Crystallography Division
Fachgruppe Kristallographie (KR)

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Overview of the Sessions

(Lecture Room H9; Poster B2)

Sessions

KR 1.1–1.10	Mon	9:30–12:00	H3	**Multiferroics 1 (MA jointly with DF, DS, KR, TT)**
KR 2.1–2.13	Mon	15:00–18:30	H3	**Multiferroics 2 (MA jointly with DF, DS, KR, TT)**
KR 3.1–3.3	Mon	15:00–16:00	H11	**Electrical and mechanical properties (DF jointly with KR)**
KR 4.1–4.8	Tue	9:30–12:15	H5	**Quantitative Materialanalyse (MI jointly with KR)**
KR 5.1–5.6	Wed	15:00–17:30	Poster B2	**Poster - Crystallography**
KR 6	Thu	17:45–18:30	H9	**Mitgliederversammlung FG KR**
KR 7.1–7.12	Fri	9:30–12:45	H32	**Resistive Switching (DS jointly with DF, KR, HL)**

Annual General Meeting of the Crystallography Division

Donnerstag 17:45–18:30 H9

- Bericht der Fachgruppenleiterin
- Aktivitäten auf der DPG-Tagung 2014
- Weiterentwicklung der Fachgruppe Kristallographie
- Verschiedenes

KR 1: Multiferroics 1 (MA jointly with DF, DS, KR, TT)

Time: Monday 9:30–12:00 Location: H3

KR 1.1 Mon 9:30 H3

Magnetoelectric coupling at the n-doped interface $BaTiO_3/SrTcO_3$ studied from first principles — •Vladislav Borisov[1], Sergey Ostanin[1], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Antiferromagnetically induced magnetoelectric coupling at the interface $BaTiO_3/SrTcO_3$, which combines a robust ferroelectric and a stable antiferromagnetic perovskite, is studied from first principles. For the BaO/TcO_2-terminated interface, the magnetic order may change from G- to C-type antiferromagnetism upon the electric polarization reversal in the ferroelectric side. By inspecting the two-dimensional band structure and orbital occupation of the Tc 4*d*-states we conclude that the polarization-dependent charge transfer is responsible for a two-dimensional electron gas at the interface between two insulating perovskites. The case of paraelectric $BaTiO_3$ is also discussed in the context of the effect.

KR 1.2 Mon 9:45 H3

Observation of novel multiferroic-like effect in C60-Co nanocomposites — •Masashi Shiraishi[1], Eiiti Tamura[1], Yutaka Sakai[1], Toyokawa Shuhei[1], Eiji Shikoh[1], Vlado Lazarov[2], Atsufumi Hirohata[3], Teruya Shinjo[1], and Yoshishige Suzuki[1] — [1]Graduate School of Engineering Science, Osaka Univ., Japan — [2]Department of Physics, Univ. York, UK — [3]Department of Electronics, Univ. York, UK

A novel magnetoelectric effect is found to appear in a C60-Co nanocomposite. Although Co is well-known as a ferromagnet, its nanoparticles embedded in a C60 matrix can exhibit enhancement of magnetoresistance ratio due to a combination of Coulomb-blockade and higher order co-tunneling [1], and also multiferroic-like behavior [2], i.e., an electric field controls magnetic alignment of the nanoparticles and a magnetic field controls their charged states. This novel effect enables a strong magnetic switching effect for which the on/off ratio is ca. 1e4. Such an effect has been expected to exist and these findings show this magnetoelectric coupling for the first time.

[1] D. Hanataka, M. Shiraishi et al., Phys. Rev. B79, 235402 (2009).
[2] Y. Sakai, E. Tamura, M. Shiraishi et al., Adv. Func. Mat. 22, 3845 (2012).

KR 1.3 Mon 10:00 H3

Investigation of magnetic ordering in $Eu_{1-x}Y_xMnO_3$ using full polarization analysis at P09 beamline — •Arvid Skaugen, Dinesh K. Shukla, Helen Walker, Sonia Francoual, and Jörg Strempfer — Deutsches Elektronen-Synchrotron, Harmburg, Germany

Varying multiferroic properties with strong ME coupling have been reported for $Eu_{1-x}Y_xMnO_3$ [1]. The crystal structure of $Eu_{1-x}Y_xMnO_3$ is similar to the one of $TbMnO_3$ with comparable lattice distortions. However, the effect of rare earth magnetism is eliminated since Eu^{3+} ($4f^6$) and Y^{3+} ($4f^0$) ions both are non-magnetic. The compound $Eu_{0.8}Y_{0.2}MnO_3$ first shows a phase transition at T_N = 45K from a paramagnetic to an antiferromagnetic and paraelectric state with a presumably sinusoidal collinear AFM structure, in analogy to $TbMnO_3$. At T_C = 30K the magnetic structure changes to weak ferromagnetism, attributed to a cone-like structure that breaks inversion symmetry and gives rise to ferroelectricity with the polarization along the a-axis.

We have investigated $Eu_{0.8}Y_{0.2}MnO_3$ using resonant x-ray diffraction as function of temperature, magnetic field and incident polarization at beamline P09 at PETRA III. The method of full polarization analysis has been used to investigate the different resonances showing up at the Mn K-edge. From the polarization scans, it is possible to draw conclusions on the complex magnetic order. Preliminary results suggest a helicoidal SDW structure of the Mn moments rather than a cone-like structure.

[1] J. Hemberger et al., Phys. Rev. B 75, 035118 (2007)

KR 1.4 Mon 10:15 H3

Electrostatic tuning of large-distance sputtered LSMO/PZT heterostructures — •Philipp Moritz Leufke, Ajay Kumar Mishra, Wang Di, Robert Kruk, and Horst Hahn — Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

In order to obtain a physical picture and quantitative characteristics of a magnetoelectric coupling at ferromagnetic/ferroelectric interfaces, epitaxial $La_{0.87}Sr_{0.13}MnO_3$/Pb(Zr,Ti)O_3 (LSMO/PZT) heterostructures were deposited by large-distance magnetron sputtering[1,2]. The remarkably high lateral uniformity achieved in such films allowed for a ferroelectric device area of more than 6 mm^2.

This has enabled for the first time *in-situ* SQUID measurements of the magnetic response to the systematically varied remanent ferroelectric polarization. Temperature dependence of the magnetic modulation upon charging and the magnetic response to the ferroelectric stimulation indicates a field-effect dominated coupling mechanism and generally confirms the concept of electrostatic hole (h^+) doping of LSMO.

For small charge modulations at low temperature, a linear tuning coefficient of $\approx 3.6\,\mu_B/h^+$ has been determined. This suggests the activation of an antiferromagnetic coupling, even for very small surface charge densities. Simultaneously a shift in the magnetic transition temperature at higher surface charge concentration indicates the presence of a ferromagnetic phase at the LSMO/PZT interface.

[1] P. M. Leufke *et al.*, *Thin Solid Films* **520**, 5521 (2012).
[2] P. M. Leufke *et al.*, *AIP Advances* **2**, 032184 (2012).

KR 1.5 Mon 10:30 H3

Optimized magnetoelectric interface coupling — •Igor Maznichenko[1], Arthur Ernst[2], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany

It was shown that magnetoelectric coupling occurs at interfaces between a magnetic and a ferroelectric material. Our idea is to construct heterostructures with a particularly strong magnetoelectric coupling. We concentrate on the optimization of the magnetic layer. We demonstrate that a small magnetic moment at the interface can still transfer the magnetoelectric coupling to a strong ferromagnet and could cause significant response. The idea is supported by numerical simulations within density functional theory using the self-consistent KKR Green function method.

KR 1.6 Mon 10:45 H3

Role of electron correlation of FeO at Fe/ferroelectric oxide/Fe interface for magnetic transport properties — •Andrea Neroni, Daniel Wortmann, Ersoy Sasioglu, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Fe/ferroelectric oxide/Fe is a nanoferronic tunnel junction with exciting electronic magneto-conductive transport properties. FeO layers at the interface of Fe/oxide/Fe barriers seems to significantly alter these properties as indicated by several experiments. In order to understand the role of electron correlations in FeO at the interface on the tunneling properties of a Fe/$BaTiO_3$/Fe barrier we use an embedded Green-function approach [1] implemented within the framework of the full-potential linearized augmented plane-wave (FLAPW) method `FLEUR` [2]. Conductances are obtained for different oxidation conditions and for different magnetic configurations of the contacts. Strong correlations are taken into account employing the LDA+U approach within the framework of the density functional theory (DFT) with a Hubbard U parameter determined by constrained random phase approximation (cRPA) [3]. Work is supported by Helmholtz Young Investigators Group Program VH-NG-409.

