# MA 13: Focused Session on Ferroic Domain Walls II (DF with MA)

Part of the 3-days focus on ferroic domain walls:
Tutorial, Symposium (SYDW), three Focused Sessions, and Poster Session.
Organizers: Elisabeth Soergel (Universität Bonn) and Dennis Meier (ETH Zürich)

Time: Tuesday 9:30–13:00 Location: EB 107

**Topical Talk** MA 13.1 Tue 9:30 EB 107
**Polarization charge as a reconfigurable dopant in wide-bandgap ferroelectrics** — •Tomas Sluka — Ceramics Laboratory, EPFL Swiss Federal Institute of Technology, Lausanne, CH-1015 Switzerland — DPMC-MaNEP, University of Geneva, 24 Quai Ernest-Ansermet, 1211 Geneva 4, Switzerland

Tuning the charge carrier density in semiconductors by spatially fixed chemical impurities has been the cornerstone of electronics for over 50 years. As the miniaturization of CMOS technology approaches critical limits, efforts are turned to conceptually new devices based on emerging electronic properties of materials and interfaces. Recently it has been shown that the effect of chemical doping in semiconductors can be also induced by the polarization charge at Charged Domain Walls (CDWs) in wide-bandgap ferroelectrics. The polarization-charge doping, unlike the chemical doping, implies the intriguing possibility to write, displace, erase and re-create channels having a metallic-type conductivity inside an excellent insulator. This suggests the possible use of CDWs as real-time doping switches in hardware reconfigurable electronics. The talk will introduce methods of CDW engineering in ferroelectric crystals and thin films, the intrinsic properties of individual CDWs, their nanoscale manipulation and implementation into submicron device structures. Nanometers thick CDWs ranging from millimeters to tens of nanometers sizes and having metallic-type conductivity which exceeds $10^3$ - $10^9$ times the thermally activated conductivity of the bulk and neutral domain walls will be discussed.

MA 13.2 Tue 10:00 EB 107
**Nonlinear characteristic of ferroelectric domains: From single domain wall to the periodic structure** — •Kai Spychala[1], Moritz Grothe[1], Alex Widhalm[1], Gerhard Berth[1,2], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany

On the way to smaller periods of periodically poled structures in ferroelectrica a comprehensive acknowledgement of the domain wall's nonlinear response is necessary. In this approach the analysis of the ferroelectric domain structures have been realized by means of second harmonic (SH) microscopy. In our study the nonlinear characteristic of an isolated transition between two contrarily poled ferroelectric domains has been determined. Here for the nonlinear sequence in the region of a single domain wall, a symmetric trend transverse to the domain transition was initially detected. A detailed depth-resolved and polarization-dependent study hints at a SH-signature conditioned by the orientation of the crystals. Additionally a functional dependence on depth of such sequences was observed. Here an influence of surface charge and inner electric field distribution can be assumed. Furthermore specific nonlinear signatures which are directly connected to the period of the do-main grating were detected in the system's nonlinear response. Due to the long-range character of the correlation between the domain boundaries, an assumed direct link with the inner electric field distribution is suggested.

MA 13.3 Tue 10:20 EB 107
**Ferroelectric 180° domain wall motion controlled by biaxial strain** — •Robert Roth[1], Er-Jia Guo[1,2], Andreas Herklotz[1,2], Dietrich Hesse[3], and Kathrin Dörr[1,2] — [1]MLU Halle-Wittenberg, Institute for Physics, 06099 Halle, Germany — [2]Institute for Metallic Materials, IFW Dresden, Postfach 270116, 01171 Dresden, Germany — [3]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

Switching polarization in a ferroelectric proceeds by nucleating reversed domains which subsequently expand. Therefore, wall velocity (v) limits the speed of switching. In thin films, measured values of v are many orders below sound velocity [1], whereas bulk crystals showed larger v. Why are domain walls in films so slow? New insights can be derived from local studies of domain wall velocity by piezoresponse force microscopy in in-situ controlled elastic strain states of the sample. In c-oriented epitaxial $PbZr_{0.2}Ti_{0.8}O_3$ films on piezoelectric substrates, the velocity of non-ferroelastic 180° walls has been investigated employing the approach of Tybell et al. [2]. Remanent circular domains showed strong strain dependences of both, domain relaxation / shrinking in zero electric field and field-driven velocity. We discuss results in the light of known physical mechanisms, identify a strain-induced change of the driving field arising from built-in Schottky junctions at electrodes and suggest a new mechanism of strain-induced charging of tilted domain walls (wall sections).

