KFM 28: Focus Session: (Multi-)Ferroic States IV

The focus session is dedicated to (multi)ferroic states at interfaces and in heterostructures. The design of (emergent) properties at interfaces, modelling methods and advanced characterization tools will be of interest. Typical examples may include electrostatic and strain boundary conditions at interfaces, domains and domain walls in (multi)ferroics and applications in nano-electronic device.

Chair: Morgan Trassin (ETH Zürich)

Time: Thursday 15:00–17:45 Location: EMH 225

Invited Talk KFM 28.1 Thu 15:00 EMH 225

Every (ferroelectric) wall is a door - exploring the links between structure, dynamics, and emergent functionalities — •Patrycja Paruch — DQMP, University of Geneva, Switzerland

Ferroelectric materials can host a wide range of unusual structural features, often linked to novel functional properties. One such feature are the domain walls separating regions with different polarisation orientation, providing an intrinsically nanoscale, powerful model system for the rich physics of pinned elastic interfaces. Understanding their structure, geometry, and nonlinear dynamics is key for controlling polarisation switching and domain size, shape, and stability in memory, electro-optic, electro-mechanical and catalytic devices. In addition, at such domain walls the complex interaction between polarisation, electrostatics, and strain can lead to localised chiral polarisation textures, electrical conductivity, local mechanical responses, and charge or chemical segregation, potentially useful for nanoelectronics applications. We use a broad spectrum of primarily scanning probe microscopy techniques, coupled with machine learning analysis to investigate and disentangle the many complex and correlated physical phenomena in these materials. Considering the dual role of defects for both domain wall pinning and local electrical conduction modulation in $Pb(Zr_{0.2}Ti_{0.8})O_3$ and $PbTiO_3$ thin films, with both 180° and 90° domain walls, I will emphasise the interactions between the statistical physics approach and new insights into emergent functional properties at domain walls.

KFM 28.2 Thu 15:30 EMH 225

Nanoscale electrostatic control of polarization in ferroelectric thin films using lattice chemistry — •Ipek Efe[1], Alexander Vogel[2], William S. Huxter[1], Elzbieta Gradauskaite[1], Christian L. Degen[1], Marta D. Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]ETH Zurich — [2]Empa, Switzerland

Nanoscale electrostatic control of oxide interfaces enables functionalities beyond the realm of the bulk material, including superconductivity, multiferroicity, and topological properties. Here, by exploiting spontaneously forming charged interfaces in layered materials, we control the electrostatic boundary conditions in ferroelectric oxide heterostructures. Using in-situ optical second harmonic generation during the growth of layered Aurivillius $Bi_5FeTi_3O_{15}$ films, we correlate, in real-time, the stacking of highly charged fluorite-like $(Bi_2O_2)^{2+}$ layers with the formation of the out-of-plane antipolar ordering of electric dipoles in the unit-cell. Next, we insert multiferroic $BiFeO_3$ into the Aurivillius scaffold and show that the resulting charged layering stabilizes the ferrielectric-like ordering of the electric dipoles. Our work brings the use of polarizing charged layers of layered oxides as an additional degree of freedom towards the design of technologically relevant electric dipole orderings in epitaxial thin films.

KFM 28.3 Thu 15:50 EMH 225

First-principles predictions of HfO2-based ferroelectric superlattices — •Binayak Mukherjee[1], Natalya S. Fedorova[1], and Jorge Íñiguez-González[1,2] — [1]Department of Materials Research and Technology, Luxembourg Institute of Science and Technology, L-4362, Esch-sur-Alzette, Luxembourg — [2]Department of Physics and Materials Science, University of Luxembourg, L-4422, Belvaux, Luxembourg

The metastable nature of the polar phase of HfO2 is a significant impediment to its industrial application as a functional ferroelectric material. In fact, no polar phases exist in the bulk phase diagram of HfO2, which shows a non-polar monoclinic ground state, and this requires polar orthorhombic HfO2 to be kinetically stabilized. Here, we propose an alternative approach, demonstrating the feasibility of thermodynamically stabilizing polar HfO2 through superlattices with other simple oxides. Using the composition and stacking direction of the superlattice as design parameters, we obtain heterostructures that can be fully polar, fully antipolar or mixed, with improved energetics compared to the orthorhombic polar HfO2 in bulk form. Our results suggest that combining HfO2 with an oxide that does not have a monoclinic ground state generally drives the superlattice away from this non-polar phase, favoring the stability of the ferroelectric structures that minimize the elastic and electrostatic penalties. As such, these diverse and tunable superlattices hold promise for various applications in thin-film ferroelectric devices.

KFM 28.4 Thu 16:10 EMH 225

Localized oxygen reorganization under sub-millisecond switching in ferroelectric epitaxial hafnia-based films — •Nives Strkalj[1,2], Megan O. Hill[2], Ji Soo Kim[2], Moritz L. Müller[2], Maximilian T. Becker[2], Dibya Phuyal[2,3], Sunil Taper[2], Manisha Bansal[4], Babak Bakhit[3], Tuhin Maity[4], Giuliana Di Martino[3], and Judith L. MacManus-Driscoll[3] — [1]IoP, Zagreb, Croatia — [2]UCAM, UK — [3]KTH, Sweden — [4]IISER TVM, India

The discovery of ferroelectricity in nanoscale films of binary oxides based on hafnia spurred renewed interest in the emergence of ferroelectric properties on the nanoscale. The unusual size dependence of polarization in hafnia is a topic of intense research with explanations including flat phonon bands, and coupling to an antipolar phase or an electrochemical state. Though polarization switching and electrochemical reactions have been shown to co-occur in hafnia-based films, their relationship remains unclear.

