

DF 15: Ferroics - Domains, Domain Walls and Skyrmions III

Chair: Weida Wu

Time: Wednesday 15:00–17:30

Location: WIL B321

Topical Talk

DF 15.1 Wed 15:00 WIL B321

Domain and fluctuation dynamics in magnetoelectric multiferroics — ●JOACHIM HEMBERGER — Institute of Physics II, University of Cologne, Germany

Multiferroic systems comprise hybrid order parameters which couple e.g. non-collinear spin structures to ferroelectric polarization. This talk raises the question concerning the dynamics of the corresponding fluctuations and discusses results for exemplary magnetoelectric systems on the basis of broadband linear and non-linear dielectric spectroscopy.

E.g. in MnWO_4 one observes a critical slowing down of a magnetoelectric soft-mode above the multiferroic transition [1], while the dielectric response within the ordered phase is dominated by the dynamics of domains [2]. Thus both electric field driven phenomena resemble the behavior of canonical ferroelectrics, but an analysis of the corresponding dynamical exponents reveals differences reflecting the magnetic nature of the underlying order parameter.

Similar findings can be reported for other spin-spiral multiferroics like TbMnO_3 , $\text{Ni}_3\text{V}_2\text{O}_8$, or even the spin chain LiCuVO_4 effected by quantum fluctuations. In addition, the merely magnetic field induced domain and fluctuation dynamics in the non-multiferroic but linear magnetoelectric TbPO_4 shall be discussed.

[1] D. Niermann, C.P. Grams, P. Becker, L. Bohatý, H. Schenck, and J. Hemberger, *Phys. Rev. Lett.* **114**, 037204 (2015)

[2] D. Niermann, C.P. Grams, M. Schalenbach, P. Becker, L. Bohatý, J. Stein, M. Braden, and J.H., *Phys. Rev. B* **89**, 134412 (2014)

DF 15.2 Wed 15:30 WIL B321

Probing polar order in improper ferroelectric thin films using SHG — ●JOHANNA NORDLANDER¹, GABRIELE DE LUCA¹, MARTA D. ROSSELL², MANFRED FIEBIG¹, and MORGAN TRASSIN¹ — ¹Departments of Materials, ETH Zürich, Switzerland — ²Electron Microscopy Center, EMPA, Switzerland

Improper ferroelectrics are materials whose ferroelectricity is driven by a non-polar order parameter. This type of ferroelectricity can lead to exotic properties which do not exist in standard ferroelectrics. For example, improper ferroelectricity in hexagonal YMnO_3 (YMO), which is geometrically driven through a lattice trimerization, leads to a topological domain vortex pattern. There has been a revival in the growth of improper ferroelectric thin films, and these bulk-like ferroelectric domain vortices were also reported in YMO thin epitaxial layers. In order to understand the behavior of ultrathin YMO, and in particular in order to investigate the influence of epitaxial strain on the ferroelectric trimerization, we use optical second harmonic generation (SHG) to non-invasively probe the ferro state of these thin films for different epitaxial growth conditions. Here, we demonstrate the growth of highly oriented, epitaxial hexagonal YMO thin films by pulsed laser deposition on various substrates. We report reversible scanning-probe-tip-induced ferroelectric switching and the subsequent spatially resolved SHG analysis. The temperature-dependent emergence of the coexisting magnetic and electric orders is investigated by SHG. Ultimately, we provide a deeper insight into the mechanism of ferroelectric domain vortex formation and antiferromagnetism in thin film YMO.

DF 15.3 Wed 15:45 WIL B321

Inner structure of topological defects in hexagonal manganites — KOSTANTIN SHAPOVALOV¹, MEGAN HOLTZ², JULIA MUNDY², DAVID MULLER², ZEWU YAN³, EDITH BOURRET-COURCHESNE³, DENNIS MEIER⁴, and ●ANDRÉS CANO¹ — ¹CNRS, Univ. Bordeaux, ICMCB, Bordeaux, France — ²Cornell University, Ithaca, NY, USA — ³Lawrence Berkeley National Laboratory, Berkeley, CA — ⁴Norwegian University of Science and Technology, Trondheim, Norway

Structural domain walls and vortices are two different incarnations of topological defects in the hexagonal manganites RMnO_3 . These entities display intriguing functional features related to their local transport properties and can be regarded as analog systems for the study of the formation of cosmic strings in the early universe. We develop a field-theory description of their inner structure supporting the experimental characterization of these defects by means of HAADF scanning transmission electron microscopy. Our theory reveals novel features

such as the emergence of a continuous $U(1)$ symmetry at the vortex cores and a multipolar charge (re-)distribution that become universal in these regions. These inner features are expected to bring forth an additional degree of functionality to these topological defects.