[1] A. Grigoriev et al., Phys. Rev. Lett. 96, 187601 (2006)
[2] T. Tybell et al., Phys. Rev. Lett. 89, 097601 (2002)

**Topical Talk** MA 13.4 Tue 10:40 EB 107
**Influence of defects on domain wall mobility in ferroelectrics** — •Susan Trolier-McKinstry[1], Daniel Marincel[1], Stephen Jesse[2], Sergei Kalinin[2], Huiaruo Zhang[3], and Ian Reaney[3] — [1]Penn State University, University Park, PA, USA — [2]ORNL — [3]University of Sheffield

The dielectric and piezoelectric properties of ferroelectric thin films depend both on the intrinsic response of the material, as well as the motion of domain walls. There are a host of factors that can affect domain wall motion, including grain boundaries, other ferroelectric or ferroelastic domain walls, phase boundaries, dislocations, point defects, some electrode/dielectric interfaces, and core-shell microstructures. One of the challenges that faces the field is the difficulty in isolating the role played by a single type of pinning center or domain wall in controlling the response of an electroded ferroelectric. Instead the amalgamated response of millions of domains and domain walls is probed. This paper will describe the use of scanning probe microscopy and transmission electron microscopy to characterize the motion of domain walls in ferroelectric films, with a concentration on how mechanical stresses at the film * substrate interface and grain boundaries influence the correlated motion of domain walls. Measurements were made on 3 compositions of PZT with a variety of different grain boundary angles. It was found that the domain structure at the grain boundary controlled the width of influence on the domain wall motion. Depending on the angle this width ranged from 0 to hundreds of nm from the boundary.

**10 min break**

**Topical Talk** MA 13.5 Tue 11:20 EB 107
**The electronic structure of longitudinal domain walls: a DFT perspective** — •Gustav Bihlmayer, Kourosh Rahmanizadeh, Daniel Wortmann, and Stefan Blügel — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Whenever ferroelectric domains meet "head-on", a local accumulation of charge and/or defects compensating this charge can arise. As there is no general atomistic picture of these charged domain walls (DWs), ab-initio studies are still rather scarce. Motivated by detailed transmission electron microscopy images of transversal and longitudinal DWs in PZT [1,2], we studied these walls in $PbTiO_3$ using density functional theory (DFT). We explore the possibility of introducing defects acting as electron-acceptors or -donors at the DWs, as well as the localization of electrons due to correlation effects at the Ti site and compare the DW profiles with experimental data. Our calculations allow to investigate the distribution of defects in the DWs as well as the electronic structure of the bands hosting the accumulated charges. We find that states with magnetic- charge- and orbital order allow to realize an insulating (or semiconducting) behavior even in charged DWs [3]. We further discuss spin-polarization effects in the electron gas forming at the DWs due to relativistic phenomena in charged 90° walls.
[1] C. L. Jia et al., Nature Mater. **7**, 57 (2008). [2] Y. L. Tang et al., Sci. Rep. **4**, 4115 (2014). [3] K. Rahmanizadeh et al., Phys. Rev. B **90**, 115104 (2014). *Financial support of the EU grant NMP3-LA-2010-246102 (IFOX) is gratefully acknowledged.*

MA 13.6 Tue 11:50 EB 107

**_Ab initio_ investigation of ferroelectric domain walls in barium fluorides** — •Maribel Núñez Valdez and Nicola Spaldin — Materials Theory, ETH Zürich, Wolfgang-Pauli-Strasse 27, CH-8093 Zürich, Switzerland

We present results of first-principles calculations of the ferroelectric domain walls in the layered perovskite-related barium fluorides, $BaMF_4$ (M = Mg, Zn).

