KFM 10: Ferroics - Domains and Domain Walls

Time: Tuesday 9:30–12:50 Location: H47

KFM 10.1 Tue 9:30 H47

Ferroic transition in single-crystal $BaTiO_3$ — Asaf Hershkovitz[1], •Florian Johann[2], Maya Barzilay[1], Alon Avidor[1], and Yachin Ivry[1] — [1]Department of Materials Science and Engineering, Technion, Israel Institute of Technology, Haifa, Israel — [2]Asylum Research, an Oxford Instruments company, Wiesbaden, German

Variable-temperature piezoresponse force microscopy was used to image real-time dynamics of ferroelastic domains during the orthorhombic-tetragonal ferroic phase transition in single-crystal BaTiO3. We demonstrate multiscale stress releasing mechanism at the time space. This mechanism comprises domain wrinkling at the pre-transition state, followed by domain wedging during the transition and ending with domain zipping after the transition, in which striped ferroelastic domains are broadened.

KFM 10.2 Tue 9:45 H47

External-field induced domain wall dynamics in $LiNbO_3$ and $BaTiO_3$ single crystals imaged by in-situ 3D Cherenkov second harmonic generation microscopy — •Benjamin Kirbus, Christian Godau, Lukas Wehmeier, Elke Beyreuther, Alexander Haussmann, and Lukas Eng — Institut für Angewandte Physik, TU Dresden, Nöthnitzer Str. 61, 01187 Dresden

Cherenkov second harmonic generation (CSHG) microscopy poses a powerful new tool [1,2] for the 3D imaging of ferroelectric domain walls (DWs). Investigating $LiNbO_3$ crystals, 10-nm-thick Cr electrodes were deposited onto the samples. The z^+ side was grounded and a ramped potential applied to the z^- side. When increasing the field up to +4.0 kV/mm, laser-poled hexagonal domains were observed in real-time and *in-situ* to collapse into inclined, coned structures, forming highly conductive head-to-head DWs [3]. Consequently, the domain-wall current (DWC) increased by over 4 orders of magnitude, reaching values of >1 μA. A reversed poling field down to -3.6 kV/mm led to reversible and irreversible domain-shape recovery. Expansion of spike domains increased the DWC up to >1 mA.

The crystal symmetry of $BaTiO_3$ allows much more complex domain patterns [4], such as 90° domain walls. Their kinetics upon phase transition will also be discussed using 3D CSHG imagery.

[1] L. Wehmeier et al. *Phys. Status Solidi RRL* **11**, 1700267 (2017).
[2] T. Kämpfe et al. *Phys. Rev. B* **8**, 035314 (2014).
[3] C. Godau et al. *ACS Nano* **11**, 4816 (2017).
[4] J. Döring et al. *J. Appl. Phys.* **120**, 084103 (2016).

KFM 10.3 Tue 10:00 H47

Tuning ferroelectric phase transition temperatures in epitaxial $K_xNa_{1-x}NbO_3$ thin films — •Leonard von Helden[1], Laura Bogula[1], Pierre-Eymeric Janolin[2], Michael Hanke[3], Martin Schmidbauer[1], and Jutta Schwarzkopf[1] — [1]Leibniz Institute for Crystal Growth, Berlin, Germany — [2]Laboratoire SPMS, CNRS-École Centrale Paris, France — [3]Paul-Drude-Institute for Solid State Electronics, Berlin, Germany

$K_xNa_{1-x}NbO_3$ is a promising material for, e.g., surface acoustic wave (SAW) sensors based on ferroelectric thin films. For these systems a strong enhancement of SAW transmission coefficients in the vicinity of phase transition temperatures has been reported, recently.[1] Hence, it is desirable to deliberately tune those phase transitions.

Here, we present a first systematic study in which ferroelectric phase transition temperatures in epitaxial $K_xNa_{1-x}NbO_3$ films could be altered by choice of different (110) oriented rare earth scandate substrates and variation of the K-to-Na ratio in the film. Sample preparation was conducted by liquid delivery metal organic vapor phase epitaxy (MOVPE). Our results reveal the possibility to continuously shift the ferroelectric-ferroelectric transition between monoclinic M_C and c-phase by about 400 K via application of compressive strain. The phase transition was investigated in detail by temperature dependent piezoresponse force microscopy (PFM), X-ray diffraction (XRD) and laser interferometry.