DF 15.4 Wed 16:00 WIL B321

Modeling domain wall dynamics in multiferroic hexagonal manganites — XIAOYU WU¹, URKO PETRALANDA², LU ZHENG¹, YUAN REN¹, RONGWEI HU³, SANG-WOOK CHEONG³, ●SERGEY ARTYUKHIN², and KEJI LAI¹ — ¹Department of Physics, University of Texas at Austin, Austin, Texas 78712, USA — ²Quantum Materials Theory, Istituto Italiano di Tecnologia, Genova, Italy — ³Rutgers Center for Emergent Materials and Department of physics and Astronomy, Rutgers University, Piscataway, NJ 08854

Multiferroic materials with coexisting magnetic and ferroelectric orders hold promise for the manipulation of magnetism by applied electric fields. These effects were demonstrated [1] to be controlled by the dynamics of strongly interacting domain walls of different types. We report on modeling the electric field - driven dynamics of ferroelectric domain walls in hexagonal manganites, where ferroelectric polarization is produced due to condensation of a trimerization mode [2]. The dynamics is studied using a tight-binding model with parameters derived from first-principles calculations.

[1] Y. Tokunaga et al. *Nature Materials* **8**, 558 (2009) [2] S. Artyukhin, K.T. Delaney, N.A. Spaldin, and M. Mostovoy, *Nature Materials* **13**, 42 (2014) [3] C. J. Fennie and K. M. Rabe, *Phys. Rev. B* **72**, 100103(R) (2005)

15 min. break

DF 15.5 Wed 16:30 WIL B321

A numerical approach to optical second harmonic generation imaging of multiferroic domains — ●THOMAS LOTTERMOSER, CHRISTOPH WETLI, AMADÉ BORTIS, and MANFRED FIEBIG — Department of Materials, ETH Zürich, Zürich, Switzerland

Due to its direct coupling to symmetry optical second harmonic generation (SHG) has been established as a versatile tool for the investigation of magnetoelectric multiferroics. As the only method it allows a non-invasive and simultaneous access to both, the electric and magnetic order of a multiferroic in a single experiment. It not only gives access to the often complex and interlinked interactions of the related order parameters on a macroscopic level, but also spatially resolved on the level of domains. Nevertheless, as any optical imaging method also SHG imaging is limited by the optical resolution of about one micron. Here we present a numerical model based on a statistical analysis of the domain imaging to overcome this limitation and to reveal information of the domain topology and their size distribution even several orders of magnitude below the resolution limit. The model is tested numerically against different domain topologies like the well known antiferromagnetic and ferroelectric domain structures that occur in the multiferroic hexagonal manganites. We can distinguish these different structures by the respective intensity of the SHG response, even if their domains are of equal lateral size.

DF 15.6 Wed 16:45 WIL B321

Local structure and structural coherence across the ferroelectric phase transition of h-YMnO_3 — ●SANDRA HELEN SKJAERVØ¹, QUINTIN MEIER², EMIL BOŽIN³, SIMON BILLINGE^{3,4}, MIKHAIL FEYGENSON⁵, NICOLA SPALDIN², and SVERRE SELBACH¹ — ¹Dept. Mat. Sci. Eng, NTNU, Norway — ²Dept. Mat., ETH Zürich, Switzerland — ³Brookhaven Natl. Lab., Condensed Matter Phys. & Mat. Sci. Dept., Upton, USA — ⁴Columbia Univ, Dept. Appl. Phys. & Appl. Math., New York, USA — ⁵Forschungszentrum Jülich, JCNS