[1] www.flapw.de
[2] D. Wortmann, H. Ishida, and S. Blügel, PRB **65**, 165103 (2002)
[3] E. Şaşıoğlu, C. Friedrich, and S. Blügel, PRB **83**, 121101(R) (2011)

KR 1.7 Mon 11:00 H3

Multiferroic Aurivillius Phases: the Case of $Bi_5FeTi_3O_{15}$ by *ab initio* — •Yael Birenbaum, Nicola Spaldin, and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

The Aurivillius phases form a family of naturally-layered perovskite-

related materials with good ferroelectric properties. $Bi_5FeTi_3O_{15}$ (BFTO) is perhaps the simplest known member of this family that also incorporates magnetic degrees of freedom. Using *ab initio* electronic structure calculations, we establish the ferroelectric and magnetic properties of BFTO. We then discuss a possible site preference of the Fe^{3+} cation, which so far has not been found experimentally, and quantify the magnetic coupling between adjacent Fe cations. In addition, we analyse the different structural distortions, in order to relate BFTO to other members of the Aurivillius phases.

KR 1.8 Mon 11:15 H3

Strain effect on magnetic properties of $La_{0.7}Ca_{0.3}MnO_3/SrRuO_3$ Superlattices — •Sujit Das[1,2], Andreas Herklotz[1,2], and Kathrin Doerr[1,2] — [1]IFW Dresden, Postfach 270116, 01171 Dresden, Germany — [2]Institute for Physics, MLU Halle-Wittenberg, 06099 Halle, Germany

Coherent interfaces between magnetic oxides such as $La_{0.7}$ $Sr_{0.3}MnO_3$ and $SrRuO_3$ may induce an intense magnetic coupling [1]. Recent work indicated an impact of elastic strain on the strength and even the sign of the coupling [2]. Superlattices (SL) of $La_{0.7}$ $Ca_{0.3}MnO_3/SrRuO_3$ with layer thicknesses below 10 unit cells were grown by pulse laser deposition simultaneously on $SrTiO_3$(001) (STO), $LaAlO_3$(001) (LAO) and piezoelectric $0.72Pb(Mg_{1/3}Nb_{2/3})O_3$-$0.28PbTiO_3$ (001) (PMN-PT) substrates and structurally characterized by X-ray diffraction (XRD). On LAO, the SL assumes a compressive strain state, i. e. the lattice parameter is larger out-of-plane than in-plane, whereas on PMN-PT it shows a tensile strain state and on STO an intermediate strain value. Magnetization measurements demonstrate a strong antiferromagnetic (AFM) coupling in SLs on STO and LAO substrates which is due to superexchange interaction between Ru and Mn ions. The AFM coupling seems to decrease under tensile strain. The coupling is much weaker on PMN-PT, probably because of higher interface roughness. In order to probe the effect of elastic strain directly, magnetization loops in reversibly controlled strain states have been recorded for SLs on PMN-PT. [1] M. Ziese et al., PRL 104, 167203 (2010), [2] J. W. Seo et al., PRL 105, 167206 (2010) .

KR 1.9 Mon 11:30 H3

Tuning the multiferroic phase of CuO with impurities — •Johan Hellsvik[1], Marcello Balestieri[1], Alessandro Stroppa[2], Anders Bergman[3], Lars Bergqvist[4], Olle Eriksson[3], Silvia Picozzi[2], and José Lorenzana[1] — [1]ISC-CNR, Rome, Italy — [2]CNR-SPIN, L'Aquila, Italy — [3]Uppsala University, Uppsala, Sweden — [4]KTH, Stockholm, Sweden

The discovery that CuO is a multiferroic with a high antiferromagnetic transition temperature of 230 K opened a possible route to room-temperature multiferroicity with a strong magnetoelectric coupling [1]. CuO belongs [2] to a new class of multiferroic materials where the so called 'order by disorder mechanism' [3] plays a crucial role. In this work we study the effect of different impurities on the phase diagram of CuO aiming at engineering the multiferroic properties. Extensive density functional theory (DFT) calculations were performed for a large number of fixed spin configurations in pure CuO and CuO doped with a small fraction of the Cu atoms substituted with the nonmagnetic elements Mg, Zn or Cd, or the magnetic elements Ni or Co. Our computations established that the energy difference between the low-temperature collinear AF1 phase and the intermediate temperature multiferroic AF2 phase decreased monotonously with increasing doping level confirming that impurities favour the multiferroic phase. The magnetic phase diagram has been mapped out in Monte Carlo simulations for classical Heisenberg spins. [1] T. Kimura et al., Nature Mat. 7, 291 (2008); [2] G. Giovannetti et al., Phys. Rev. Lett. 106, 026401 (2011); [3] C. L. Henley, Phys. Rev. Lett. 62, 2056 (1989)

KR 1.10 Mon 11:45 H3

Charge-mediated magnetoelectric coupling in patterned multiferroic heterostructures — •daniele preziosi[1], dietrich hesse[1], marin alexe[1], martin wahler[2], and georg schmidt[2] — [1]Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, 06120 Halle(Saale) Germany — [2]Martin-Luther-Universität Halle-Wittenberg Von-Danckelman-Platz 3, 06120 Halle(Saale) Germany

Several studies on single phase multiferroics demonstrate that the coupling between the ferroelectric and the (ferro)magnetic order parameters tends to be small. Engineering of artificially structured systems could provide a reliable way to improve the MagnetoElectric (ME) coupling. Devices based on charge-mediated ME effect represent a viable alternative. The electric field produced by the polarization of the ferroelectric material can induce, at the interface with an ultrathin strongly correlated magnetic oxide, a change in the magnetization. The ME coupling would be in this case the consequence of the spin-dependent screening of the electric field. Patterned hetero-structures of La1-xSrxMnO3 (LSMO) and PbZr0.2Ti0.8O3 (PZT) have been fabricated. Transport and magnetic measurements show that the switching of the PZT polarization influences significantly the competing electronic ground states of the LSMO, modulating the resistivity as well as the magnetization value.

KR 2: Multiferroics 2 (MA jointly with DF, DS, KR, TT)

Time: Monday 15:00–18:30 Location: H3

KR 2.1 Mon 15:00 H3

Magnetization control in thin two-phase multiferroic structures via external electric fields — •Alexander Sukhov[1], Paul P. Horley[2], Chenglong Jia[3], and Jamal Berakdar[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06120 Halle/Saale, Germany — [2]Centro de Investigation en Materiales Avanzados, S.C. (CIMAV), 31109 Chihuahua, Mexico — [3]Key Laboratory for Magnetism and Magnetic Materials of the Ministry of Education, Lanzhou University, Lanzhou 730000, China

We present a theoretical study of the coupled magnetization and polarization dynamics in a thin multiferroic junction related to a $BaTiO_3$ (rhombohedral phase) layer in contact with Fe-layer. The dynamical properties are discussed in the context of different interfacial magnetoelectric coupling mechanisms. For the magnetoelectric coupling induced by the screening of the spin-polarized electrons in Fe we investigate the minimum strength of the coupling constant which is required for the full switching of the magnetization [1]. In the case of a strain-induced magnetoelectric interaction we show an electric field-induced magnetic switching in the plane perpendicular to the magneto-crystalline easy axis while the total magnetization remains stable [2]. In addition, the response of the multiferroic structure to magnetic radio-frequency fields by means of ferromagnetic resonance and dependent on the applied electric field is studied. [1] P.P. Horley, A. Sukhov, C.-L. Jia, E. Martinez, J. Berakdar, Phys. Rev. B **85**, 054401 (2012). [2] C.-L. Jia, A. Sukhov, P.P. Horley, J. Berakdar, Europhys. Lett. **99**, 17004 (2012).

KR 2.2 Mon 15:15 H3

Magnetic field induced charge anisotropy in $CoFe_2O_4/BaTiO_3$ nanocomposite — •Carolin Schmitz-Antoniak[1], Detlef Schmitz[2], Sven Stienen[1], Pavel Borisov[3], Anne Warland[1], Bernhard Krumme[1], Wolfgang Kleemann[1], and Heiko Wende[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, D-47048 Duisburg — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, D-12489 Berlin — [3]Department of Chemistry, University of Liverpool, Liverpool L69 7ZD

The system of $CoFe_2O_4$ nanopillars in a $BaTiO_3$ matrix represents a multiferroic nanocomposite in which strong ferrimagnetism and strong ferroelectricity coexist at room temperature [1]. The magnetostrictive CFO nanopillars and the piezoelectric BTO matrix are coupled by strain so that it is possible to change the electric properties by a magnetic field and the magnetic properties by an electric field. The charge anisotropy of Ti ions is probed by x-ray linear dichroism (XLD) and the magnetisation of Co ions by x-ray magnetic circular dichroism (XMCD) giving the unique possibility to study the effect of the coupling on a microscopic level as a function of magnetic field strength and direction. The occurrence of significant in-plane components of the electric polarisation is discussed. They are due to shear forces acting on the $BaTiO_3$ matrix while taking into account non-diagonal piezoelectricity components.

