MA 41: Ferroics - Domains and Domain Walls (joint session KFM/MA)

Time: Wednesday 15:00–18:20 Location: TOE 317

MA 41.1 Wed 15:00 TOE 317

Ferroelectric Domain Structure In Hexagonal Yttrium Manganite Thin Films - A Phase Field Study — •Amadé Bortis, Manfred Fiebig, and Thomas Lottermoser — Department of Materials, ETH Zurich, Zurich, Switzerland

The topologically protected vortex domains in hexagonal rare-earth manganites exhibit rich physics, both from a fundamental and application point of view. In thin films, however, the nanoscale domain size has thus far hindered the experimental investigation of domain patterns - the existence of vortex domains remains elusive. Here, we use a phase-field model based on a known Landau expansion of the free energy and incorporate boundary conditions for a thin film. With this model, we investigate up to which thickness a thin films retains the bulk-like vortex-string network - closed loops of connected vortices. We simulate the evolution of the structural domains for different thicknesses. In the ultrathin regime, we find straight lines of vortices emerging perpendicular to the films surface, similar to stacked 2D vortex patterns. As the thickness increases, we find an intermediate regime where the vortex lines start bending and merging, while still not being connected into closed loops. Finally, the bulk-like vortex-strings are recovered for a thickness of about 50 unit cells. Our work shows an effective 2D to 3D transition in rare-earth manganite thin films, revealing the impact of confined dimensionality on the domain topology.

MA 41.2 Wed 15:20 TOE 317

Dielectric nonlinearity in $0.5(Ba_{0.7}Ca_{0.3})TiO_3$–$0.5Ba(Zr_{0.2}Ti_{0.8})O_3$ ferroelectric thin film capacitors — •Maximilian Becker[1,2], Claus Burkhardt[1], Reinhold Kleiner[2], and Dieter Koelle[2] — [1]NMI Natural and Medical Sciences Institute at the University of Tübingen, Reutlingen, Germany — [2]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, University of Tübingen, Germany

We use the recently developed Rayleigh analysis based on impedance spectroscopy to investigate dielectric nonlinearity caused by irreversible motion of domain walls in lead-free ferroelectric $0.5(Ba_{0.7}Ca_{0.3})TiO_3$–$0.5Ba(Zr_{0.2}Ti_{0.8})O_3$ (BCZT) thin films. Impedance spectra from 10 Hz to 1 MHz were collected at different excitation fields on pulsed laser deposited polycrystalline and epitaxial BCZT thin film capacitors. Rayleigh plots were created by fitting the measured complex impedance to an equivalent-circuit model containing the Rayleigh element. For a polycrystalline film, we observed nonlinear behavior in good agreement with the Rayleigh law at a threshold field $E_T \approx 55\,\mathrm{kV/cm}$ with Rayleigh constant $\alpha' = 0.407 \pm 0.035\,\mathrm{cm/kV}$. For the epitaxial counterpart, we found Rayleigh-like behavior which is not in full agreement with the Rayleigh law at $E_T \approx 3.75\,\mathrm{kV/cm}$ with $\alpha' = 1.836 \pm 0.031\,\mathrm{cm/kV}$, indicating a significantly higher domain wall mobility. Our results demonstrate the superiority of Rayleigh analysis based on impedance spectroscopy over the commonly used single-frequency approach.

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MA 41.3 Wed 15:40 TOE 317

Soft modes and effective Hamiltonian for the antiferroelectric NaNbO3 — •Niloofar Hadaeghi and Hongbin Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

To understand the antiferroelectric(AFE) phase transition in prototype $NaNbO_3$, we carried out detailed symmetry analysis and first-principles calculations. The primary modes have been identified together with the coupling terms up to the fourth order based on symmetry. The corresponding energy landscape is obtained by constraint calculations with specific mode(s) frozen-in, and is further fitted to get the effective Hamiltonian. It is observed that there are three dominant modes for the AFE phase of $NaNbO_3$; R_5^-, T_2, and Δ_5. Our results reveal that it is not possible for the system to adopt the coupling of R_5^- and T_2 modes, since there is a strong mutual repulsion between them. However, coupling of both R_5^- and Δ_5, and T_2 and R_5^- are essential in the reduction of energy. Theses couplings are cooperative to stabilize the AFE phase. That is, the trilinear coupling is essential for the occurrence of the AFE phase. We also investigated the unfolded band structure to understand the effects of such soft modes on the electronic structure.

