KFM 10: Focus session: Polar Materials Meet Energy demands

Polar materials, in particular in (anti-) ferroelectrics, play an important role in future energy storage and energy harvesting devices and have a high potential for ultra-low power memory and logic devices as well as energy efficient cooling technologies. The aim of this focus-session is to bring together scientists from theory and experiment to improve the fundamental understanding and optimization of the underlying material properties and microstructures in a multiphysics and multidisciplinary scenario.

Organizers: Prof. Dr. Anna Grünebohm (Bochum) and Prof. Dr. Bai-Xiang Xu (TU Darmstadt)

Chair: Prof. Dr. Anna Grünebohm (Bochum University)

Time: Tuesday 9:30–12:25 Location: H5

Prize Talk KFM 10.1 Tue 9:30 H5

Einfluss des Sauerstoffgehalts auf das Koerzitivfeld für die Polarisationsumschaltung in HfO_2 aus der Dichtefunktionaltheorie — •Luis Azevedo Antunes — Hochschule für angewandte Wissenschaften München — Laureate of the Georg-Simon-Ohm-Prize 2022

Die fortschreitende Miniaturisierung in der Mikroelektronik stößt beim Thema Energieeffizienz zunehmend an ihre Grenzen. Der Grund sind die Speicher- und Schaltkonzepte, welche auf dem Schalten von elektrischen Strömen basieren. Einen Ausweg könnte hier der ferroelektrische Feldeffekt-Transistor (FeFET) bieten, welcher stromsparend und ohne Kondensator viel besser skalierbar ist. Mit dem vor 15 Jahren in einem Industrielabor in Dresden gefundenen ferroelektrischen HfO_2 und ZrO_2 gibt es ein Material, welches die Anforderungen bei sehr kleinen Bauelementen zu erfüllen scheint. Die Fluorit-struktur basierte ferroelektrische Phase des HfO_2 weist im Vergleich zu den Perowskit basierten Ferroelektrika jedoch ein höheres Koerzitivfeld auf, welches die Zuverlässigkeit einschränkt. Derzeit wird der Einfluss von Dotierstoffen sowie von Sauerstoff auf die Eigenschaften des Koerzitivfeldes und weiterer Eigenschaften untersucht. In dem Vortrag wird über First-Principle-Berechnungen dieser Eigenschaften berichtet, welches Übergangszustände in den kristallinen Materialien betrachtet. Die Ergebnisse führen zu einem grundlegenden Verständnis von Sauerstoffdefekten auf die Bindungsstruktur und weiterführend auf das Koerzitivfeld. Die Ergebnisse werden mit experimentell gemessenen Koerzitivfeldern verglichen.

Invited Talk KFM 10.2 Tue 10:00 H5

Negative capacitance and voltage amplification in ferroelectric heterostructures — •Jorge Iniguez — Luxembourg Institute of Science and technology — University of Luxembourg

My group is interested in the behavior of ferroelectric materials that present non-trivial polar orders (vortexes, skyrmions) and properties (chirality, negative capacitance) in situations of reduced dimensionality (ultra-thin layers or films) and/or subject to suitable electrostatic boundary conditions. In this talk I will review our most recent theoretical results for one of the model systems in the field, the $PbTiO_3$/$SrTiO_3$ ferroelectric/dielectric superlattices where many of the above effects were first demonstrated. In particular, I will discuss the negative-capacitance response of such materials, with an emphasis on the attendant voltage amplification. I will show that this anomalous behavior is actually quite frequent, occurring in regular multi-domain structures as well as in novel topological states. Further, I will explain its atomistic underpinnings and show how it can be optimized (to obtain voltage amplifications beyond x10) if the polar layers are tuned to display an incipient ferroelectric state.

Most of the work done in collaboration with M. Graf and H. Aramberri (postdocs at the Luxembourg Institute of Science and Technolgoy) and funded by the Luxembourg National Research Fund through Grants INTER/RCUK/18/12601980 and C18/MS/12705883/REFOX. Other key contributors include P. Zubko (UC London), J. Junquera (U. Cantabria), R. Ramesh (UC Berkeley), etc.

Topical Talk KFM 10.3 Tue 10:30 H5

Advanced Phase-field Simulation of Ferroelectrics and Antiferroelectrics — •Bai-Xiang Xu — Division Mechanics of Functional Materials, Institute of Materials Science, TU Darmstadt

Featured by high power density and high cyclic stability, ferroelectric (FE) and antiferroelectric (AFE) perovskites are distinct type of materials for energy storage and conversion particularly in pulse power equipment, miniaturized electronic devices and electronic control system in electric vehicles. The key issue is to increase the energy storage density, which is strongly related to ferroelectric domain structure in the materials and its interaction with defects.

