time, and more recently topological magnon band structures and other aspects were discussed. However, switching, one of the most important processes from the viewpoint of applications, has not been discussed in the context of topology until recently, when magnetoelectric switching in GdMn2O5 [1], the first known topologically protected ferroic switching phenomenon, was discovered. Here we discuss electric field induced switching in spiral multiferroics, where topology plays an important role.

[1] Louis Ponet, SA, Th. Kuhn et al., Nature 607, 81 (2022).

KFM 13.3 Wed 10:20 EMH 225

Atomic-scale control of exchange bias at ferroelectric BaTiO3 and ferromagnetic La0.67Sr0.33MnO3 interface — •Manisha Bansal[1], Tuhin Maity[1,2], and Judith L. MacManus-Driscoll[2] — [1]School of Physics, Indian Institute of Science Education and Research Thiruvananthapuram, Thiruvananthapuram, Kerala 695551, India — [2]Department of Materials Science and Metallurgy, University of Cambridge, CB3 0FS, UK

The atomic-scale interfaces in 3D transition-metal oxides give rise to intriguing phenomena, including magnetoelectric coupling and unconventional exchange bias (EB) coupling. They hold promises for the next-generation nanoscale spintronics applications such as high-density memory and sensor technologies. We demonstrate EB coupling (~40Oe at 2 K) at the interface of epitaxially grown ferromagnetic (FM) La0.67Sr0.33MnO3 (LSMO)-ferroelectric (FE) BaTiO3 (BTO) bilayer thin films on TiO2 terminated SrTiO3 (STO) substrates in the absence of any conventional antiferromagnetic (AFM) material due to strain induced FE screening effect by BTO. Such EB is only observed when the thickness (t) of BTO is 5<t<10 unit cells (uc) and LSMO is only a few unit cells (<=14uc). The out-of-plane (OOP) polarization is lost in thicker BTO followed by the negligible EB due to multi domains formation. STEM and DFT confirms the OOP polarized Ti atoms which further displaces the interfacial Mn sites from their centrosymmetric positions in LSMO. This modifies the d-orbital occupancy of interfacial Mn, favoring an interface induced EB in LSMO-BTO bilayer films without any AFM material.

KFM 13.4 Wed 10:40 EMH 225

Unraveling Coupled Martensitic and Magnetic Microstructure of Freestanding Multiferroic Ni-Mn-based Heusler Films — •Satyakam Kar[1,2,3], Yuki Ikeda[4], Kornelius Nielsch[1,2], Heiko Reith[1], Robert Maass[4,5], and Sebastian Fähler[3] — [1]Leibniz IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [4]Federal Institute of Materials Research and Testing, Berlin, Germany — [5]University of Illinois Urbana-Champaign, Illinois, USA

Ni-Mn-based Heusler alloys combine ferroelasticity and ferromagnetism to achieve multifunctional applications like high stroke actuation, multicaloric effects, and thermomagnetic energy harvesting. The underlying principle in these applications is a reversible martensitic phase transformation. In bulk, this first-order transformation is governed by an invariant plane, connecting both phases: austenite and martensite. Theory predicts that this plane should converge to a line for ultrathin films, but experimental evidence is missing. Here, we examine 500 nm thick freestanding epitaxial Ni-Mn-Ga films using electron microscopy and magnetic force microscopy techniques and demonstrate that a line constraint controls the martensitic microstructure. This line constraint results in a complex martensitic and magnetic microstructure, differing from the bulk and the constrained film microstructures. Using a simple phenomenological model, the martensite microstructure can be deduced from a line constraint. Our findings show that finite size effects on martensitic transformation are accessible at a film thickness suitable for microsystem technologies.

10 min. break

KFM 13.5 Wed 11:10 EMH 225

Experimental evidence for the PJTE in alkali niobates — •Leif Carstensen and Wolfgang Donner — Technical University of Darmstadt, Germany

The electronic origin of antiferroelectricity is considered not fully understood by most of the scientific community. Sodium niobate evolves from a paraelectric cubic to an antiferroelectric orthorhombic structure via a series of phonon instabilities. A combination of Rietveld refinement and Maximum Entropy Method is performed to gain insight into the differences between ferroelectrics and antiferroelectrics with respect to their electron density. Using this technique, the electron density distributions of room temperature sodium niobate and potassium niobate have been calculated from powder diffraction experiments to study the extent to which the Pseudo-Jahn-Teller effect changes the electron distribution from the originally fully ionic bonding proposed for the cubic structures of these perovskites. This study delivers experimental results to back up the PJTE theory and proves that the Rietveld-MEM approach is not limited to large radiation facility data, making it much more commonly available.