Funded by DFG (SFB491) and BMBF (05 ES3XBA/5).

[1] H. Zheng et al., Science 303, 661 (2004)

KR 2.3 Mon 15:30 H3

Multiferroic CoFe2O4/ BaTiO3 with core shell structure nanoparticles — •Morad Etier[1], Vladimir V.Shvartsman[1], Yanling Gao[1], Joachim Landers[2], Heiko Wende[2], and Doru C.Lupascu[1] — [1]University of Duisburg-Essen, Institute for Materials Science, Essen, Germany — [2]University of Duisburg-Essen, Faculty of Physics, Duisburg, Germany

Multiferroic materials exhibit ferroelectricity and ferromagnetism simultaneously. Combining piezoelectricity and magnetostriction components in the same composite received more interests in the modern researches. In this work we report synthesis and properties of cobalt iron oxide barium titanate composite with a core shell structure. To synthesize the samples we combine co-precipitation and organosol method. Phases content, microstructure and morphology were studied by x-ray diffraction, SEM and TEM. Multiferroic properties were proved by home-built Sawyer-Tower circuit and SQUID magnetometry. Temperature dependence of magnetic moment was measured in zero field cooling (ZFC) and field cooling (FC) and compared with those cobalt iron oxide nanopowder. The dielectric properties were studied using impedance spectroscopy.

KR 2.4 Mon 15:45 H3

Strain-induced changes of magnetic anisotropy in epitaxial spinel-type cobalt ferrite films — •Stefania Florina Rus[1,2], Andreas Herklotz[2,4], Iuliu Grozescu[3], and Kathrin Dörr[4] — [1]Politehnica University of Timişoara, 300006 Timişoara, Romania — [2]IFW Dresden, 01171 Dresden, Germany — [3]Institute for Research and Development in Electrochemistry and Condensed Matter, 300224 Timisoara, Romania — [4]Martin-Luther-Universität Halle-Wittenberg, Institute for Physics, 06099 Halle, Germany

We present results on the effect of biaxial strain on the magnetic anisotropy of thin films of the parent compound CoFe2O4 and films with a partial substitution of Co and Fe by Zr and Pt, respectively. The strain states of the epitaxially grown films are controlled twofold: (i) statically by epitaxial misfit strain via an appropriate choice of substrates and buffer layers and (ii) reversibly by strain transfer from piezoelectric $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$ (001) (PMN-PT) substrates. Due to large negative magnetostriction all films show an out-of-plane magnetic easy axis under tensile strain and an in-plane easy axis under compressive strain. Our reversible strain measurements show that the magnetic anisotropy can be efficiently altered by the application of an electric field to the ferroelectric PMN-PT substrates. The effect of substitution with Zr and Pt on the magnetoelectric effect will be discussed. This work is supported by the strategic grant POSDRU ID77265 (2010), co-financed by the European Social Fund, within the Sectoral Operational Programme Human Resources Development 2007-2013. Advising by P. Vlazan is greatly acknowledged.

KR 2.5 Mon 16:00 H3

***Ab initio* study of magneto-phonon interaction in $GaFeO_3$** — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Magnetoelectric (ME) coupling provides a handle for manipulating the magnetization of a material with an electric field, giving a perspective for a new type of non-volatile memory. Unfortunately, materials with ME coupling that is large enough for industrial applications are scarce. Moreover, among the materials which are both ferroelectric and magnetic at room temperature, only $BiFeO_3$ is known. Unfortunately, the ordering of spins in this material is antiferromagnetic (whereas ferro/ferrimagnetic coupling is desired) and the ME coupling is small.

$GaFeO_3$ (GFO) is the first material observed to simultaneously present a strong ME coupling and a resulting magnetization in a single phase. It has the polar structure $Pc2_1n$, which allows disorder in A and B cation sites. By increasing the iron content its Curie temperature can be increased above room temperature [1].

To understand the mechanism of the strong ME coupling in $GaFeO_3$ at the microscopic level, we performed *ab initio* calculations based on density functional theory of the structural properties and magneto-phonon interaction in stoichiometric $GaFeO_3$ compounds in different structures, as well as with different occupancies of the A and B sites.

We acknowledge the support by Helmholtz Young Investigators Group Programme VH-NG-409 and GALIMEO Consortium.

[1] T. Arima *et al.*, Phys. Rev. B **70**, 064426 (2006)

KR 2.6 Mon 16:15 H3

The effect of ion doping on multiferroic $MnWO_4$ — •safa golrokh bahoosh[1,3], julia m. wesselinowa[2], and steffen trimper[3] — [1]Max Planck Institute of Microstructure Physics,Weinberg 2, 06120 Halle, Germany — [2]University of Sofia, Department of Physics,Blvd. J. Bouchier 5, 1164 Sofia, Bulgaria — [3]Institute of Physics, Martin-Luther-University, 06120 Halle, Germany

We have studied the ion doping effects on different transition temperatures in the multiferroic compound $MnWO_4$ based on a microscopic model and within the framework of Green functions technique. It is shown that the exchange interaction constants can be changed due to the different ion doping radii. This leads to reduction of the magnetic phase transition temperature T_N by doping with non-magnetic ions,such as Zn, Mg, whereas T_N is enhanced by doping withtransition metal ions, such as Fe, Co. The different behavior of the temperature T_1 (where up-up-down-down collinear spin structure appears) by Fe and Co doping could be explained taking into account the single-ion anisotropy.

15 min. break

KR 2.7 Mon 16:45 H3

Hybrid improper ferroelectricity in a Multiferroic and Magnetoelectric Metal- Organic Framework — •Alessandro Stroppa[1], Paolo Barone[1], Prashant Jain[2], Manuel Perez-Mato[3], and Silvia Picozzi[1] — [1]CNR-SPIN Via Vetoio, 67100, L'Aquila (Italy) — [2]Los Alamos National Lab, 30 Bikini Atoll Rd Los Alamos, NM 87545-0001 (505) 664-5265 — [3]Departamento de Fisica de la Materia Condensada, Facultad de Ciencia y Tecnologia, UPV/EHU, Bilbao (Spain)

Metal-organic frameworks (MOFs) show increasing promise as candidates for various applications. Of particular interest are MOFs with the perovskite topology showing hydrogen bonding-related multiferroic phenomena. By using state-of-the-art-ab-initio calculations, we show that in [C(NH2)3]Cr(HCOO)3 MOF, interaction between the cooperative antiferro-distortive Jahn-Teller distortions and the C(NH2)3 cations breaks the inversion symmetry through hydrogen-bonding and induces a ferroelectric polarization. Interestingly, the polar behavior arises due to a trilinear coupling between two unstable modes, namely a Jahn-Teller and a tilting mode, and one stable polar mode. Therefore, this compound represents the first example of hybrid improper ferroelectric in the family of metal-organic compounds. Since rotational modes in perovskite-inorganic compounds usually freeze-in at elevated temperatures (300 K), the trilinear coupling in MOF compounds may provide an interesting route to realize room temperature multiferroic. Last but not least, we show that switching of polarization direction implies the reversal of a large weak ferromagnetic component.

KR 2.8 Mon 17:00 H3

Ferroelectric properties of $(Ba,Sr)TiO_3/La_{0.7}Sr_{0.3}MnO_3$ multilayered thin films — •Markus Michelmann[1], Johannes Aprojanz[1,2], Arseni Buryakov[2], Elena Mishina[2], Markus Jungbauer[1], Sebastian Hühn[1], and Vasily Moshnyaga[1] — [1]I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Moscow State Institute of Radioengineering, Electronics and Automation, Prosp. Vernadskogo 78, 119454 Moscow, Russia

$Ba_xSr_{1-x}TiO_3$ (BSTO) epitaxial thin films became feasible for room temperature applications in contrast to the bulk material due to a possibility to enhance the ferroelectric Curie temperature under biaxial compressive strain. Using $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) thin films as metallic electrodes, we have grown highly strained BSTO/LSMO bilayers and LSMO/BSTO/LSMO trilayers on $SrTiO_3$ (100) substrates with BSTO layer thicknesses of 10 - 200 nm by means of metalorganic aerosol deposition. Ferroelectric switching was studied both electrically and by nonlinear optics (second harmonic generation (SHG)). Capacitance-voltage characteristics in a frequency range of $f = 1-10^6$ Hz and PUND measurements prove a ferroelectric hysteretic behavior up to room temperature with a remanent polarization of several $\mu C/cm^2$ and a switching fields in the range of 10−100 kV/cm. This was also supported by the SHG measurements. A detailed study of multiferroic properties will be performed for temperatures, $T = 10-400$ K, and applied magnetic field, $B = 0-9$ T. This work was supported by IFOX of the European Community's 7th Framework Programme.