MA 41.4 Wed 16:00 TOE 317

Dimerized phases in IrTe2: phase diagram from a first-principles-derived model — Gabriele Saleh and •Sergey Artyukhin — Italian Institute of Technology, Genova, Italy

Materials with strong spin-orbit coupling have attracted recent interest due to their non-trivial magnetism and topological properties. IrTe2 combines some of the strongest spin-orbit-coupled cations and anions, and shows below 220 K a puzzling sequence of ordered phases with different patterns of short Ir-Ir bonds (dimers), some of which break the inversion symmetry. In spite of active efforts of the community, first principles simulations have struggled to describe the energetics of these phases, especially when the spin-orbit coupling is accounted for. Here we discuss a simplified model that captures dimer energetics, and use it to calculate the phase diagram and discuss the structure of domain walls. The choice of the model parameters is guided by first-principles simulations.

MA 41.5 Wed 16:20 TOE 317

Robust In-Plane Ferroelectricity in Ultrathin Epitaxial Aurivillius Films — •Elzbieta Gradauskaite[1], Marco Campanini[2], Banani Biswas[3], Christof W. Schneider[3], Manfred Fiebig[1], Marta D. Rossell[2], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]Electron Microscopy Center, Empa, Switzerland — [3]LMX, Paul Scherrer Institut, Switzerland

Layered ferroelectrics exhibit functionalities beyond those of the classical ferroelectric perovskite compounds due to their highly anisotropic structure. Unfortunately, the layered architecture has been impeding their growth as single crystalline thin films, and thus their integration into oxide-electronic devices. We show that deposition of layered ferroelectric $Bi_5FeTi_3O_{15}$ (BFTO) thin films on a lattice-matching $NdGaO_3$ (001)-oriented orthorhombic substrate supports the epitaxial single-crystal form of this Aurivillius compound. Layer-by-layer growth is demonstrated, permitting in-situ control of thickness with sub-unit-cell accuracy and resulting in atomically flat surfaces. The achievement of twin-free films significantly enhances their uniaxial ferroelectric properties. In the ultrathin regime, such films exhibit in-plane polarization with a periodic arrangement of ferroelectric domains, which, in conjunction with uniaxial ferroelectric anisotropy, results in nominally charged domain walls. Hysteresis measurements reveal a remnant polarization of 16.5 μC cm^{-2} with a remarkable endurance after 10^{10} switching cycles. The uniaxial in-plane ferroelectricity of Aurivillius thin films breaks new ground for alternative device paradigms less susceptible to the depolarizing-field effects.

20 min. break

MA 41.6 Wed 17:00 TOE 317

Ferroelectric domain wall imaging by focused ion beam — •Erik Roede[1], Aleksander Mosberg[1], Donald Evans[1], Theodor Holstad[1], Zewu Yan[2], Edith Bourret[3], Antonius van Helvoort[1], and Dennis Meier[1] — [1]NTNU, Trondheim, Norway — [2]ETH, Zurich, Switzerland — [3]Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Charged ferroelectric domain walls (DWs) have received much attention for their functional properties and potential applications [1]. The orientation of a DW relative to the ferroelectric polarization determines the charge state and electronic properties of the wall. Therefore, the propagation of DWs through a crystal has drastic effects on the properties measured at the surface. Still, research on DWs has so far been dominated by surface techniques.

