MM 29: Topical session: Caloric effects in ferroic materials III - Electrocalorics

Time: Wednesday 10:15–11:45 Location: H39

MM 29.1 Wed 10:15 H39

Abnormal electrocaloric effect studied by lattice based Monte-Carlo simulations — •Kai-Christian Meyer, Constanze Kalcher, Alexander Stukowski, and Karsten Albe — TU Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt

The abnormal electrocaloric effect (ECE) was first found by Peräntie *et al.* in 2010 in PMN-PT single crystals. [1] Contrary to the normal ECE, an increase of the electric field leads in these materials to a decrease of the temperature. In this work we show that the abnormal ECE can be described within a lattice based random bond model that only includes next neighbor interactions and an external electric field. The negative temperature change can be observed when the electric field lowers the order (configurational entropy) of the polarization vectors. This is the case when the system is in a antiferroelectric state or polar defects with polarization antiparallel to the external field are present. These findings are in agreement with a more elaborate model which includes long-range dipole-dipole interaction and gradient terms. [2]

[1] J. Peräntie, *et al.*, Phys. Rev. B 82, 134119 (2010)
[2] Y. Ma, *et al.*, arXiv:1507.05004

MM 29.2 Wed 10:30 H39

Role of polarization anisotropy in epitaxial PMN-PT thin films for electrocaloric studies — •Michael Mietschke[1,2], O. Mey[1,2], C. Molin[3], S. Gebhardt[3], P. Chekonin[1], S. Fähler[1], K. Nielsch[1], L. Schultz[1], and R. Hühne[1] — [1]IFW Dresden — [2]TU Dresden — [3]Fraunhofer IKTS Dresden

A prominent example for electrocaloric (EC) materials are $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT) compounds, which are typically used for high performance actuator applications due to its outstanding piezoelectric properties. As the structural and functional properties of these materials are well-known they might serve as a suitable model system to study the interplay between microstructure and EC properties. Since ferroic materials exhibit a strong anisotropy, we will probe the role of polarization anisotropy on the ECE by variation of the film orientation. Epitaxial films are a useful tool to analyze this correlation in order to optimize the performance of these materials.

Therefore, epitaxial 0.9PMN-0.1PT films were grown by pulsed laser deposition on (001)-oriented and (111)-oriented $SrTiO_3$ single crystalline substrates using an epitaxial $La_{0.7}Sr_{0.3}CoO_3$ buffer as bottom electrode and additional Au top electrodes. The structural properties were studied by high resolution XRD, AFM and TEM. The anisotropy of the ferroelectric domain structure was investigated by vertical and lateral piezoresponse force microscopy. The indirect determination of the EC properties was performed by temperature dependent polarization measurements at different electric fields. Funded by SPP 1599.

MM 29.3 Wed 10:45 H39

Electric field direction dependence of the electrocaloric effect in $BaTiO_3$: a first principles effective Hamiltonian approach — •Madhura Marathe[1], Damian Renggli[1], Anna Grünebohm[2], and Claude Ederer[1] — [1]Materials Theory, ETH Zürich, Switzerland — [2]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany

The electrocaloric (EC) effect describes heating/cooling of a material on adiabatically applying/removing an external electric field. Currently, extensive work in this area is motivated by its huge potential for solid-state cooling devices.

We have performed molecular dynamics simulations for a first principles-based effective Hamiltonian to study the EC effect. In bulk $BaTiO_3$, there are three phase transitions – one paraelectric (PE) to ferroelectric (FE) and two FE to FE – with different polarization direction in each FE phase. The EC effect has been mainly studied at the PE to FE phase transition. We calculate the EC temperature change ΔT also at the two FE-FE transitions observed in the bulk. In particular, we consider the effect of the direction of the applied field on ΔT at each transition. The largest ΔT is observed at the PE-FE transition, however a smaller, but finite effect is also observed at the other two transitions. This is very interesting for applications because one of the FE-FE transitions occurs near room temperature. Further, we observe an "inverse" EC effect, that is, heating on field removal, when the applied field is not along the polarization direction of the ferroelectric phase of the system.

MM 29.4 Wed 11:00 H39

Direct Electrocaloric Effect Measurements in $BaTiO_3$-based Ferroelectric Ceramics — •Mehmet Sanlialp, Vladimir V. Shvartsman, and Doru C. Lupascu — Universität Duisburg-Essen, Institut für Materialwissenschaft

Nowadays small size and high performance of electronic components are highly demanded. However, use of miniaturized high power electronic devices often faces large heat dissipation, which reduces the performance of these devices. Recently, solid-state refrigeration based on the electrocaloric effect (ECE) has been proposed as a promising solution of this problem. ECE is a change of temperature or entropy of a dielectric material under an applied electric field at adiabatic or isothermal conditions, respectively. ECE based refrigerators should combine high efficiency, low cost, be environmental friendly and easy scalable. Therefore, search for materials with large ECE is important. We report on development of two experimental setups to measure the ECE directly: a modified differential scanning calorimeter and a self-made quasi-adiabatic calorimeter. We performed the ECE measurements in several lead-free ferroelectric ceramics: (1-x)$Ba(Zr_{0.2}Ti_{0.8})O_3$-x$(Ba_{0.7}Ca_{0.3})TiO_3$, 0.55$Ba(Zr_{0.2}Ti_{0.8})O_3$-0.45$(Ba_{0.7}Ca_{0.3})TiO_3$ with Fe and Nb doping, (1-x)$Ba(Sn_{0.15}Ti_{0.85})O_3$-x$(Ba_{0.7}Ca_{0.3})TiO_3$. Temperature, electric field, and composition dependences of the electrocaloric effect have been studied. Furthermore, we compare results of the direct measurements with frequently used indirect estimations based on Maxwell relations to judge the compatibility of these measurement methods.

MM 29.5 Wed 11:15 H39

Electrocaloric Effect in $BaZr_xTi_{1-x}O_3$: Simulation vs Experiment — •Yang-Bin Ma[1], Christian Molin[2], Vladimir Shvartsman[3], Doru Constantin Lupascu[3], Sylvia Gebhardt[2], Bai-Xiang Xu[1], and Karsten Albe[1] — [1]Technischen Universität Darmstadt — [2]Fraunhofer-Institut für Keramische Technologien und Systeme IKTS — [3]Universität Duisburg-Essen

The electrocaloric effect (ECE) and the relaxor behavior of $BaZr_xTi_{1-x}O_3$ (BZT) are investigated as function of Zr content, computationally and experimentally. A lattice-based Ginzburg-Landau-type Hamiltonian is used. A multi-well Landau-type term is applied for unit cells containing Ti, and a single well for Zr. The high-frequency permittivity entering the dipole-dipole interaction is assumed composition-dependent. In experiment, the ECE in $BaTiO_3$ and BZT ($x = 0.12$ and 0.2) ceramics is studied. The domain patterns are revealed by Piezoresponse Force Microscopy, together with the hysteresis and the ECE at various temperatures. The relaxor behavior is related to the relative standard deviation of the internal field distribution. With increasing Zr content, the domain size becomes smaller, and the hysteresis becomes slimmer. For Zr contents ranging from 0 to 0.3 there is a sharp drop of the ECE peak value, while the drop becomes moderate when Zr contents are larger. Meanwhile, the ECE peak shifts to lower temperature with increasing Zr content, and the temperature change decreases. The phenomena are interpreted explicitly by the domain patterns. It presents a good qualitative consistence between the phenomena observed in simulation and experiment.

15 min. coffee break