KR 2.9 Mon 17:15 H3

Epitaxial thin films of the multiferroic double perovskite Bi_2FeCrO_6 — •Vikas Shabadi, Mehran Vafaee, Mehrdad

BaghaieYazdi, Aldin Radetinac, Philipp Komissinskiy, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt, Germany

Co-existence of magnetism and ferroelectricity was theoretically predicted in the ordered double perovskite Bi_2FeCrO_6 (BFCO) [1]. We report epitaxial BFCO thin films grown by pulsed laser deposition from a 20% Bi-rich ceramic target on single crystal $SrTiO_3$(100) substrates. The degree of the Fe-Cr cation ordering in the BFCO films was calculated based on the X-ray diffraction patterns. The magnetic moments of the BFCO films were measured with a SQUID magnetometer and analyzed as a function of the Fe-Cr ordering. The discrepancies in the previously reported values of the magnetic moment of BFCO [2,3] are most likely connected to the varying degree of the Fe-Cr cation ordering in the samples. In a recent experiment more than 90% spontaneous B-site ordering in a similar Fe-Cr based double perovskite system has been achieved [4]. Anti-site disorder control is a key challenge to design double perovskite multiferroics.

[1]P. Baettig and N. A. Spaldin, Appl. Phys. Lett. **86**, 012505 (2005)
[2]Kim *et al.*, Appl. Phys. Lett. 89, 102902 (2006)
[3]R. Nechache *et al.*, J. Appl. Phys. **105**, 061621 (2009)
[4]S. Chakraverty *et al.*, Phys. Rev. B **84**, 064436 (2011)
The authors acknowledge support from DAAD.

KR 2.10 Mon 17:30 H3

Growth of multiferroic heterostructures — •Sergiu Stratulat, Dietrich Hesse, and Marin Alexe — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Coupling two materials with different order parameters gives great flexibility in engineering multifunctional devices. In achieving the maximum interfacial effects, vertical heterostructures present the maximum potential. Creating well-ordered vertical multiferroic heterostructures is not a trivial task, especially on large areas. We are focusing our attention on the system comprising ferrimagnetic CoFe2O4 and ferroelectric/antiferromagnetic BiFeO3, using pulsed laser deposition as a synthesizing technique. Considering a time-viable process to create the pillar-matrix configuration, we used anodic aluminum oxide masks to pattern the nucleation sites for the cobalt ferrite on previously deposited SrRuO3 bottom electrode on SrTiO3. After removal of the mask, deposition by means of a mixed target leads to ordered arrays of CFO pillars embedded in a BFO matrix. Scanning electron microscopy was employed at every step of the experiments to show the development of the samples, and X-ray diffraction probed the structural parameters. Testing the ferroelectric and magnetic properties locally gives an indication on the coupling influences present in the thin films.

KR 2.11 Mon 17:45 H3

Self-assembled composite multiferroic films in controlled strain states — •Mohsin Rafique[1,2,3,4], Andreas Herklotz[3,4], Er-Jia Guo[3,4], Kathrin Doerr[3,4], and Sadia Manzoor[1,2] — [1]Magnetism Laboratory, COMSATS Institute of Information Technology, Park Road 44000, Islamabad, Pakistan — [2]Center for Micro and Nano Devices (CMND), COMSATS Institute of Information Technology, Park Road 44000, Islamabad, Pakistan — [3]IFW Dresden, Postfach 270116, 01171 Dresden, Germany — [4]Institute for Physics, Martin-Luther-University Halle-Wittenberg, 06099 Halle, Germany

Self-assembled thin-film nanocomposites of piezoelectric and magnetostrictive materials have stimulated increasing research activities because of their potential to exhibit a large magnetoelectric response exploitable in multifunctional devices. Epitaxial thin films of $CoFe_2O_4$ and $BaTiO_3$ (CFO-BTO) composites were grown on $SrTiO_3$ (001) and piezoelectric $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$(001) (PMN-PT) substrates by pulsed laser deposition. Self-assembled nanostructures consisting of spinel nanopillars heteroepitaxially embedded in the ferroelectric perovskite matrix form. X-ray diffraction is utilized to estimate the lattice parameters. The magnetic properties studied by SQUID magnetometry show an out-of-plane easy axis of the CFO nanopillars and a strengthening of the out-of-plane anisotropy with increasing compression along the nanopillar axis. The magnetoelectric coupling in the composite film is revealed at a structural transition of the BTO matrix. Electrically controlled substrate strain of PMN-PT is applied to modify the magnetic anisotropy of the nanopillars.

KR 2.12 Mon 18:00 H3

Low-lying magnetic excitations in the distorted triangular lattice antiferromagnet α-$CaCr_2O_4$ — •Michael Schmidt[1], Zhe Wang[1], Sandor Toth[2], Bella Lake[2], A.T.M.Nazmul Islam[2], Alois Loidl[1], and Joachim Deisenhofer[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany

We will discuss our results on α-$CaCr_2O_4$ obtained by FIR and Terahertz spectroscopy. This compound orders below $T_N = 42.6$ K in a proper screw 120° magnetic order, but shows additional low-lying magnetic modes indicative for the vicinity of a more complex magnetic order [1], [2]. Our spectra obtained by FTIR and THz-TD spectroscopy show several optical magnons appearing below the magnetic ordering with anomalous temperature dependence. We will discuss their polarization dependence and a possible magnetoelastic coupling of these modes.

[1] S. Toth *et al.*, Phys. Rev. B 84, 054452 (2011)
[2] S. Toth *et al.*, PRL 109, 127203 (2012)

KR 2.13 Mon 18:15 H3

Multiferroic $Ni_3V_2O_8$ measured in THz range at low temperatures and in high magnetic fields — •Malte Langenbach[1], Tobias Hissen[1], Komalavalli Thirunavukkuarasu[1], Holger Schmitz[1], Iván Cámara Mayorga[2], Rolf Güsten[2], Joachim Hemberger[1], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Köln, Germany; — [2]Max-Planck-Institut für Radioastronomie, Bonn, Germany;

THz spectroscopy in high magnetic fields is an important technique to probe materials with strong magneto-electric coupling. Here, we discuss the Kagomé-staircase compound $Ni_3V_2O_8$. The triangle-based lattice gives rise to a frustration of the short-range antiferromagnetic couplings. This causes a rich variety of magnetic and structural phases at low temperatures.
Below $T_N = 9.8$ K, a incommensurate phase with collinear sinusoidal spin structure is established. This phase is followed by a cycloidal spin structure which is accompanied by the onset of ferroelectricity. Finally, below 3.9 K, the structure changes to a commensurate canted antiferromagnetic phase [1].
We report on elementary excitations in the THz range observed between 2 K and 50 K in fields up to 8 T.

Work supported by the DFG through SFB 608.

[1] G. Lawes et al., Phys. Rev. Lett. **95**, 087205 (2005)

KR 3: Electrical and mechanical properties (DF jointly with KR)

Time: Monday 15:00–16:00 Location: H11

KR 3.1 Mon 15:00 H11

High-pressure crystal structure of $Bi_{12}GeO_{20}$ sillenite — •Leonore Wiehl, Alexandra Friedrich, Eiken Haussühl, Wolfgang Morgenroth, and Björn Winkler — Institut für Geowissenschaften, Goethe-Universität, Frankfurt/Main, Germany

$Bi_{12}GeO_{20}$ crystallizes in the sillenites structure type with the noncentrosymmetric cubic space group $I23$. Sillenites $Bi_{12}MO_{20}$ (M = Si, Ge, Ti) are used in technical applications because of their outstanding electrical and nonlinear optical properties, especially the photorefractive effect. These properties are assumed to be correlated with the stereochemical activity of the $6s^2$ lone electron pair of Bi^{3+}.

The evolution of the $Bi_{12}GeO_{20}$ crystal structure under high pressure was investigated by experiment and theory using single-crystal X-ray diffraction and density functional theory (DFT) calculations. The crystal structure was determined from X-ray intensity data collected at ambient conditions in house and at high pressure with synchrotron radiation at HASYLAB (D3). Pressures up to 21 GPa were generated in diamond anvil cells. DFT calculations were performed up to 50 GPa. The pressure dependence of interatomic distances indicates a reduced eccentricity of the Bi^{3+} coordination at high pressure, but

not a collapse of the Bi^{3+} lone electron pair. The results are discussed in comparison with the isotypic Si sillenite [1].

Financial support from the DFG (HA 5137/3-1) and from HASYLAB is gratefully acknowledged. We thank HASYLAB for synchrotron beamtime and Martin Tolkiehn for assistance at D3.

[1] Wiehl L, et al. (2010) J. Phys.: Condens. Matter 22, 505401

KR 3.2 Mon 15:20 H11

Ripening of ZnO nanoparticles - influence of the stabilizing layer — •Torben Schindler, Martin Schmiele, Thaer Kassar, and Tobias Unruh — Lehrstuhl für Kristallographie und Strukturphysik, Friedrich-Alexander Universität Erlangen Nürnberg, Staudtstr. 3, 91058 Erlangen

ZnO semiconductor nanoparticles (NPs) exhibit promising electro-optical properties for applications in e.g. solar cells or light emitting devices due to the quantum size effect. Thus, the preparation of well-defined, stable ZnO-NPs is of high interest and therefore knowledge about the nucleation and growth processes is crucial.

