DF 11: Ferroics - Domains, Domain Walls and Skyrmions II

Chairs: Tadej Rojac and Istvan Keszmarki

Time: Wednesday 9:30–13:00 Location: WIL B321

Topical Talk DF 11.1 Wed 9:30 WIL B321

Implications of domain evolution during the growth of ferroelectric superlattices — Rui Liu, Benjamin Bein, Hsiang-Chun Hsing, Anna Gura, Mohammed Humed Yusuf, Giulia Bertino, Jin-Wen Lai, and •Matthew Dawber — Dept of Physics and Astronomy, Stony Brook University, Stony Brook, NY, USA

In ferroelectric superlattices the constituent materials are often under considerable epitaxial strain, raising their ferroelectric transition temperatures to the point where they are comparable to or exceed the growth temperature. This has a number of important consequences for the growth of the superlattice and it's eventual properties. For example, the polarization domain structure is markedly different depending on whether the overall structure's transition temperature lies constantly below, constantly above, or oscillates around the growth temperature. Perhaps more surprisingly, we have found that the ferroelectric polarization of a growing structure has a strong effect on the rate at which it grows, which is critical information if high quality samples with well defined layer thicknesses are to be achieved. A useful approach to investigating these questions is x-ray diffraction performed in-situ during the growth process. The precise control of both layer thicknesses and the arrangement of polarization domains are particularly important for applications of ferroelectric materials that rely on their polar surface structure, such as photocatalysis or the nanoscale control of the charge state of 2D materials.

DF 11.2 Wed 10:00 WIL B321

Probing in situ the polar states in growing multiferroic heterostructures — •Morgan Trassin, Gabriele De Luca, Sebastian Manz, and Manfred Fiebig — ETH Zurich, Switzerland

In ferroelectric thin films, the polarization state, i. e. orientation and domain architecture, defines the macroscopic ferroelectric properties such as the switching dynamics. Ferroelectric domain engineering is in permanent evolution from the epitaxial strain tuning to the chemical control on interface atomic termination. Technology promising complex polar flux closure or vortices architecture have been recently demonstrated in ferroelectric heterostructures. However the determination of the role of depolarizing field and local strain in the formation of these complex polar states remains challenging. The optical second harmonic generation process is an efficient and non-invasive tool for thin films ferroic properties probing. Here, we investigate the emergence of the ferroelectric polarization in ultra-thin ferroelectric and multiferroic films and monitor in situ the optical non-linear response of the film during the growth. We find that, the ferroelectric critical thickness and domain state can be measured in situ during the film deposition. Using a combination of epitaxial strain engineering and surface termination control in $(BiFeO_3/SrRuO_3)_n$ multilayers, we determine the $BiFeO_3$ net polarization orientation in each layer and in real-time, exempt from substrate contribution. Our work provides direct observation of ferroelectric states during the growth as well as new insights towards further control of ferroelectric based heterostructure.

DF 11.3 Wed 10:15 WIL B321

Early stage of ferroelectricity in $BaTiO_3$ multilayers — •Nives Bonacic[1], Gabriele De Luca[1], Marco Campanini[2], Marta D Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]ETH Zürich, Department of Materials — [2]EMPA, Switzerland

Progress in the growth quality of transition-metal oxide heterostructures by pulsed-laser deposition greatly faciliated research of ultra-thin ferroelectrics with respect to their technological potential. In the thickness regime of a few unit cells, maintaining a large, stable and switchable ferroelectric polarization relies on the control of the strain state, thickness and interface termination in multilayers. Due to the complex interplay of these parameters, open questions remain about the intrinsic ferroelectric properties in the ultra-thin thickness regime. In order to understand the emergence of the ferroelectric polarization and determine the critical thicknesses involved, we use optical second harmonic generation (SHG) during the film deposition to probe the formation of the ferroelectric order directly. Taking $(BaTiO_3\text{-}SrRuO_3)_n$-based multilayers as an example, we access the polarization of each ferroelectric layer separately and of the ferroelectric interlayer coupling using SHG. Within each $BaTiO_3$ layer, an abrupt transition from single domain to multi-domain state is evidenced. By tracking the SHG signal during growth continuously, we show that reduced dimension and electrostatic environment induce intermediate polar states not visible in the final structure. Following the dynamics of ferroelectricity emergence and evolution in-situ paves the way to definite answers on size-reduction effects and the dynamics of complex domain formation.

