KFM 6: Ferroelectric Domain Walls II (joint session KFM/TT)

Organizer: Sergey Artyukhin - Istituto Italiano di Tecnologia - Genova (Italy)

Time: Monday 15:00–18:30 Location: EMH 225

Invited Talk KFM 6.1 Mon 15:00 EMH 225

First-principles studies of ferroelectric and ferroelastic domain walls — •Jorge Íñiguez — Materials Research and Technology Department, Luxembourg Institute of Science and Technology, Avenue des Hauts-Fourneaux 5, L-4362 Esch/Alzette, Luxembourg

I will present our latest theoretical predictions on how to control the properties of functional oxides, and even induce completely new behaviors, by appropriately engineering their nano-structure, domains or domain walls. I will focus on two different research directions. On one hand, I will discuss ways to engineer ferroelectric and ferroelastic domain walls so they acquire specific properties (conductive, magnetic, topological) not present in the surrounding domains. On the other hand, I will show predictions that ferroelectric domain walls can be used to control heat currents, and can even act as phonon filters. Finally, I will also describe briefly the first-principles-based (second-principles) large-scale simulation methods that we use in most of our investigations.

Works done in collaboration with many colleagues, in particular H.J. Zhao, M.A.P. Gonçalves and C. Escorihuela-Sayalero (LIST); M. Royo, J.A. Seijas-Bellido and R. Rurali (ICAMB-CSIC); and J. Junquera and P. García-Fernández (U. Cantabria). Work at LIST funded by the Luxembourg National Reserach Fund through the CORE (Grant C15/MS/10458889 NEWALLS), PEARL (Grant P12/4853155/Kreisel COFERMAT) and AFR (Grant No. 9934186) programs.

KFM 6.2 Mon 15:30 EMH 225

First-principles prediction of electric skyrmions — •Mauro Gonçalves[1,2], Carlos Escorihuela-Sayalero[1], Pablo García-Fernández[2], Javier Junquera[2], and Jorge Íñiguez[1] — [1]Luxembourg Institute of Science and Technology, Belvaux, Luxembourg — [2]Universidad de Cantabria, Santander, Spain

Nowadays, nontrivial topological spin structures like skyrmions are a focus of interest, as they open the door to novel nano-technologies with huge potential impact. Some authors have discussed electric skyrmions, whereby an exotic arrangement of electric dipoles would yield skyrmion-like structures in ferroelectric materials. Indeed, the recent experimental discovery of a dipole vortices in $PbTiO_3/SrTiO_3$ superlattices [1] has added to earlier theoretical predictions of skyrmions in ferroelectric nano-composites [2], and the possibility of stabilizing electric skyrmions currently attracting a lot of attention.

Following these ideas, we have used first-principles model potentials and large-scale lattice-dynamical simulations [3] to investigate the behavior of ferroelectric nano-domains immersed in a big domain of opposite polarization. Our simulations yield the first prediction of an electric skyrmion in a single phase material. We have also found that these dipole structures can be controlled applying an epitaxial strain or external electric fields, which may open the door to interesting physics and applications.

[1] Damodaran, A. R. et al., Nature Materials **16**, 1003 EP (2017).
[2] Nahas, Y. et al., Nature Communications **6**, 8542 EP (2015).
[3] J.C. Wojdeł, et al., J. Phys.:Condens. Matter **25**, 305401 (2013).

KFM 6.3 Mon 15:45 EMH 225

The impact of domains on phase transitions and the electrocaloric effect - an ab initio based study of $BaTiO_3$. — •Anna Grünebohm[1], Madhura Marathe[2], and Claude Ederer[3] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Institut de Ciència de Materials de Barcelona, Spain — [3]Materials Theory, ETH Zürich, Switzerland

The electrocaloric effect (ECE) is the adiabatic temperature change induced by a varying external electrical field [1]. Although large temperature changes arise at field-induced first order phase transitions, this response may be irreversible due to thermal hysteresis [1-3]. We present an *ab initio* based study of the impact the domain structure makes on such transitions, their thermal hysteresis, and the (reversible) caloric response. As example, we focus on the tetragonal and orthorhombic phases of $BaTiO_3$ [4].

[1] X. Moya, *et al.*, Nature Mater. **13**, 439 (2014).
[2] M. Marathe, *et al.*, Phys. Rev. B **96**, 014102 (2017).
[3] M. Marathe, *et al.*, PSS (b), **1521**, 1700308 (2017).
[4] A. Grünebohm *et al.* Euro. Phys. Lett. **115**, 47002 (2016).