To elucidate the relationship between the polarization state and the electrochemical state, we perform direct observations of the electrochemical state in areas with preset polarization directions for hafnia-based films using hard x-ray photoelectron spectroscopy (HAXPES). Because we observe more pronounced electrochemical changes in films with lower polarization, we propose that the polarization and the electrochemical change are not directly linked. Our results present a step forward in disentangling the origin of the ferroelectric response in hafnia-based films.

15 min. break

KFM 28.5 Thu 16:45 EMH 225

Conduction mechanisms in $Al_{1-x}Sc_xN$-based thin-film ferroelectric capacitors — •Vinay Lulla[1], Georg Schönweger[2,3], Simon Fichtner[2,3], Hermann Kohlstedt[1,4], and Adrian Petraru[1] — [1]Chair of Nanoelectronics, Institute of Electrical and Information Engineering, Faculty of Engineering, Kiel University, Kaiserstraße 2, D-24143 Kiel, Germany — [2]Chair of Microsystems and Technology Transfer, Institute of Material Science, Faculty of Engineering, Kiel University, Kaiserstraße 2, D-24143 Kiel, Germany — [3]Fraunhofer Institute of Silicon Technology, Fraunhoferstraße 1, 25524 Itzehoe, Germany — [4]Kiel NanoSurface and Interface Science KiNSIS, Kiel University, Christian-Albrechts-Platz 4, D-24118 Kiel, Germany

Current $Al_{1-x}Sc_xN$ based devices are limited by the high electric switching fields that require to operate the capacitors in a regime where the breakdown is highly likely, i.e., close to 4 MV/cm. In this work, ferroelectric capacitors with the layer sequence $Pt/Al_{1-x}Sc_xN/Pt$ have been investigated. The electrodes and the $Al_{1-x}Sc_xN$ were deposited by DC sputtering and pulsed DC sputtering, respectively. These devices exhibit high leakage currents, especially for films thinner than 100 nm. In order to understand the transport mechanisms, the electric field dependence and temperature dependence (300 K - 77 K) of the leakage currents were investigated. The experiments showed that Richardson-Schottky conduction is likely to dominate the transport in high electric field regime (4 MV/cm), while domain wall conduction and Poole-Frenkel were valid mechanisms in the low-field regime (2 MV/cm).

KFM 28.6 Thu 17:05 EMH 225

Point Defects and Domain Walls in Soft Ferroelectric CsGeX3 (X = Cl, Br, I) — •Kristoffer Eggestad, Benjamin Albert Dobson Williamson, Dennis Gerhard Meier, and Sverre Magnus Selbach — Department for Materials Science and Engineering - NTNU

Conductive domain walls (DWs) hold promise for nanoscale, energy-efficient multi-level diodes and neuromorphic circuitry. In CsGeX3, caesium and halogen vacancies are intrinsic point defects that can induce electrons and holes, respectively. Controlling the formation and position of vacancies can in principle give switchable local n-type or p-type conductivity at DWs and enable new concepts for DW-based circuitry. This requires a material where mobile point defects of both positive and negative charge can accumulate at DWs. CsGeX3 is here chosen as our model system due to the possibility of having mobile caesium and halogen vacancies.

Using hybrid density functional theory (DFT) we investigate electronic structure and defect formation energies in bulk, showing highly mobile holes and free electrons, as well as relatively shallow defect levels. Moreover, a study on point defect mobility in bulk, reveals exceptionally mobile anion vacancies with migration barriers comparable to Li vacancies in the best solid-state electrolytes. Furthermore, we show that Y-type 71-degree DWs are the most stable and that they are extremely mobile, implying that polarisation can easily be switched. Finally, the possibility of reversible p- and n-type conductivity in DWs in CsGeX3 and other similar materials is discussed.

KFM 28.7 Thu 17:25 EMH 225

Ferroelectricity in epitaxially strained thin films of a binary oxide — •Zhuotong Sun, Nives Strkalj, Sunil Taper, Atif Jan, Chuck Witt, Bartomeu Monserrat, Giuliana Di Martino, and Judith Driscoll — University of Cambridge, Cambridge, UK

Interest in ferroelectric materials for processing, memory and sensing devices has been spurred by the discovery of nanoscale ferroelectricity in insulating binary oxides based on HfO2 and ZrO2. However, stabilizing the ferroelectric phase and achieving good ferroelectric performance in these materials is challenging because several non-ferroelectric phases have similar formation energy to the ferroelectric phase. The search for other binary oxide ferroelectrics which can be achieved by industry-friendly processes is therefore still ongoing. Here, we report the stabilization of epitaxial films of a binary oxide at temperatures below 400°C using atmospheric pressure chemical vapor deposition. In these films, strain imposed by the substrate gives rise to the spontaneous polarization evidenced by piezo-response force microscopy. Exploring ferroelectricity in binary oxide films could provide a new platform for polarization-controlled memory applications and allow combining ferroelectric and photosensitive properties for photoferroelectrics applications.