[1] S. Liang et al., Appl. Phys. Lett. 113, 052901 (2018)

KFM 10.4 Tue 10:15 H47

Transient depolarizing field effects leading to domain formation in the ultrathin regime — •Nives Strkalj[1], Gabriele De Luca[1], Marco Campanini[2], Shovon Pal[1], Jakob Schaab[1], Chiara Gattinoni[1], Nicola A. Spaldin[1], Marta D. Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]EMPA, Switzerland

A major challenge for the ferroelectric-based device miniaturization is to stabilize a robust polarization. In the ultrathin regime, however, the interface-related effects can drastically alter the polarization behavior and in extreme case lead to annihilation of the ferroelectric state. Because the ferroelectric layers are usually grown below their Curie temperature, their polarization state is set during the heterostructure growth. We thus track the evolution of polarization state using in situ optical second harmonic generation [1]. Taking $SrRuO_3$-$BaTiO_3$-$SrRuO_3$ capacitor heterostructure as a model system, we observe an abrupt domain formation leading to a net polarization quench during the top electrode deposition. We show a reduced conductivity in the ultrathin regime of the top electrode, leading to an inferior charge screening efficiency and therefore transient depolarizing field enhancement [2]. We demonstrate a healing route to the single domain state by post-growth thermal annealing above the strain-engineered Curie temperature. Our in-situ approach addresses transient electrostatic effects during the deposition and sheds light on the emergence of complex domain architectures in ferroelectric superlattices. [1] G. De Luca et al. Nat. Commun. 8, 1419 (2017) [2] N. Strkalj et al. (submitted)

KFM 10.5 Tue 10:30 H47

Deconvoluting conductance contributions at charged ferroelectric domain walls — •Theodor Secanell Holstad[1], Donald Malcolm Evans[1], Didrik René Småbråten[1], Joshua Agar[2], Stephan Krohns[3], Zewu Yan[4], Edith Bourret[4], Sverre Magnus Selbach[1], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, Norwegian University of Science and Technology, Norway. — [2]Department of Materials Science and Engineering, University of Lehigh, USA. — [3]Center for Electronic Correlations and Magnetism, University of Augsburg, Germany. — [4]Materials Sciences Division, Lawrence Berkeley National Laboratory, USA.

Ferroelectric domain walls are spatially mobile interfaces that naturally occur in materials that develop a spontaneous electric polarization. Because of their unique electronic properties, such walls hold great promise as functional 2D systems, but the characterization of their intrinsic transport properties remains a challenging task. Here, we combine scanning probe microscopy (SPM) with machine learning to gain new insight into the local electronic domain wall properties and to enhance the informational value of local conductance measurements. As a model case, we study the transport at ferroelectric domain walls in ($Er_{0.99}$, $Zr_{0.01}$)MnO_3: At low voltages, head-to-head domain walls appear to be conducting. At higher voltages, however, the same domain walls are insulating. Using machine learning, we disentangle different conduction contributions and explain these seemingly contradictory results, highlighting how machine detection enhances the SPM output.

KFM 10.6 Tue 10:45 H47

Interplay of domain structure and phase transitions and its impact on functional responses — •Anna Grünebohm[1] and Madhura Marathe[2] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Institut de Ciència de Materials de Barcelona, Spain

It is well established that the domain structure of ferroelectrics depends on crystal structure as well as the elastic and electric boundary conditions. However, the knowledge on the interplay of domain structure and structural phase transitions is incomplete. In this *ab initio* based study we focus on the domain structure at the tetragonal to orthorhombic phase transition in $BaTiO_3$ which has been less studied than the high temperature paraelectric to ferroelectric transition [1]. In particular, we show how domain engineering may allow to reduce the thermal hysteresis of the transition and how this allows to optimize functional responses such as the electrocaloric effect.

[1] T. Limboek and E. Soergel, Appl. Phys. Lett. **105**, 152901, 2014

Break

KFM 10.7 Tue 11:35 H47

Electric-field poling of an improper ferroelectric — Alexander Ruff[1], Jakob Schaab[2], Manfred Fiebig[2], Dennis Meier[3], and •Stephan Krohns[1] — [1]Experimental Physics V, Center for Electronic Correlation and Magnetism, University of Augsburg, Augsburg 86159, Germany — [2]Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [3]Department of Materials Science and Engineering, Norwegian University of Science and Technology

Manipulation of domains within ferroelectric semiconductors has attracted attention in recent years for potentially allowing domains and domain walls to be used as functional elements in nanoelectronics. Hexagonal manganites have shown particular potential because of their unusual, improper ferroelectric properties. Here, we provide an electric-field poling study of h-$ErMnO_3$. From a detailed dielectric analysis [1], we deduce the temperature- and frequency-dependent range for which single-crystalline h-$ErMnO_3$ exhibits purely intrinsic dielectric behavior [2]. In this temperature range, the ferroelectric switching kinetics, which is mainly driven by domain-wall motion, is investigated without superimposing extrinsic contributions. Controlling the domain walls via electric fields will bring us an important step closer to their utilization in domain-wall-based electronics [3].

[1] E. Ruff et al., Phys. Rev. Lett. 118, 036803 (2017).
[2] A. Ruff et al., Appl. Phys. Lett. 112, 182908 (2018).
[3] J. Schaab et al., Nature Nanotechnology, 13, 1028 (2018).

