KFM 9: (Multi)ferroic States: From Fundamentals to Applications (IV)

This focus session explores the intricate properties of (multi)ferroic states, spanning from fundamental understanding to cutting-edge applications. Topics include the design and control of (multi)ferroic states and domain structures at interfaces, domain walls, and in heterostructures. Emphasis will be placed on theoretical models, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices.

Chair: Morgan Trassin (ETH Zurich)

Time: Tuesday 11:45–13:00 Location: H9

KFM 9.1 Tue 11:45 H9

Investigating Self-Heating of Conducting Domain Walls Using Scanning Thermal Microscopy — •Lindsey Lynch, Kristina Holsgrove, Marty Gregg, and Raymond McQuaid — Queen's University Belfast

Domain walls (DWs) in ferroelectrics are an exciting category of reconfigurable functional interface, with properties that can differ from bulk. Lab-level transistor [1] and memristor devices [2] have been demonstrated, where functionality is derived entirely from electrically conducting DWs. Here, the DWs perform the equivalent role of conductive nanofilaments in metal-oxide resistive switching memories. While self-heating and local temperature are important factors in oxygen-vacancy based resistive switching [2,3], much less is known about the intrinsic self-heating of domain walls and its influence on device operation. We have been investigating the electrothermal properties of LiNbO3 domain wall devices using Scanning Thermal Microscopy (SThM). This involves using the scanning probe as a mobile nanoscale temperature sensor to map self-heating in domain wall devices. Temperature hot spots on the order of 10K are detected and PFM corroborates that their origin is due to sub-surface domain wall heating. Since heat spreading occurs within the surrounding ferroelectric film and top electrode, the measured surface temperatures likely represent a lower bound for the intrinsic rise in domain wall temperature.

[1] Nat. Commun. 11, 2811 (2020). [2] Adv. Funct. Mater. 30, 2000109 (2020). [3] Sci. Adv. 8, eabk1514 (2022). [4] ACS Appl. Mater. Interfaces 14, 29025 (2022).

KFM 9.2 Tue 12:00 H9

Thermoelectricity from domain wall formation in a polar metal — •Feifan Wang[1,2], Carl Romao[1], and Manfred Fiebig[1] — [1]Dept. of Materials, ETH Zurich, Switzerland — [2]Institute of Physics, Beijing 100190, China

Simultaneous optimization of the electronic and phononic properties of a thermoelectric material is essential to achieve a high thermoelectric performance. This has been realized in the polar metal compounds by making use of the high configurational entropy, Rashba effect and ferroelectric anharmonicity, tuned at the atomic level. What has been overlooked in this process is the role of macroscopic effect such as the role of domain and domain wall formation in further enhancing the thermoelectric performance. Using GeTe as a prototype, we show that microdomain formation determines the thermal conduction in the polar metal examined by the spatial correlation between the domain structure and the thermal conductivity. In particular, the thermal conductivity decreased by a factor of five following the appearance of the micro-sized antiparallel-aligned domains. Conductive force microscopy shows that the electrical conduction does not change in spite of the presence of domain discontinuities. This is in line with the band gap reduction and the electron–phonon decoupling from density-functional theory calculations. The direct visualization of the association between microdomain formation and thermal/electrical transport suggests the domain and domain wall engineering as a key ingredient in advancing polar-metal-based thermoelectrics.

KFM 9.3 Tue 12:15 H9

Hybrid ferroelectric-antiferroelectric domain walls in noncollinear antipolar oxides — •Ivan N. Ushakov[1], Mats Topstad[1], Muhammad Z. Khalid[1], Niyorjyoti Sharma[2], Christoph Grams[3], Ursula Ludacka[1], Jiali He[1], Kasper A. Hunnestad[1], Mohsen Sadeqi-Moqadam[1], Julia Glaum[1], Sverre M. Selbach[1], Joachim Hemberger[3], Petra Becker[3], Ladislav Bohaty[3], Amit Kumar[2], Antonius T. J. van Helvoort[1], and Dennis Meier[1] — [1]Norwegian University of Science and Technology — [2]Queen's University Belfast — [3]University of Cologne

Antiferroelectrics are emerging as advanced functional materials and are fertile ground for unusual electric effects. For example, they enhance the recoverable energy density in energy storage applications and give rise to large electromechanical responses. In my talk, I will present noncollinearity in dipolar order as an additional degree of freedom, unlocking physical properties that are symmetry-forbidden in classical antiferroelectrics. I will show that noncollinear order of electric dipole moments in $K_3[Nb_3O_6|(BO_3)_2]$ leads to a coexistence of ferroelectric and antiferroelectric behaviors. Besides the double-hysteresis loop observed in antiferroelectrics, a pronounced piezoresponse and electrically switchable domains are observed, separated by atomically sharp and micrometer-long charged domain walls. Similar hybrid ferroelectric-antiferroelectric responses are expected in a wide range of noncollinear systems, giving a new dimension to the research on antiferroelectrics and multifunctional oxides in general.

KFM 9.4 Tue 12:30 H9

Step sintering process on sol-gel synthetized Bi0.5Na0.5TiO3 for enhanced temperature stability of relaxor ferroelectric state and energy storage properties — •Thomas Fourgassie[1], Cécile Autret-Lambert[1,2], and Pierre-Eymeric Janolin[2] — [1]Laboratoire GREMAN, UMR 7347 Université de Tours, CNRS, INSA CVL, Université de Tours UFR Sciences & Techniques, 37200 Tours, France — [2]Laboratoire SPMS, UMR 8580 Université Paris-Saclay, CNRS, CentraleSupélec, 91190 Gif-sur-Yvette, France

With the ever-growing need for energy in our society, researchers are striving to obtain new materials with better energy storage properties capable of replacing current lead-based materials. Among all lead-free materials that have been synthesized, Bi0.5Na0.5TiO3 (BNT) has attracted the attention of many. The main reasons are his high temperature of maximum permittivity called Tm at 320°C, a huge maximum polarization and relaxor ferroelectric properties making his phase transition very diffuse in temperature. However, the good energy storage properties only apply at a temperature higher than the depolarizaition temperature Td (200°C). Usually, to reduce Td, researchers either make solid solutions with other perovskite ceramics or use donor dopants. Here we show the results we obtained while keeping the pristine BNT phase by optimizing the sol-gel synthesis process used. The BNT exhibits sub-micrometric grain size thanks to a multi-step sintering process lowering Td (around 160°C). This BNT has enhanced relaxor ferroelectric at lower temperatures. Results about donor dopants reducing dielectric losses on this BNT will also be shown.

KFM 9.5 Tue 12:45 H9

Composite quadrupole order in ferroic and multiferroic materials — •Matthias Geilhufe — Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden

The formalism of composite and intertwined orders has been remarkably successful in discussing the complex phase diagrams of strongly correlated materials and high-Tc superconductors. Here, we propose that composite orders are also realized in ferroelectric and ferromagnetic materials when lattice anisotropy is taken into account. This composite order emerges above the ferroic phase transition, and its type is determined by the easy axis of magnetization or polarization, respectively. In multiferroic materials, where polarization and magnetization are coupled, composites of both orders are possible. This formalism of composite orders naturally accounts for magnetoelectric monopole, toroidal, and quadrupole orders. More broadly, composite orders may explain precursor phenomena in incipient ferroic materials, arising at temperatures above the ferroic phase transition and potentially contributing to the characterization of currently hidden orders.

[1] R Matthias Geilhufe, J. Phys.: Condens. Matter, 37, 05LT01 (2025)