KFM 13.6 Wed 11:30 EMH 225

Charged twin domain walls in antiferroelectric-like $K_3[Nb_3O_6(BO_3)_2]$ — •Ivan N. Ushakov[1], Kasper A. Hunnestad[1], Christoph Grams[2], Joachim Hemberger[2], Petra Becker[2], Ladislav Bohatý[2], Thomas M. Tybell[1], and Dennis Meier[1] — [1]Norwegian University of Science and Technology (NTNU), Trondheim, Norway — [2]University of Cologne, Cologne, Germany

Antiferroelectric materials exhibit an anti-polar alignment of electric dipoles, giving rise to intriguing physical properties and functional behaviors. In this work, we apply different scanning probe microscopy techniques to image and investigate the domains and domain walls in $K_3[Nb_3O_6(BO_3)_2]$, a ferroelectric with antiferroelectric-like structure and properties. Using piezoresponse force microscopy, we show that the domains exhibit a pronounced piezoresponse, consistent with the non-centrosymmetric crystal structure. At the nanoscale, a chevron-like pattern of twin domains develops, where the crystallographic structure changes by 120° across the domain walls. Interestingly, we observe

the formation of charged twin walls with distinctly different piezoelectric and electrostatic responses, arising from a small canted electric moment of the otherwise anti-polar arrangement of electric dipoles. Furthermore, the charged domain walls can be controlled by local electric fields. Our findings provide insight into novel types of ferroic domain walls with unusual mechanical and electronic properties.

KFM 13.7 Wed 11:50 EMH 225

Origin of antiferroelectric-like behaviour in a quaternary compound: Multiscale insights from first principles and phase-field simulations — •Muhammad Zeeshan Khalid[1], Ivan Ushakov[1], Bai-Xiang Xu[2], Dennis Meier[1], and Sverre Magnus Selbach[1] — [1]Department of Materials Science and Engineering, Norwegian University of Science and Technology,Trondheim, NO-7491,Norway. — [2]Mechanics of Functional Materials, Department of Materials and Geoscience, Technical University of Darmstadt, Darmstadt, 64287, Hessen, Germany

Understanding domain switching behavior in ferroelectric and antiferroelectric materials is pivotal for optimizing their utility in diverse applications. Here, we investigate the domain characteristics of K3Nb3B2O12, which was recently reported to exhibit antiferroelectric-like switching behavior. Employing the ab-initio calculation and the Landau theory , we parameterize the Landau potential, exploring the mechanisms governing the domain switching from the non-centrosymmetric high-temperature P-62m phase to the room-temperature phase Pma21. Following the calculations of phase-field coefficients and potentials, we conduct multiscale simulations to analyze the domain formation and evolution. External electric fields are applied to reproduce the antiferroelectric-like hysteretic switching, providing new insight into the switching dynamics of K3Nb3B2O12 at the level of the domains.

KFM 13.8 Wed 12:10 EMH 225

Structural and electrical properties of Bi0.5Na0.5TiO3-based ceramics synthetize by optimized sol-gel method — •Thomas Fourgassie[1,2], Cécile Autret-Lambert[1,2], Pierre-Eymeric Janolin[2], and Brahim Dkhil[2] — [1]Laboratoire GREMAN, UMR 7347 Université de Tours, CNRS, INSA CVL, 37200 Tours, France — [2]Laboratoire SPMS, UMR 8580 Université Paris-Saclay, CNRS, CentraleSupélec, 91190 Gif-sur-Yvette, France

The energetic needs of our society seems to grow endlessly, that is why we need to increase our energy storage capacity for a sustainable future. Novel lead-free solid solutions are promising candidates to replace lead-based piezoelectric ceramics such as Pb(Zr,Ti)O3. Among the lead-free material, Bi0,5Na0,5TiO3 (BNT) ceramics have attracted a large attention for their excellent and competitive dielectric properties. Our goal is to synthetize a new lead-free material based on BNT presenting high energy storage properties in a wide range of temperature. BNT was chosen as a base material for his high maximum polarization (Pmax) and his relaxor properties making his phase transition more diffuse, resulting in broad peaks of dielectric permittivity . In order to improve the electrical properties for our final material, we decided to work on the optimization of the base material BNT by sol-gel method. We therefore report the impact of different synthesis processes, with different temperature of calcination or different time of calcination on the structural and dielectric properties of BNT, as well as the impact of the addition of dopants or excess of already present cations on the high leakage current usually seen in pure BNT.