In this work, we introduce the use of focused ion beam (FIB) techniques [2] for 3D domain and DW imaging in ErMnO3[3] with nanoscale resolution. This enables relating the measured surface properties to the 3D domain wall geometry, enabling a move towards a comprehensive knowledge of the intrinsic properties of charged ferroelectric domain walls and their application in future nanoelectronic devices.

[1] D. Meier et al., Nature Materials, 11, 284-288 (2012) [2] A. Mosberg et al., Appl. Phys. Lett. 115, 122901 (2019) [3] Z. Yan et al., J. Cryst. Growth, 409, 75-79 (2015)

MA 41.7 Wed 17:20 TOE 317

Functional bubble domains in ferroelectric superlattices — •Anna Grünebohm[1] and Claude Ederer[2] — [1]ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Materials Theory, ETH Zürich, 8093 Zürich, Switzerland

In this contribution we revisite the phase diagram of $BaTiO_3$–$SrTiO_3$ superlattices by means of ab initio based molecular dynamics simulations [1]. We discuss the stabilization of domain walls by epitaxial strain and the interplay of depolarization and anisotropy energy. Excitingly, transitions between stripe and bubble domains can be induced by an electrical field in close analogy to stray-field stabilized skyrmions in magnetic films. The local and global properties of the superlattices differ considerably in the vicinity of this transition. Thus exceptional functional responses such as negative capacitance may be realized.

[1] T. Nishimatsu et al., Phys. Rev. B **78**, 104104 (2008).

MA 41.8 Wed 17:40 TOE 317

Tracing domain formation in ferroelectric PZT films in-situ — •Martin Sarott, Manfred Fiebig, and Morgan Trassin — Department of Materials, ETH Zurich, Switzerland

The pronounced impact of growth conditions on the formation of domains in ferroelectric thin films obstructs the effective design of devices based on ferroelectrics that require controlled polarization states and deterministic switching dynamics. Here, we overcome this notorious difficulty by tracking in-situ, during growth, the emergence of domains in ultrathin ferroelectric layers. We use a combination of in-situ optical second harmonic generation (ISHG) and reflection high energy electron diffraction to directly observe the formation of in-plane oriented a-domains in an otherwise c-domain matrix in technologically relevant PZT films. By monitoring ISHG, we correlate the signal to the domain structure and identify a signature of mixed in-plane/out-of-plane domain patterns. Furthermore, we reveal the impact of epitaxial strain on the emergence of a-domains in a c-domain matrix. Our in-situ approach allows us to disentangle the influence of various growth parameters on the domain structure and thus enables the design of thin films with predefined domain states for reliable ferroelectric properties in the ultrathin regime.

MA 41.9 Wed 18:00 TOE 317

Photovoltage from ferroelectric domain walls in $BiFeO_3$ — •Sabine Körbel[1,2], Stefano Sanvito[1], and Jirka Hlinka[2] — [1]School of Physics & CRANN, Trinity College Dublin, Ireland — [2]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

Ferroelectric domain walls are objects capable of creating local electric fields in ferroelectric materials, and therefore in principle allow for a domain-wall driven photovoltaic effect. However, up to now the magnitude of such a domain-wall photovoltage was never measured nor calculated directly: experimentally it is hard to distinguish between domain-wall and bulk photovoltaic effect; first principles calculations used only an indirect approach based on the ionic polarization in the dark state, neglecting the electronic polarization. In order to directly calculate the domain-wall photovoltage in $BiFeO_3$, we modeled the excitonic charge density upon light irradiation from first principles and determined the potential variations at the domain walls and consequently the domain-wall photovoltage. We find indeed that excitons form an electric dipole layer at the domain walls resulting in a domain-wall driven photovoltage, and that the excitonic dipole moment is aligned parallel to the net polarization, not, as previously assumed, antiparallel. By comparing the calculated domain-wall photovoltage to the total photovoltage measured in experiment, we conclude that the domain-wall effects are relatively small and cannot account for the major part of the measured photovoltage. This indicates that bulk effects, not domain-wall effects, dominate the photovoltage in $BiFeO_3$.