15 min. break

DF 11.4 Wed 10:45 WIL B321

Domain wall architecture in tetragonal ferroelectric thin films — •Gabriele De Luca[1], Marta D. Rossell[2], Jakob Schaab[1], Nathalie Viart[3], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]Electron Microscopy Center, EMPA, Switzerland — [3]Institut de Physique et Chimie des Matériaux de Strasbourg, France

Ferroic domain walls separate regions with a different orientation of the order parameter. The resulting lowering of the local symmetry enables properties that are otherwise not allowed in the bulk rendering them attractive for potential applications. Lead Zirconate Titanate (PZT) is the most important ferroelectric material to date, and its performance largely depends on the behaviour of its domains and domain walls. For example, in PZT thin films, out-of-plane-polarized c-domains are typically interspersed by in-plane-polarized a-domains that obstructs the controlled migration of 180° domain walls due to pinning at surface dislocations. Combining scanning transmission electron microscopy and nonlinear optics we determine the relation between strain, film thickness, local electric fields and the resulting domain and domain-wall structure across the entire thickness of various PZT films [1]. We find that the voltage-induced c-domain walls are inclined and exhibit a mixed Ising-Néel-type rotation of polarization across the wall with a specific nonlinear optical response. The domain wall tilt leads to a macroscopic tail-to-tail polarization component where accumulation of screening charges can be expected.

[1] G. De Luca et al., Adv. Mater. 28 (2016)

DF 11.5 Wed 11:00 WIL B321

Monoclinic superdomains in ferroelectric $K_{0.7}Na_{0.3}NbO_3$ thin films on $TbScO_3$ — •Leonard von Helden[1], Martin Schmidbauer[1], Dorothee Braun[1], Christoph Feldt[1], Michael Hanke[2], and Jutta Schwarzkopf[1] — [1]Leibniz Institut für Kristallzüchtung, Max-Born-Str. 2, 12389 Berlin — [2]Paul-Drude-Institut für Festkörperelektronik, Hausvogteipl. 5-7, 10117 Berlin

$K_xNa_{1-x}NbO_3$ is a promising material for lead free ferro- and piezoelectric applications. Enhanced piezoelectric properties can be achieved by incorporating anisotropic lattice strain in epitaxial thin films. Monoclinic domains, which are favorable as they enable a continuous rotation of the polarization vector within the monoclinic mirror plane, were shown to be stabilized in $K_{0.7}Na_{0.3}NbO_3$ thin films grown by MOCVD on $TbScO_3$ substrates.[1]

In this study we present the coexistence of four variants of superdomains in $(001)_{pc}$ oriented $K_{0.7}Na_{0.3}NbO_3$ films on $TbScO_3$ with a film thickness of 30 nm. Below this thickness, only two types of superdomains occur. Each superdomain consists of periodically ordered stripe domains which are characterized by their vertical and lateral response in piezoresponse force micrographs (PFM) indicating different local piezoelectric coefficients. The domain structure can tentatively be described by monoclinically distorted unit cells, whose in-plane orientation is rotated by 90° between the stripe domains. A domain model is presented based on X-Ray diffraction experiments using a nano-focused beam.

[1] J. Schwarzkopf et al., J. Appl. Crys., 49, 375-384, (2016)

DF 11.6 Wed 11:15 WIL B321

Controlling the intrinsic polarization state in RF sputtering grown ferroelectric ultrathin films — •Christian Weymann, Céline Lichtensteiger, Stéphanie Fernandez, Jean-Marc Triscone, and Patrycja Paruch — DQMP, University of Geneva, Geneva, Switzerland

Ferroelectric ultrathin films are technologically promising. Crucial to all applications is their intrinsic polarization state. To maintain a uniform polarization state, the depolarizing field must be compensated either by external free charges or by internal mobile charges from within the ferroelectric itself. The built-in field also affects the polarization state, as it favors one polarization direction over the other. It results from an asymmetry in the screening or from internal sources, such as trapped charges or strain gradients leading to flexoelectricity.

We show that we can manipulate both these fields, acting on the electrostatic boundary conditions via the use of dielectric spacer layers to increase the depolarizing field, or modulating the built-in field through changes in the growth temperature of PbTiO3 thin films.

Quality and production costs are also major issues for applications. Off-axis radio frequency (RF) magnetron sputtering is a reliable technique to grow these structures. However, the relatively low cost of such a system compared to other thin film deposition techniques traditionally brings the disadvantage of lower control over the sample quality. Here we present a slow kinetics intermittent sputtering (SKIS) approach which greatly enhances the sample quality, opening a pathway towards an affordable method to grow high quality epitaxial thin films.