For the synthesis ethanolic solutions of zincacetate and lithiumhydroxide are simply mixed. The nucleation of the NP occurs instantly, while a further ripening of the ZnO-NPs starting from about 2.5 nm as a function of temperature was observed using UV/Vis measurements. The ripening process is further investigated in detail using temperature- and time-dependent small angle x ray scattering (SAXS) measurements. To determine the influence of the stabilizing acetate layer for the particle growth, small angle neutron scattering (SANS) is used and first results will be presented.

KR 3.3 Mon 15:40 H11

Localization Effects in Dielectric Disordered Crystals and Random Materials — Anton Lebedev, Marius Dommermuth, and •Regine Frank — Institut für Theoretsiche Physik, Universität Tübingen

Anderson localization, the counterpart of hyper diffusion, more than ever is of high interest to the semiconductor community. We apply diagrammatic quantum field theory beyond Lippmann-Schwinger equation to derive and explain localization effects in disordered photonic crystals and random media. Mie-Scattering als well as other scatterers are considered and we present self-consistent fit-parameter free 'ab initio' calculations and results.

KR 4: Quantitative Materialanalyse (MI jointly with KR)

Time: Tuesday 9:30–12:15 Location: H5

Invited Talk KR 4.1 Tue 9:30 H5

Quantitative Röntgenspektrometrie für die Analyse nanostrukturierter Materialien — •Matthias Müller, Burkhard Beckhoff, Philipp Hönicke, Beatrix Pollakowski, Cornelia Streeck und Rainer Unterumsberger — Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin

Die physikalischen und chemischen Eigenschaften nanostrukturierter Materialen bestimmen maßgeblich deren Funktionalität. Für eine zielführende und effektive Materialentwicklung ist es deshalb entscheidend, dass eine zuverlässige Analytik verfügbar ist. Die quantitative Röntgenspektrometrie hat sich für die Materialcharakterisierung als leistungsfähige und zuverlässige Methode etabliert.

Die Nutzung von Röntgenstrahlung geringer Divergenz an Synchrotronstrahlungslaboren hat die Entwicklung der RFA unter streifendem Einfall ermöglicht, wodurch die tiefensensitive Charakterisierung von Nanoschichtsystemen erreicht wurde. Der Einsatz von durchstimmbarer Synchrotronstrahlung hat die Weiterentwicklung von Quantifizierungsmodellen unterstützt, welche auf der Fundamentalparametermethode basieren. Eine weitere deutliche Verbesserung lässt sich durch den Einsatz radiometrisch kalibrierter Instrumentierung erreichen, wodurch eine referenzprobenfreie Quantifizierung erreicht werden kann.

Der Vortrag gibt einen Überblick über die verschiedenen Quantifizierungsmodelle, deren Vor- und Nachteile sowie die Entwicklungsperspektiven. Anhand aktueller Arbeiten der PTB bei BESSY II werden ausgewählte Anwendungsfelder der quantitativen Röntgenspektrometrie für die Entwicklung nanostrukturierter Materialien vorgestellt.

KR 4.2 Tue 10:15 H5

Advances in Low Energy X-ray Analysis with state of the art Silicon Drift Detectors using EPMA, SEM and STEM — •T. Salge[1], R. Terborg[1], M. Falke[1], O. Tunckan[2], A. Kearsley[3], D. Pereira da Silva Dalto[4], M.J.O.C. Guimarães[4], R. Ferhati[5], I. Bjurhager[6], S. Turan[2], M.E.F. Garcia[4], and W. Bolse[5] — [1]Bruker Nano GmbH, Berlin, Germany — [2]Anadolu University, Eskisehir, Turkey — [3]Natural History Museum, London, UK — [4]UFRJ, Rio de Janeiro, Brazil — [5]University of Stuttgart, Germany — [6]Ångström Laboratory, Uppsala, Sweden

Element analysis of ever smaller structures in bulk samples requires low electron beam energy to enhance spatial resolution. To separate overlapping peaks at low energy X-ray lines (e.g. N-K/Ti-L), the line deconvolution algorithms in EDX software is important. We describe features at the submicron scale (e.g. ceramic-metal joints) using SDDs in conventional geometries. The annular four channel SDD placed between the pole piece and sample covers a large solid angle of 1.1sr. Features with high topography from experiments with wafer irradiation and hypervelocity impact craters can be analyzed as well as beam sensitive polymer composites. For cultural heritage and biological samples, carbon coating can be avoided during low vacuum acquisition. Nano- and atomic scale analysis of electron transparent samples ideally requires not only high solid angle detector design but also adjustments in pole piece and sample holder geometry as well as a high quality electron probe. This approach will be demonstrated to allow 1 sr solid angle and single atom spectroscopy even at 0.1 sr and 60 kV.

KR 4.3 Tue 10:30 H5

Quantitative Analysis of Pyramid Textured Silicon Wafers and Size Dependence of Optical and Electronic Properties — •Jan Kegel[1,2], Heike Angermann[2], Uta Stürzebecher[3], Erhard Conrad[2], and Bert Stegemann[1] — [1]Hochschule für Technik und Wirtschaft, Berlin, Germany — [2]Helmholtz Zentrum Berlin, Berlin, Germany — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, Erfurt, Germany

Wet-chemical etching in alkaline solution is used to texture monocrystalline silicon wafers for high-efficiency solar cells. This texturing result in micron-sized random pyramids on the wafer surface which reduce reflection losses and increase the absorption probability. Successful texturing is evaluated by reflection and charge carrier lifetime measurements. Both parameters are found to be influenced by the geometric surface properties as well. Thus, elaborated image processing is applied for precise and reproducible evaluation of pyramid number and size distribution. The results show a distinct dependence of the total reflection and the minority charge carrier lifetime on the pyramid size distribution. Based on these results etching parameters can be adjusted to produce optimal surface properties with respect to highest solar cell efficiencies.

KR 4.4 Tue 10:45 H5

phase diagram of nano-hydride formation: consequences for hydrogen embrittlement — •Gerard Paul Leyson, Blazej Grabowski, Johann von Pezold, and Jörg Neugebauer — Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Local hydride formation around dislocations induces stress-shielding effects and is the underlying mechanism for hydrogen-enhanced local plasticity (HELP). In this work, we present an analytic model for hydride formation around fcc Ni edge dislocations that takes input from atomistic calculations. The hydrogen-hydrogen interaction is modeled using information obtained from a semi-empirical embedded atom method (EAM) potential. Within this approach, the equilibrium concentration and the binding energies of hydrogen around the dislocation are self-consistently calculated. At 300K, local hydride formation is observed with bulk hydrogen concentrations on the order of ~500ppm, consistent previous studies [1]. The onset of nano-hydride formation and with it the activation of the HELP mechanism is predicted through a parametric study of the hydride size as a function of temperature and bulk hydrogen concentration.

[1] von Pezold J, Lymperakis L and Neugebeauer J. Acta Materialia 59 (2011), 2969-2980.

KR 4.5 Tue 11:00 H5

Diffuse scattering and stacking faults in (Bi,Na)TiO3 single crystals — •Wolfgang Donner[1], Marton Major[1], and John Daniels[2] — [1]Fachbereich Materialwissenschaft, Technische Universität Darmstadt — [2]School of Materials Science and Engineering, University of New South Wales, Sydney

In our previous work we found diffuse streaks in the x-ray diffraction from the single crystal relaxor BNT-4BT [1]. These streaks connect half-order reflections associated with octahedral tilts in the sample. The diffuse streaks and diffuse half-order peaks react upon the application of an external electric field. Similar diffuse scattering patterns had been found in electron diffraction [2] from pure BNT samples and were interpreted as arising from stacking faults in the octahedral tilt sequence. The stacking fault structure could also be viewed as a twin structure of two rhombohedral domains. Here we present results from simulations of the diffuse scattering pattern based on certain stacking faults in the R3c structure and show that the model can be applied to estimate the amount of stacking faults. The stacking fault probability in turn can be used to estimate the size of the nanopolar regions in BNT-BT giving rise to the relaxor behavior.