We use pair distribution function (PDF) analysis to investigate the nature of the high-temperature (~ 1270 K) structural phase transition in multiferroic hexagonal YMnO_3 . Upon the phase transition, the unit cell is known to triple as the Mn-O_5 polyhedra tilt in trimers and the Y atoms alternatively displace along the tilt axis, with a ferroelectric polarization arising from a coupling to a secondary Y displacement. Whether the polarization emerges simultaneously with the high-temperature structural distortion or a many hundred degrees

lower remains controversial [1,2]. We have measured high-temperature neutron total scattering data at Oak Ridge Natl. Lab. We analyse the data as PDFs to investigate the short range order and structural coherence. We see that the transition shows both displacive and order-disorder character, and we explain the short range mechanisms behind the ferroelectric transition. [1] Lilienblum, M. et al. "Ferroelectricity in the multiferroic hexagonal manganites". Nature Physics, 11, 2015. [2] Nénert, G. et al., "Experimental evidence for an intermediate phase in the multiferroic YMnO_3 ". J. Phys.: Condensed Matter 19, no. 46, 2007.

DF 15.7 Wed 17:00 WIL B321

Kibble-Zurek mechanism in RMnO_3 — •QUINTIN MEIER¹, ANDRES CANO^{1,2}, MARTIN LILIENBLUM¹, MANFRED FIEBIG¹, and NICOLA A. SPALDIN¹ — ¹ETH Zürich, Department of Materials, Zürich, Switzerland — ²CNRS, Univ. Bordeaux, ICMCB, UPR 9048, F-33600 Pessac, France

We use density functional and Landau-Ginzburg theories to investigate the role of critical fluctuations on the structural phase transition in the ferroelectric hexagonal manganites RMnO_3 ($R = \text{Y}$ or a element of the rare-earth series). These multiferroic materials are of interest because their improper ferroelectricity leads to an unusual domain structure that has been interpreted in terms of the Kibble-Zurek mechanism in the fluctuation dominated Ginzburg regime [1]. We discuss the effect of critical fluctuations and their influence on the Kibble-Zurek mechanism by studying trends in the domain-formation behavior across the series by comparing with new experimental data.

[1]Griffin, S. M., Lilienblum, M., Delaney, K. T., Kumagai, Y.,

Fiebig, M., & Spaldin, N. A. (2012) Physical Review X, 2(4), 041022.

DF 15.8 Wed 17:15 WIL B321

Interstitial oxygen as a source of p-type conductivity in RMnO_3 hexagonal manganites — SANDRA H. SKJAERVØ, ESPEN T. WEFRING, SILJE K. NESDAL, NIKOLAI H. GAUKÅS, GERHARD H. OLSEN, JULIA GLAUM, THOMAS TYBELL, and •SVERRE M. SELBACH — NTNU Norwegian University of Science and Technology, 7491 Trondheim, Norway

We use a combination of experiments and first principles electronic structure calculations to elucidate the effect of interstitial oxygen anions, O_i , on the electrical and structural properties of h-YMnO_3 . Hexagonal manganites, h-RMnO_3 ($R = \text{Sc}, \text{Y}, \text{Ho-Lu}$) have been intensively studied for their multiferroic properties and magnetoelectric coupling, topological defects and electrically conducting domain walls. Although point defects strongly affect the conductivity of transition metal oxides, the defect chemistry of h-RMnO_3 has received little attention. Enthalpy stabilized interstitial oxygen anions are here shown to be the main source of p-type electronic conductivity, without reducing the spontaneous ferroelectric polarization [1]. A low energy barrier interstitialcy mechanism is inferred from Density Functional Theory calculations to be the microscopic migration path of O_i . Since the O_i content governs the concentration of charge carrier holes, controlling the thermal and atmospheric history provides a simple and fully reversible way of tuning the electrical properties of h-RMnO_3 .

[1] S. H. Skjaervø, E. T. Wefring, S. K. Nesdal, N. H. Gaukås, G. H. Olsen, J. Glaum, T. Tybell, S. M. Selbach, Nat. Commun. 7, 13745 (2016).