DF 11.7 Wed 11:30 WIL B321

Analysing the orientation distribution function of ferroelectric domains using vector piezoresponse force microscopy — •Markus Kratzer[1], Michael Lasnik[1,2], Felice Bombieri[1,2], Sören Röhrig[2], Marco Deluca[2], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversität Leoben, Aiustria — [2]Materials Center Leoben Forschung GmbH, Austria

An important figure of merit for analyzing and improving the behavior of commercial piezoelectric actuators is the orientation distribution function (ODF) of the domains in ferroelectric ceramics. A common method to visualize piezoelectric domain orientations is Piezoresponse Force Microscopy (PFM). In principle, a three-dimensional reconstruction of the domain polarization can be obtained by measuring the out-of-plane and in-plane components of the domains (Vector PFM). On the basis of the material's piezoelectric tensor and multiple measurements on one sample, the vertical (1D) and lateral (2D) orientations of the domains are obtained, and the ODF can be reconstructed. Utilizing Vector PFM we investigated differently polarized lead zirconate titanate ceramics and commercial piezoceramic actuators. A newly developed data treatment algorithm allowed fast and reliable reconstruction of the domain ODF from three-dimensional Vector PFM data.

DF 11.8 Wed 11:45 WIL B321

Smart correction of SPM time series: can data analytics help us extract correlations? — •Iaroslav Gaponenko[1], Philippe Tückmantel[1], Benedikt Ziegler[2], Guillaume Rapin[1], Manisha Chhikara[1], and Patrycja Paruch[1] — [1]Department of Quantum Matter Physics, University of Geneva, 1211 Geneva, Switzerland — [2]Combine AB, 413 04 Gothenburg, Sweden

Since its inception, scanning probe microscopy (SPM) has established itself as the tool of choice for probing surfaces and functionalities at the nanoscale. Although recent developments in the instrumentation have greatly improved the metrological aspects of SPM, it is still plagued by the drifts and nonlinearities of the piezoelectric actuators underlying the precise nanoscale motion.

In this work, we present a novel computer-vision-based distortion correction algorithm for offline processing of functional SPM images, allowing two images to be directly overlaid with minimal error - correlating the position with time evolution and local functionality.

The algorithm is applied to two very different systems. First, the characteristics of surface folds and wrinkles in CVD graphene deposited on a polyethylene substrate are probed as a function of applied strain. Secondly, we demonstrate the tracking of polarization switching in an epitaxial $Pb(Zr_{0.2}Ti_{0.8})O_3$ thin film during high-speed continuous scanning under applied tip bias. Thanks to the precise time-location-polarization correlation we can extract the regions of domain nucleation and track the motion of domain walls until the merging of the latter in avalanche-like events.

15 min. break

Topical Talk DF 11.9 Wed 12:15 WIL B321

The electro-caloric effect in $BaTiO_3$ from first principles — •Claude Ederer — Materials Theory, ETH Zürich, Switzerland

The electro-caloric effect (ECE), a temperature change observed in certain materials under application or removal of an electric field, provides an attractive perspective for future solid state cooling. Here, we use molecular dynamics simulations for a first-principles-based effective Hamiltonian to study the ECE in the prototypical ferroelectric (FE) material $BaTiO_3$. Our simulations allow to gain a better understanding of the underlying mechanisms and to identify routes for optimizing the electro-caloric response towards future device applications. In particular, we discuss the anisotropy of the ECE for different directions of the applied electric field, and analyze the origin of an inverse effect (i.e. decreasing temperature under application of an electric field) that occurs at FE-FE phase transitions for certain orientations of the applied field. Finally, we explore ways to optimize the caloric response through epitaxial strain in thin films of $BaTiO_3$. We show that strain can be used to shift the largest caloric response to both higher and lower temperatures, depending both on the type of strain (compressive or tensile) and on the orientation of the applied field.

DF 11.10 Wed 12:45 WIL B321

Influence of domain walls on the electrocaloric effect — •Anna Grünebohm[1], Madhura Marathe[2], and Claude Marathe[2] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Materials Theory, ETH Zürich, Switzerland

The electrocaloric effect (ECE) is the adiabatic temperature change of a material in a varying external electrical field which is promising for novel cooling devices [1]. However, a large ECE is restricted to a small temperature range, which is above room temperature for standard ferroelectrics such as $BaTiO_3$. One way to shift the operation temperature is epitaxial strain [2,3]. Most important, tensile strain stabilizes a multi-domain ferroelectric phase which can enhance the caloric response in a broad temperature interval. We discuss the coupling between ferroelectric domains and the external electric field and its impact on the ECE by means of *ab initio* based simulations.

[1] X. Moya, *et al.*, Nature Mater. **13**, 439 (2014).
[2] M. Marathe, *et al.*, Appl.Phys.Lett, **104**, 212902 (2014).
[3] A. Grünebohm *et al.* Euro. Phys. Lett. **115**, 47002 (2016).