[1] J. Daniels, W. Jo, J. Rödel, D. Rytz and W. Donner, Appl. Phys. Lett. 98, 252904 (2011) [2] V. Dorcet, G. Trolliard, Acta Mat. 56, 1753 (2008)

15 min. break

KR 4.6 Tue 11:30 H5

Comparative Study of Ion Sputtering in XPS Depth Profiling for Thin Film Analysis. — •Andrey Lyapin[1], Stefan Reichlmaier[1], Saad Alnabulsi[2], Sankar Raman[2], John Moulder[2], Scott Bryan[2], and John Hammond[2] — [1]Physical Electronics GmbH, Fraunhoferstr. 4, D-85737, Ismaning, Germany — [2]Physical Electronics, 18725 Lake Drive East, Chanhassen, MN, 55317, USA

The objective of successful XPS sputter depth profiling is to accurately identify the layer thicknesses and chemical composition of materials within thin film structures. Cluster ion beam sputtering has been widely used in recent years with the intent to address this essential analytical goal for a broader range of materials, including organic materials. C_{60} cluster ion beam sputtering provided the first access to quantitative chemical state information below the surface for many polymers, organic and inorganic oxide materials.

The recent introduction of argon gas cluster ion beam sputtering to the XPS community has further expanded the capability of successful depth profiling with an emphasis on preserving the chemical structure of challenging polymer and organic materials that exhibit rapid radiation induced damage due to the mobility and reactivity of free radicals that are formed during the sputtering process when other ion sources are used.

The purpose of this study is to present a comparative evaluation to quantify the benefits of using either C_{60} or argon gas cluster ion beam sputtering for XPS compositional depth profiling.

KR 4.7 Tue 11:45 H5

Analysis of impurity diffusion and recrystallisation processes of Fe and FeNi polycrystals with low energy electron microscopy — •Benjamin Borkenhagen, Gerhard Lilienkamp, and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstraße 4, 38678 Clausthal-Zellerfeld

We use low energy electron microscopy (LEEM) and laterally resolved low energy electron diffraction (μLEED) to characterize surface properties of polycrystalline materials as well as structural and dynamic properties of grain boundaries. In this contribution, we report on our analyses of segregation and diffusion processes taking place at the surface of polycrystalline Fe and FeNi. Previously we have shown that bulk impurities, mostly sulphur, segregate from the bulk of a heated polycrystal to the surface and form two-dimensional impurity islands. At a suitable temperature we observe Ostwald ripening of these islands and, at elevated temperature, dissolution of the islands. Here we present a quantitative study of impurity diffusion processes, which yields both linear and $t^{1/2}$ time dependencies for the impurity concentrations on different grains. These different time dependencies point to different bulk impurity concentration profiles in different grains. In addition to impurity diffusion, we studied recrystallisation processes and their effects on surface topography in real time. By measuring tripel-point speeds and geometries of the grain boundaries, the rate-limiting step of the recrystallisation process – grain boundary mobility or tripel point mobility – was identified.

KR 4.8 Tue 12:00 H5

Microscopic Understanding of Ionic Thermophoresis — Mario Herzog, •Maren Reichl, Alexandra Götz, and Dieter Braun — Systems Biophysics, LMU, München, Germany

A number of microscopic models for thermophoresis has been proposed recently. Here we measured short DNA and RNA molecules over a wide parameter range (0.4-14 nm Debye length, 5-75°C base temperature, 5-50 bases, 11 different electrolytes) [1]. The measurements confirm the capacitor model of thermophoresis with the following details [2]:

1. Thermophoresis is proportional to the Debye length when the latter is smaller than the molecule radius, but saturates for Debye lengths exceeding the molecule radius. This confirms the predicted size transition between the plate and spherical limit of the capacitor model. The fitted effective charges depend on DNA length predicted by molecular dynamics simulations of Manning condensation.

2. Depending on the electrolyte, a constant additive contribution for the Seebeck effect of the electrolyte is confirmed. It can be understood from literature data without fitting parameters.

The model allows non-trivial predictions of thermophoresis. Our work confirms in detail a local equilibrium approach to thermophoresis. The finding is likely to improve biomolecule binding studies using microscale thermophoresis (Nanotemper Technologies).

[1] Herzog M and Braun D, under review

[2] Dohnt J, Wiegand S, Duhr S and Braun D, Langmuir 23, 1674-1683 (2007)

KR 5: Poster - Crystallography

Time: Wednesday 15:00–17:30 Location: Poster B2

KR 5.1 Wed 15:00 Poster B2

Determination and correction of distortions and systematic errors in low-energy electron diffraction — •Falko Sojka[1], Matthias Meissner[1], Christian Zwick[1], Roman Forker[1], Claudius Klein[2], Michael Horn-von Hoegen[2], and Torsten Fritz[1] — [1]University of Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany — [2]University of Duisburg-Essen, AG Horn-von Hoegen, Lotharstr. 1-21, 47048 Duisburg, Germany

LEED on epitaxial layers is a powerful tool to examine long-range ordering at the interface. However, due to limitations like distortions of the LEED images, additional efforts have to be made in order to derive precise epitaxial relations from the measured LEED patterns.

We developed and implemented an algorithm to determine and correct systematic distortions in LEED images. The procedure is independent of the design of the device (conventional LEED, MCP-LEED, SPA-LEED). Therefore, only a calibration sample with a well-known structure and a suitably high number of diffraction spots is required. The algorithm provides a correction matrix which can be used to rectify all further measurements generated with the same device. Additionally, we found an axial distortion which occurs due to a tilted sample surface. This axial distortion can be described theoretically, and thus it is possible to correct those measurements, too.

Only corrected LEED images represent an unaffected view of the reciprocal space. So we can use them for the determination of the lattice parameters or epitaxial relations by numerical optimization achieving a very high accuracy.

KR 5.2 Wed 15:00 Poster B2

Digital electron diffraction: a new approach for determining crystal symmetry at the nanometre scale — Richard Beanland[1], Paul J Thomas[2], David I Woodward[1], Pam A Thomas[1], and •Rudolf A Römer[1,3] — [1]Department of Physics, The University of Warwick, Coventry CV4 7AL, UK — [2]Gatan UK Ltd, 25 Nuffield Way, Abingdon, Oxon, OX14 1RL, UK — [3]Centre for Scientific Computing, The University of Warwick, Coventry CV4 7AL, UK

The functional properties of materials are normally determined by their symmetry. This is equally true on the nano-scale as it is at the macro-scale. Whilst for bulk material the structure and symmetry can routinely be solved by X-ray diffraction, there is no comparable technique for nanostructured materials. Electron diffraction has the required nano-scale resolution and sensitivity, but overlapping data from different diffracted beams has limited its use to date. Here, we demonstrate that computer control of beam tilt and image capture in a conventional transmission electron microscope can be used to overcome this problem, quickly providing very rich diffraction datasets. The technique requires no new hardware, no more expertise than conventional electron diffraction and takes less than two minutes to acquire and process a complete data set. We apply the new technique to the question of a centrosymmetry phase of VO2 and show large differences between theory and experiment for every oxide so far examined.

KR 5.3 Wed 15:00 Poster B2

Structure, mechanical, and tribological properties of C:Ni nanocomposite films grown by IBAD — •S. Gemming[1,2], M. Krause[1,3], T. Kunze[1,3], A. Mücklich[1], M. Fritzsche[1], R. Wenisch[1], M. Posselt[1], A. Schneider[1], and G. Abrasonis[1] — [1]HZ Dresden-Rossendorf, D-01314 Dresden — [2]TU Chemnitz, D-09107 Chemnitz — [3]TU Dresden, D-01062 Dresden

The mechanical and tribological properties of nanostructured carbon:nickel films on silicon substrates are investigated by a multi-scale experimental and theoretical approach. The C:Ni nanostructures comprising either tilted columns or three-dimensionally self-organized nanopatterns are grown by ion-beam assisted deposition (IBAD). Complex layer architectures were obtained by sequential deposition by rotating the substrate in relation to the assisting ion beam after each deposition step. Atomic composition of the films was determined by ion beam analysis. The phase structure of carbon was analyzed by Raman spectroscopy, that of nickel by X-ray diffraction. The microstructure of the films was determined by high resolution transmission electron microscopy. The films show good adhesion as probed by scratch tests. The film hardness is about 20 GPa, and the elastic modulus 200 GPa. Friction coefficients on the order of 0.1 are found for oscillating wear conditions under ambient conditions. Atomistic computer simulations assist the experimental findings for dry and liquid contacts. The simulation shows a complex behaviour for the carbon-carbon interaction, e.g. resulting in the formation of a tribo-layer. Support by the ECEMP excellence cluster is acknowledged.