The ferroelectricity in the barium fluorides is driven by the softening of a single polar phonon mode consisting of both rotations of the $MF_6$ octahedra and polar displacements of Ba cations. This so-called "geometric ferroelectricity" is a strikingly different mechanism from that in conventional ferroelectrics [C. Ederer and N.A. Spaldin Phys. Rev. B **74**, 024102,2006].

Using density functional theory (DFT) within the general gradient approximation (GGA) we perform detailed structural relaxations of neutral domain walls (parallel to the polar $c$ axis) and calculate the corresponding energies.

Based on comparisons of the total energies, we determine which domain wall orientations and configurations are most likely to form, and we compare their structural and electronic properties to those of domain walls in conventional ferroelectrics.

Finally we explore the strain dependence of the ferroelectric polarization, again comparing to that of conventional ferroelectrics.

MA 13.7 Tue 12:10 EB 107

**Advanced characterization of functional ferroelectric domain walls by X-ray photoelectron emission microscopy** — •Jakob Schaab[1], Ingo P. Krug[2,3], Zewu Yan[4], Edith Bourret[4], Claus M. Schneider[3], Ramamoorthy Ramesh[4,5], Manfred Fiebig[1], and Dennis Meier[1] — [1]Department of Materials, ETH Zürich — [2]Institut für Optik und Atomare Physik, TU Berlin — [3]Forschungszentrum Jülich, PGI-6 — [4]Materials Science Division, LBNL Berkeley — [5]Department of Materials Science and Engineering, UC Berkeley

The observation of anomalous electronic transport at ferroelectric domain walls and its significance for nano-electronics triggered tremendous scientific interest. To date, the transport behavior and potential barriers at domain walls have been predominantly scrutinized by scanning probes. This, however, convolutes the intrinsic electronic properties with contact resistance and inhomogeneous probe fields, so that the detailed origin of the behavior remains obscured.

Here, we report on the capability of high-resolution X-ray photoemission electron microscopy (X-PEEM) to image and characterize ferroelectric domain walls contact-free and with nanometer resolution. In the ferroelectric semiconductor $ErMnO_3$, we visualize ferroelectric domain walls by exploiting photo-induced charging effects and generate an electronic conduction map by analyzing the kinetic energy of photoelectrons. With this we open a pathway for non-destructive and element-specific studies of electronic and chemical domain-wall structures bypassing previous experimental limitations and significantly expanding the accessible parameter space.

**Topical Talk** MA 13.8 Tue 12:30 EB 107

**Electronic reconstruction and transport at ferroelectric domain walls** — •Dennis Meier — ETH Zürich, Switzerland

Unusual electronic properties arise at ferroelectric domain walls due to the low local symmetry and hypersensitivity of these natural oxide interfaces to electrostatics and strain. Such domain walls can, for instance, be highly conducting even when the host material is rather insulating. A major challenge is to understand the complex domain wall physics at the nanoscale and gain control of their properties with the ultimate goal to exploit them for designing domain-wall-based next-generation devices. In my talk I will discuss the case of domain walls in so-called improper ferroelectrics, i.e., systems in which the ferroelectric domain formation is determined by a primary order parameter other than the polarization. Due to the secondary nature of the polarization unusual domain wall configurations are stabilized, which leads to novel degrees of freedom and functionalities. Here, the multiferroic hexagonal manganites are a striking example. I will show that both positively and negatively charged ferroelectric domain walls naturally form in the as-grown state. Driven by the polarity mismatch at these walls, a variety of exotic interface effects emerge giving rise to, e.g., orientation-dependent conduction properties as well as local variations in the electrochemical interface structure. Results gained by electron microscopy, scanning-probe microscopy, and nonlinear optics will be shown, providing novel insight to the domain-wall physics across all relevant length scales from the nanometer to the millimeter regime.