KFM 10.8 Tue 11:50 H47

Local manipulation of improper ferroelectric domains in $YMnO_3$ using scanning probe microscopy at low temperatures — •L. Kuerten[1], P. Schoenherr[1], S. Krohns[2], D. Meier[3], E. Pomjakushina[4], K. Conder[4], Th. Lottermoser[1], and M. Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]Experimental Physics V, University of Augsburg — [3]Department of Materials Science and Engineering, NTNU, Trondheim — [4]Laboratory for Scientific Developments and Novel Materials, PSI, Villigen

In hexagonal manganites, the conductivity can differ by orders of magnitude between ferroelectric domains and domain walls. In order to utilize this technological potential, control over the domain wall position and orientation is necessary. In $YMnO_3$, switching of the bulk polarization has been achieved at low temperatures using co-planar electrodes. However, the microscopic mechanism of domain switching and the role played by domain wall motion and domain nucleation are still unknown. In particular, the multi-domain state of the surface appears unaffected when observed at room temperature before and after switching. Here, we investigate the microscopic mechanism of domain manipulation in situ at low temperature using piezoresponse force microscopy (PFM). By applying DC voltages to the PFM tip, we reveal signatures of polarization reversal at the sample surface indicating local domain switching. However, charge injection via the tip also plays a crucial role, which is demonstrated for regions on the nanometer scale. These charged regions remain stable for days at low temperatures, but vanish for increased temperatures.

KFM 10.9 Tue 12:05 H47

Charge-carrier localization at ferroelectric domain walls in $BiFeO_3$ — •Sabine Körbel and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, Ireland

$BiFeO_3$ is a prototype material for investigating the photovoltaic effect in ferroelectrics, and it has been suggested that ferroelectric domain walls in $BiFeO_3$ and other ferroelectrics are beneficial for separating charge carriers.

In order to elucidate the role of the domain walls in the separation of photogenerated charge carriers, we studied electron and hole localization at ferroelectric domain walls in $BiFeO_3$, using density-functional theory.

In this talk we will discuss the localization behavior of separate electrons and holes and that of electron-hole pairs.

KFM 10.10 Tue 12:20 H47

Hall effect probed within highly- conducting ferroelectric domain walls in single-crystalline Lithium Niobate — •Henrik Beccard, Benjamin Kirbus, Alexander Haussmann, Elke Beyreuther, and Lukas M. Eng — Institute of Applied Physics, TU Dresden, Nöthnitzer-Str. 61, 01187 Dresden, Germany

Conducting domain walls (CDWs) in single-crystalline lithium niobate (LNO) are promising candidates for generating a manifold of possible nanoscale devices, especially based on electronic and optical properties [1]. Much works focused on improving imaging methods [2] and developing new devices utilizing CDWs. Moreover, novel protocols have been proposed that allow to tuned the domain wall current up to the mA regime [3]. Nevertheless, some of the most fundamental properties of charge carrier transport within these CDWs could not be measured accurately. We thus thoroughly inspected a single CDW in LNO using macroscopic Hall transport measurements. As a result, the mobility and charge carrier density of CDWs in LNO could be determined. Additionally, the influence of UV illumination on charge the charge carrier density within the wall was investigated. Utilizing Cherenkov second-harmonic generation, we were also able to record 3D images of these domain walls hence correlating [4] the Hall transport current to the local inclination of the domain within the LNO single crystal.

[1] G. Catalan et al. Rev. Mod. Phys. 84, 119 (2012).
[2] T. Kämpfe et al. Phys. Rev. B 8, 035314 (2014).
[3] C. Godau et al. ACS Nano 11, 4816 (2017).
[4] B. Wolba et al. Adv. Electron. Mater. 4, 1700242 (2017).

KFM 10.11 Tue 12:35 H47

Nonlinear optical crystals in tightly focused laser beams: A spatially resolved second-harmonic analysis in the focal plane — •Kai Spychala, Peter Mackwitz, Alex Widhalm, Gerhard Berth, and Artur Zrenner — Department Physik, Universität Paderborn, 33098 Paderborn, Germany

In this work the nonlinear light-matter interaction in tightly focused optical systems is characterized. The study comprises the development of a theoretical model and a detailed experimental verification of the behaviour of second-harmonic (SH) generation in nonlinear optical crystals by focused light beams. We apply a direct imaging technique which records the spatial distribution of the second-harmonic signal in the back focal plane. Besides a profound understanding of the interaction which takes place in the focal region, the objective of this work is to develop the necessary numerical tool kit for in-depth data analysis. Our rigorous simulation, which is based on a vectorial description of the propagating light-fields, models the generated nonlinear signal in the case of (high NA) SH-microscopy and is verified via focal plane mapping in lithium niobate and potassium titanyl phosphate in a surface near regime. The calculations predict the symmetry and shape of the corresponding signals very well. In combination with experimental results it is now possible to extract information about the crystal symmetry. In this respect, our experiments verify the vectorial interaction processes, which lead to a specific and well-understood response in the SH signal.