KR 5.4 Wed 15:00 Poster B2

Modelling the growth of ZnO nanocombs synthesized by vapor-liquid-solid method — •Farzaneh Fattahi Comjani[1], Ulrike Willer[2], Stefan Kontermann[1], and Wolfgang Schade[1,2] — [1]Fraunhofer Heinrich Hertz Institute, Am Stollen 19B, Goslar, Germany — [2]Institute of Energy Research and Physical Technologies, Clausthal University of Technology, Am Stollen 19B, Goslar, Germany

Generally, ZnO nanocombs are synthesized by the carbothermal reduction process between graphite and ZnO powder. Mechanisms for the growth of ZnO nanocombs have been proposed, which relate the formation of nanocombs with a self catalytic effect related to the Zn cluster at the defective site on the polar +(0001) surface of the ZnO nanobelt or the enrichment of Zn at the growth front +(0001). However, these mechanisms cannot explain why the ZnO nanowires grow equally spaced on the polar +(0001) surface of the backbone nanobelt. This work reports on the synthesis of ZnO nanocombs by the vapor-liquid-solid (VLS) method. For this, we use the molar ratio ZnO:C (2:3) instead of the standard molar ratio (1:1). Additional emphasis is laid on the development of a model for the growth of nanocombs based on the piezoelectric character of ZnO. Applying the perturbation and elasticity theory and using the Fourier expansion, the induced mechanical strain and piezoelectric potential distribution in the backbone nanobelt are approximated. The coupling of the mechanical strain to the piezoelectric field across the nanobelt thickness explains the equidistant growth of nanowires on the polar +(0001) surface of the nanobelt as a consequence of a self catalytic growth process.

KR 5.5 Wed 15:00 Poster B2

BL 10 at DELTA, an interesting new beamline for crystallographers — •Anne Kathrin Hüsecken[1], Konstantin Istomin[1], Ralph Wagner[2], Stefan Balk[2], Dirk Lützenkirchen-Hecht[2], Ronald Frahm[2], and Ullrich Pietsch[1] — [1]Universität Siegen — [2]Bergische Universität Wuppertal

DELTA is a small synchrotron in Dortmund performing at 1.5 Gev and a maximum current of 130 mA. After the commissioning of the beamline BL 10 was finished in August 2012 it is now open for all users. The beamline is devoted to materials science research with the focus on X-ray diffraction and absorption spectroscopy measurements. Possible experiments are precise single crystal diffraction, charge density studies and also fatigue studies in metals, transmission and fluorescence EXAFS measurements and reflection mode EXAFS. The beamline is working at an energy range of 4.5 to 16 keV with an energy resolution of $dE/E \propto 1.6 \cdot 10^{-4}$. Depending on the aperture it is possible to measure with a beamsize between $3 \cdot 10\text{mm}^2$ and $0.5 \cdot 0.1\text{mm}^2$. The photon flux is with a focusing mirror expected to be $5 \cdot 10^9 \text{Photons/s mm}^2$. The user can decide between several detectors, a Pilatus 100K 2D, a Scintilation Counter, an Avalanche Photodiode or Ionization Chambers. First diffraction measurements with Quartz powder obtained with the 2D and point detectors show that high-quality powder diffraction measurements are possible at the beamline. And the diffraction of a BSO single crystal shows that the intensity is comparable to the now closed beamline D3 at Doris. So we close a gap for all users who do not get beamtime at big synchrotrons.

KR 5.6 Wed 15:00 Poster B2

Optical characterization of the protonation and deprotonation of pyroelectric single crystals — •Thomas Köhler, Erik Mehner, Juliane Hanzig, Hartmut Stöcker, and Dirk C. Meyer — Institut für Experimentelle Physik, Technische Universität Bergakademie Freiberg, D-09596 Freiberg, Germany

Pyroelectric crystals are used in many optical devices, therefore, understanding of structural defects is essential. It is easy to incorporate hydrogen in air-grown $LiNbO_3$ and $LiTaO_3$, however, the exact processes are only partially understood. Hence, the incorporation of hydrogen in both materials was investigated via FT-IR and UV/VIS absorption spectroscopy. Specifically the hydrogen in the congruent crystals leads to OH absorption bands with two components at $3468\,\text{cm}^{-1}$, $3485\,\text{cm}^{-1}$ in $LiNbO_3$ and at $3463\,\text{cm}^{-1}$, $3481\,\text{cm}^{-1}$ in $LiTaO_3$, respectively.

It is observed that the OH bands decrease in reduced and increase in protonated and reprotonated crystals. A third component at about $3500\,\text{cm}^{-1}$ is discernible in the protonated $LiNbO_3$. Reduced crystals show no reprotonation – only in $LiNbO_3$ crystals deprotonated above 900 °C the return of the OH band was observed. Furthermore, the varying degree of reduction of the samples has influence on the absorption in the visible range. A broad band is observed in heavily reduced crystals, which is assigned to the formation of polarons [1]. The formation of polarons is different in the two material systems and shows influence on their optical behavior and their defect structure.

[1] A. Dhar, A. Mansingh. J. Appl. Phys. 1990, 68 (11), 5804-5809.

KR 6: Mitgliederversammlung FG KR

Time: Thursday 17:45–18:30 Location: H9

Mitgliederversammlung FG KR

KR 7: Resistive Switching (DS jointly with DF, KR, HL)

Time: Friday 9:30–12:45 Location: H32

KR 7.1 Fri 9:30 H32

***Ab initio* study of defects in $SrTiO_3$ bulk and (100) surfaces** — •Ali Al-Zubi, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut (PGI) & Institute for Advanced Simulation (IAS), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Oxygen vacancies are believed to play a major role in the conduction mechanisms that enable resistive switching in oxide materials. Employing density functional theory (DFT) and the DFT+U model,we use the full-potential linearized augmented plane wave method as implemented in the `FLEUR` code to study the formation of point defects in the perovskite $SrTiO_3$ with varying coordination. We calculated the formation energy of an O-vacancy in both bulk supercells and (100) surface including different, c(2×2) and p(2×2), in-plane unit cells and different terminations. After performing full relaxation, we found that the bulk and SrO-terminated surface have a nonmagnetic, while TiO_2-terminated surface has a ferromagnetic solution. Using the c(2×2) unit cell, the vacancy formation energy was smaller for the bulk than for the SrO- and even TiO_2-terminated surface. On the other hand, the p(2×2) unit cell shows that TiO_2-terminated surface has the lowest formation energy, more than 1 eV lower than the bulk value. Similar comparisons will be presented when including the the DFT+U model that is used to correct the bulk bandgap and improve the localization of the defect states.

We gratefully acknowledge financial support of the DFG, SFB 917 Nanoswitches–A4 project.

KR 7.2 Fri 9:45 H32

Resistive switching properties in ion beam modified $SrTiO_3$ — •Jura Rensberg, Benjamin Roessler, Christian Katzer, Frank Schmidl, and Carsten Ronning — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Germany

Resistive switching phenomena, which are for instance observed in perovskite-type transition metal oxides, attract intensive attention for their potential application in future nonvolatile memory. Strontium titanate ($SrTiO_3$) exhibits bipolar resistive switching between a high- and a low-resistance state when applying an appropriate electric field. It is often proposed that the underlying mechanism for bipolar resistive switching in $SrTiO_3$ originates from oxygen-vacancy migration along filaments based on extended defects such as dislocations or grain boundaries.

Here we report on well-defined damage formation due to ion irradiation which allows a better control of the lateral and vertical defect arrangements and concentrations. Therefore, we deposited 100 nm single crystalline $SrTiO_3$ thin films with low intrinsic defect concentration on niobium doped $SrTiO_3$ substrates by pulsed laser deposition and implanted these samples with swift heavy gold ions. After irradiation the films were characterized using transmission electron microscopy and Rutherford backscattering spectrometry. Under ion irradiation, the as-deposited crystalline films undergo amorphisation due to the formation and overlap of amorphous tracks. The electrical properties of $SrTiO_3$, i.e. the resistive switching properties are discussed in terms of damage concentration.

KR 7.3 Fri 10:00 H32

Cation defect engineering in SrTiO3 thin films by PLD with Verification and implication on memristive properties — Sebastian Wicklein[1], •Chencheng Xu[1], Alessia Sambri[2], Salvatore Amoruso[2], David Keeble[3], Annemarie Köhl[1], Werner Egger[4], and Regina Dittmann[1] — [1]Peter Grünberg Institut 7, Forschungszentrum Jülich GmbH, Germany — [2]Università degli Studi di Napoli Federico II, Dipartimento di Scienze Fisiche & CNR-SPIN, I-80126 Napoli, Italy — [3]University of Dundee, School of Engineering, Physics and Mathematics, Dundee DD1 4HN, Scotland — [4]University Bundeswehr, D-85577 Munich, Germany

The origin of the c-axis expansion in homoepitaxial STO thin films is investigated by positron annihilation lifetime spectroscopy (PALS): Low laser fluence results in Ti vacancy rich sample while high laser fluence for the Sr vacancy rich sample.

XPS measurement on the ablated spot on the targets shows that increased laser fluence ablates more Ti. The ToF (Time of Flight) data from OES (optical emission spectrometry) indicate a preferred scattering of Ti because of background gas. The two effects together lead to tunable stoichiometry of the film.

In the MIM (metal insulator metal) structure Sr-rich films exhibit the most stable switching behavior and highest on/off ratio, while in the LC AFM (local conducting atomic force microscopy) switching the on/off ratio of Ti is the higest.