15 min break

KFM 6.4 Mon 16:15 EMH 225

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

Recent publications on first principles electronic structure of ferroelectric domain walls (FE DW) in $BiFeO_3$ show some variations concerning existence and magnitude of potential steps and band bending at pristine FE DW. We investigated these properties once more, trying to improve understanding by building on previous works in a systematic way. We also tested the hypothesis that FE DW modify the light absorption properties of $BiFeO_3$.

KFM 6.5 Mon 16:30 EMH 225

Formation of ferroelectric monoclinic domains in $K_{0.7}Na_{0.3}NbO_3$ thin films under different strain conditions — •Leonard von Helden[1], Martin Schmidbauer[1], Michael Hanke[2], and Jutta Schwarzkopf[1] — [1]Leibniz Institute for Crystal Growth (IKZ), Berlin — [2]Paul-Drude-Institute for Solid State Electronics (PDI), Berlin

$K_xNa_{1-x}NbO_3$ is a promising material for lead-free ferro- and piezoelectric applications due to its high piezoelectric and coupling coefficients. Moreover, monoclinic phases - which are favorable as they enable a continuous rotation of the polarization vector - can be induced by incorporating anisotropic epitaxial lattice strain in $K_xNa_{1-x}NbO_3$ thin films. Upon varying the strain conditions the symmetry and orientation of these monoclinic domains can be deliberately tailored as predicted by strain-phase calculations.[1] In order to confirm the theoretical predictions we present a systematic investigation on the ferroelectric domain formation in $K_{0.7}Na_{0.3}NbO_3$ thin films grown by MOCVD. Slightly different strain conditions were realized by the application of various (110) oriented rare earth scandate substrates. The resulting ferroelectric domain structure was investigated upon a combination of piezoresponse force microscopy and X-ray nano-diffraction. Our results reveal monoclinic M_C domains with $(001)_{pc}$ pseudocubic unit cell orientation that differ among the substrates regarding their domain wall inclination. Moreover, the additional occurrence of $(100)_{pc}$ unit cell orientation in films with a thickness above 60 nm will be discussed. [1] J. Schwarzkopf et al., Front. Mater. 4, 26 (2017).

KFM 6.6 Mon 16:45 EMH 225

Phononics at ferroelectric domain walls — •Francesco Foggetti[1,2] and Sergey Artyukhin[1] — [1]Italian Insitute of Technology, Genova, Italy — [2]University of Genova, Italy

Ferroelectric domain walls are emerging as robust 2D systems with promising functionality. Recent scanning tunneling and impedance microscopy studies revealed DC and AC conductivity, 2D electron gas and modified chemistry at ferroelectric domain walls. We study phonons localized at ferroelectric domain walls, and scattering of bulk phonons off ferroelectric domain walls using continuum theory and discrete models.

15 min. break

Invited Talk KFM 6.7 Mon 17:15 EMH 225

Probing STO domain walls with scanning SQUID microscopy — •Beena Kalisky — Department of Physics and Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Israel

The interface formed by growing LaAlO3 on SrTiO3 (STO), both non magnetic insulators, exhibits conductivity, superconductivity and even magnetism. It is not surprising that the symmetry of the STO substrate is a dominant player in the plethora of physical phenomena found at the interface. We first encountered the interplay between the STO ferroelastic domain walls and the interface while imaging the magnetic flux generated from the interfacial current flow. We found

that a big part of the current can be modulated over the STO domain walls and that macroscopic transport measurements are strongly affected. We then investigated the origin of the modulations. We applied local stress to the sample and imaged the change in resistivity. Surprisingly, we found that the resistivity changed mainly along the domain walls which are highly sensitive to pressure. Our study shows that the Scanning SQUID is very useful for the investigation of buried domain walls and their effect on nearby layers.