In this talk I will present advanced phase-field simulations on the domain scale of such energy materials. In the first part, by combining phase-field simulations with dislocation mechanics and driving force theory (Zhou et al. IJSS 2021; Höfling et al. Science, 2021), I will show simulation results and mechanistic understanding on domain wall-dislocation interaction in mechanically hardened ferroelectrics and its impact on properties. In the second part, a high order gradient phase-field model for antiferroelectrics will be presented (Liu and Xu, Script Mat. 2020). It enables simulations of the newly observed incommensurate modulations of (anti-)ferroelectric polarization configuration, which goes beyond the capability of the established models like the Kittel sublattice model. Simulations on the domain structure, hysteresis, and temperature induced FE-AFE phase transition will be shown, along with the comparison to experimental results.

15 min. break

Invited Talk KFM 10.4 Tue 11:15 H5

Magnetization processes in $SmFeO_3$ — •Thomas Schrefl[1], Alexander Kovacs[1], Roman Beigelbeck[1], Hubert Brückl[1], Shixun Cao[2], and Wei Ren[2] — [1]Department for Integrated Sensor Systems, Danube University Krems, Viktor Kaplan Straße 2E, 2700 Wiener Neustadt, Austria — [2]Department of Physics, Shanghai University, China

$SmFeO_3$ is an antiferromagnet with a canted spin structure. We analyzed the basic magnetic properties of monocrystalline $SmFeO_3$ samples through magnetic measurements and micromagnetic simulations. The measurements of the temperature dependent magnetization confirm a spin reorientation at 181°C. Hysteresis properties were found to depend on the magnetic history. We observed exchange bias at room temperature whereby the bias field is sensitive on and increases with the field which is applied after field cooling. Using the double sublattice weak ferromagnetic model we derived effective intrinsic material properties for micromagnetic simulations. The simulations show the existence of metastable multidomain states. In $SmFeO_3$ ferroelectricity is believed to arise from antiferromagnetic domain walls. In a phenomenological model, in which the electric polarization arises from the noncollinear magnetization distribution in the domain walls, the average electric polarization is directly proportional to the total number of domain walls. We show how the number of antiferromagnetic domain walls and the electric polarization changes with the applied magnetic field.

Work supported by The Austrian Research Promotion Agency (FFG) project 20087207, MagnifiSense.

KFM 10.5 Tue 11:45 H5

A first-principles study of electronic properties of lead iron niobate — •Madhura Marathe[1], Anna Grunebohm[2], Doru Lupascu[3], and Vladimir Shvartsman[3] — [1]Department of Physics and Astronomy, Uppsala University, 75120 Uppsala, Sweden. — [2]Interdisciplinary Center for Advanced Materials Simulations (ICAMS), Ruhr-University Bochum, 44801 Bochum, Germany — [3]Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 45141 Essen, Germany

Efficient and cost-effective photovoltaic devices require materials which have optimal band gaps for absorption in the visible spectrum. Several ferroelectric perovskite materials have been investigated for their photovoltaic performance, but have too large band gaps. One promising

candidate is multiferroic lead iron niobate $Pb(Fe,Nb)O_3$ (PFN) which has a narrower band gap [1].

We study the electronic and magnetic properties of PFN using density functional theory calculations. We explore how magnetic ordering and structure (ground-state rhombohedral versus high temperature cubic phases) influence the electronic structure and can thus be used to improve material performance.

References 1. N. Bartek, *et al.*, Materials, **14**, 6841 (2021).

KFM 10.6 Tue 12:05 H5

Lead-free Barium Zirconium Titanate-Based Ceramics for Energy Storage — •Eva Kröll, Vladimir Shvartsman, and Doru Lupascu — Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitätsstr. 15, 45141 Essen, Germany

The growing world population and new technical developments request advanced energy storage systems which offer long life time, high power and energy densities. Relaxor ferroelectrics promise to provide these requirements for new energy storage systems due to their high dielectric permittivity and low hysteresis losses. In this work we added bismuth compounds, $Bi(Zn_{2/3}Nb_{1/3})O_3$ and $Bi(Zn_{2/3}Ta_{1/3})O_3$, to the ferroelectric barium zirconium titanate to induce a relaxor state. The heterovalent substitution at the A- and B-sites interrupts the long-range ferroelectric order. Concurrently, Bi^{3+} and Nb^{5+} as ferro active ions improve the polarizability of the materials. The addition of Ta^{5+} should increase the breakdown strength of the ceramic which is crucial to withstand high electric fields and to increase the stored energy density. We used X-ray diffraction for the phase characterization and scanning electron microscopy for the microstructure analysis. The dielectric spectroscopy and polarization measurement show that small amounts of 1.5 mol% BZNb and BZTa induce relaxor behavior in $Ba(Ti_{0.85}Zr_{0.15})O_3$. With increasing content of dopants, the polarization loops become linear. The samples with 2 mol% BZNb and BZTa show the highest energy storage performance with 0.417 J/cm^3 and 0.423 J/cm^3 at 100 kV/cm, respectively.