KFM 6.8 Mon 17:45 EMH 225

LiNbO3 thin-film crystals: A novel class of materials for domain engineering and enhanced domain wall conductivity — •Tillmann Stralka, Alexander Hausmann, Lukas Wehmeier, and Lukas M. Eng — Institute of Applied Physics, Technische Universität Dresden, Germany

In the last years, research on ferroelectric domain wall conductivity (DWC) mostly has focused either on PLD-grown, ultra-thin ferroelectric (FE) films [1] or FE bulk-single crystals [2,3,4]. Here we extend DWC to a novel and extremely prospective class of materials, i.e. free-standing thin-film crystals made up from ultra-thin single-crystalline $LiNbO_3$ (LNO) sheets. We use 5%-Mg-doped LNO polished down to a 22-μm thickness. Beyond high-voltage- [3] and super-bandgap-illumination-induced [4] DW engineering, the sample thinness also allows to write domain patterns by low-voltage AFM lithography, resulting in fully penetrating through domains. Of central interest in these thin-film LNO crystals is the mutual interaction between neighboring DWs, hence providing a novel tool for DW shape engineering on the very local length scale. Investigations are carried out using a combination of AFM techniques (PFM, c-AFM, topography) and Cerenkov Second Harmonic Microscopy [5], as well as by monitoring the electrical transport in DWs along the crystallographic X and Y axes in LNO. [1] J. Seidel et al., Nature Mater. **8** (2009) 229. [2] T. Sluka et al., Nature Comm. **4** (2013) 1808. [3] C. Godau et al., ACS Nano **11** (2017) 4816. [4] M. Schröder et al., Adv. Func. Mater. **22** (2012) 3926. [6] L. Wehmeier et al., Phys. Stat. Solidi **11** (2017) 1700267.

KFM 6.9 Mon 18:00 EMH 225

Correlating domain wall conductivity with geometry: a real-time study via Cerenkov Second Harmonic Generation — •Christian Godau, Lukas Wehmeier, Alexander Haussmann, and Lukas Eng — Institute of Applied Physics, Technische Universität Dresden, D-01062 Dresden, Germany

Ferroelectric domain walls (DWs) have become a central topic of research these days. Especially exploring their electronic properties and domain wall conductivity (DWC) in both thin films [1,2] and single crystals (sc) [3,4,5] has become very attractive. Our recent research on sc-lithium niobate (LNO) has proven an ultra-high DWC [4] and low electronic work function [6] that both provide a solid and promising foundation for prospective electronic device application.

Here, we present a full 3D and time-resolved study by Cerenkov Second Harmonic Generation [7] when investigating the DW dynamics in sc-LNO that are subjected to electric fields. Variations of the field lead to significant changes in geometry and inclination angles of the DW, that is tracked here in real time. These changes in DW-geometry are then correlated to the current measured through the conductive DWs.

[1] J. Seidel et al., Nat. Mater. 8, 229 (2009) [2] S. Cherifi-Hertel et al., Nat. Comm. 8, 15768 (2017) [3] T. Sluka et al., Nat. Comm. 4, 1808 (2013) [4] C. Godau et al., ACS Nano 11, 4816 (2017) [5] M. Schröder et al., Mater. Res. Express 1, 035012 (2014) [6] A.-S. Pawlik et al., Nanoscale 9, 10933 (2017) [7] T. Kämpfe et al., Phys. Rev. B 89, 035314 (2014)

KFM 6.10 Mon 18:15 EMH 225

Domain wall and bulk conductance in $ErMn_{1-x}Ti_xO_3$ — •Theodor Secanell Holstad[1], Donald Malcolm Evans[1], Alexander Ruff[2], Didrik René Småbråten[1], Jakob Schaab[3], Christian Tzschaschel[3], Zewu Yan[4,5], Edith Bourret[5], Sverre Magnus Selbach[1], Stephan Krohns[2], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, NTNU, Norway. — [2]Center for Electronic Correlations and Magnetism, University of Augsburg, Germany. — [3]Department of Materials, ETH, Switzerland. — [4]Department of Physics, ETH, Switzerland. — [5]Materials Sciences Division, UC Berkeley, USA.

Ferroelectric domain walls are attracting broad attention as a novel type of spatially mobile oxide interface that can be written, erased, and moved on demand. Recently, acceptor and donor doping was adapted to optimize the behavior at ferroelectric domain walls.

In this talk, I will discuss the effect of donor doping on the electronic bulk and domain wall properties in hexagonal $ErMn_{1-x}Ti_xO_3$. Density functional theory calculations show that Ti^{4+} goes to the B-site, replacing Mn^{3+}. Scanning probe microscopy measurements confirm the robustness of the ferroelectric domain template. The electronic transport at both macro- and nanoscopic length scales is characterized. The measurements demonstrate the intrinsic nature of emergent domain wall currents and point towards Poole-Frenkel conductance as the dominant transport mechanism. Aside from the insight into the electronic properties of hexagonal manganites, B-site doping adds an additional degree of freedom for tuning the domain wall functionality.