KR 7.4 Fri 10:15 H32

Resistive Switching in thermally oxidized Titanium — •Daniel Blaschke[1], Ilona Skorupa[1], Bernd Scheumann[1], Andrea Scholz[1], Peter Zahn[1], Sibylle Gemming[1], Kay Potzger[1], Agnieszka Bogusz[2], and Heidemarie Schmidt[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, P.O. Box 510119, 01314 Dresden - Germany — [2]Dept. Electr. Eng. & Inf. Techn., TU Chemnitz, 09107 Chemnitz

In recent years the resistive switching of binary transition metal oxides like NiO, Nb2O5 and TiO2 has attracted considerable attention for application in nonvolatile memory storage systems.

For our investigations we used a thin rutile TiO2 film, which was prepared by the thermal oxidation of a 100nm thick e-beam evaporated Ti film. The oxidation temperatures were varied from 500°C to 800°C at an oxygen partial pressure of 1 atmosphere. We will present the dependence of the crystal structure and the switching behavior on the oxidation temperature as well as an interesting feature on the time-dependent evolution of the resistance during the Reset process.

The project is funded by the Initiative and Networking Fund of the Helmholtz Association (VH-VI-422).

KR 7.5 Fri 10:30 H32

Non-volatile resistive switching in multiferroic YMnO3 thin films — •Agnieszka Bogusz[1,2], Ilona Skorupa[1], Andrea Scholz[1], Oliver G. Schmidt[2,3], and Heidemarie Schmidt[2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Faculty of Electrical Engineering and Information technology, Chemnitz University of Technology, 09107 Chemnitz, Germany — [3]Institute for Integrative Nanosciences, IFW-Dresden, 01069 Dresden, Germany

Intensive research on multiferroic materials [1] is driven by the possibility of creating novel, miniaturized tunable multifunctional devices [2]. This work investigates resistive switching behavior of YMnO3 thin films, which can be utilized in new generation memory devices. Series of YMnO3 films were grown by pulsed laser deposition on Si substrates with Pt bottom electrode at temperatures varying between 500°C and 850°C. Characterization of as-grown samples by X-ray diffraction and scanning electron microscopy was followed by determination of electrical properties of films in metal-insulator-metal (MIM) configuration. Results showed that the YMnO3 films grown at 800°C exhibit the best resistive switching properties with high resistance ratio (>10000) of high over low resistance state. Switching mechanism is ascribed to the structural transitions within the film upon applied current.

[1] A. Bogusz et al., Defect Diffus. Forum 323-325, 115 (2012)

[2] Y. Shuai, H. Schmidt et al., J. Appl. Phys. 109, 124117 (2011); J. Appl. Phys. 111, 07D906 (2012)

KR 7.6 Fri 10:45 H32

Practical guide for validated memristance measurements — •Nan Du[1,2], Yao Shuai[3], Wenbo Luo[3], Christian Mayr[4], Rene Schüffny[4], Oliver G. Schmidt[1,2], and Heidemarie Schmidt[1] — [1]TU Chemnitz, Faculty of Electrical Engineering and Information Technology, 09107 Chemnitz, Germany — [2]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [3]Helmholtz Research Center Dresden-Rossendorf, 01328 Dresden, Germany — [4]TU Dresden, Department of Electrical Engineering and Information Technology, 01062 Dresden, Germany

L.O. Chua predicted rather simple charge-flux curves for active and passive memristors and presented active memristor circuit realizations already in the 70s. However, despite the fact that memristors give rise to complicated hysteretic current-voltage curves, memristors are traced in current-voltage curves. Here we give a practical guide how to use normalized charge-flux curves for the prediction of current-voltage characteristics of memristors with stable electrical characteristics in dependence on the shape and amplitude of the input voltage or input current signals. In the case of memristive BiFeO3 thin film capacitor

structures [1] the normalized charge-flux curves superimpose for different numbers of measurement points and a different measurement time per measurement point. Such normalized charge-flux curve can be used for the prediction of current-voltage characteristics of plastic synapses in neuromorphic systems [2]. [1] Y. Shuai et al., J. of Appl. Phys. 109, 124117-124117-4 (2011). [2] C. Mayr et al., NIPS 2012, in press.

Coffee break (15 min)

KR 7.7 Fri 11:15 H32

Creating an Oxygen Gradient in Nb_2O_5 by Argon Irradiation for Resistive Switching Memory — •Helge Wylezich[1], Hannes Mähne[1], Daniel Blaschke[2], Stefan Slesazeck[1], and Thomas Mikoljiack[1] — [1]NamLab gGmbH, Nöthnitzer Str. 64, D-01187 Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden

It is common knowledge that an oxygen gradient is mandatory for bipolar resistive switching [1]. We confirmed this by investigations of thin films with Nb_2O_5 as switching layer. Samples with two inert Pt electrodes are nearly symmetric and do not show bipolar resistive switching behavior. Replacing one Pt electrode with a reactive one – for example Al or Nb – results in an unsymmetrical device. These samples could be switched reproducible. It is also possible to create an oxygen gradient by depositing a stack of two different niobium oxide layers. While the first layer consists of stoichiometric Nb_2O_5 the second layer is sputtered substoichiometric [2].

A new approach is to get an oxygen gradient by irradiating the oxide layer with argon. Two effects appear: The argon sputters the surface of the Nb_2O_5 layer and so the oxide thickness decreases. Because the Nb-atoms are heavier than the O-atoms, the oxygen sputter rate is higher and the surface becomes niobium rich. The investigated samples consist of a Pt-Nb_2O_5-Pt stack. The oxide layer was irradiated by different Ar-doses before top electrode deposition. At the highest dose Φ = 3e16 cm^{-2} the resulting oxygen gradient enables resistive switching.

[1] Bertaud et al. (TSF 520, 2012)
[2] Mähne et al. (MEMCOM Workshop 2012)

KR 7.8 Fri 11:30 H32

Multilevel resistive switching in Ar+ irradiated BiFeO3 thin films — •Yao Shuai[1], Xin Ou[2], Wenbo Luo[2], Nan Du[3], Danilo Bürger[2,3], Oliver G. Schmidt[3,4], and Heidemarie Schmidt[3] — [1]State Key Laboratory of Electronic Thin Films and Integrated Devices, UESTC, China — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Germany — [3]University of Technology Chemnitz, Faculty of Electrical Engineering and Information Technology, 09107 Chemnitz, Germany — [4]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

Low energy Ar+ ion irradiation has been applied to an Au/BiFeO3/Pt capacitor structures before deposition of the Au top electrode. The irradiated thin films exhibit multilevel resistive switching without detrimental resistance degradation, which makes the intermediate resistance states more distinguishable as compared to the non-irradiated thin film [1]. The stabilization of resistance states after irradiation is discussed based on the analysis of conduction mechanism during the resistive switching in BiFeO3 with a rectifying Au top electrode and a nonrectifying Pt bottom electrode [2]. Furthermore, it is shown how the conduction mechanisms change from room temperature to 423 K. [1] Y. Shuai, X. Ou et al., IEEE Device Letters, 2012, in press. [2] Y. Shuai, S. Zhou, D. Bürger, M. Helm, H. Schmidt, J. Appl. Phys. 109 (2011), 124117-4.

KR 7.9 Fri 11:45 H32

Influence of thickness ratio on resistive switching in BiFeO3:Ti/BiFeO3 bilayer structures — •Tiangui You[1], Wenbo Luo[2], Yao Shuai[1,2], Nan Du[1], Danilo Bürger[1,3], Ilona Skorupa[3], Oliver G. Schmidt[1,4], and Heidemarie Schmidt[1] — [1]Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]University of Electronic Science and Technology of China, 610054 Chengdu, China — [3]Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany — [4]IFW-Dresden, 01069 Dresden, Germany

Nonvolatile resistive switching in BiFeO3 (BFO) [1] has attracted increasing attention; however, the underlying resistive switching mechanism is still controversial which restricts its application in nonvolatile memory devices. BFO:Ti/BFO bilayer structures with a 540 nm thick BFO layer and different thickness of BFO:Ti layer were grown on Pt/Sapphire substrates by pulsed laser deposition using the same growth conditions. Circular Au top electrodes were prepared with magnetron sputtering. Au/BFO/Pt single layer structures show a symmetric I-V curve without hysteresis due to the formation of Schottky contacts at both the top and bottom interface. However, Au/BFO/BFO:Ti/Pt bilayer structures exhibit an obvious resistive switching behavior under both voltage polarities. The influence of the thickness of BFO:Ti on the conduction mechanisms in Au/BFO/BFO:Ti/Pt bilayer structures is discussed to reveal similarities and differences between single and bilayer structures.

Reference [1] Y. Shuai et al., J. Appl. Phys., 109, 124117(2011)

KR 7.10 Fri 12:00 H32

Nanoscale resistive switching in epitaxial and polycrystalline BiFeO3 thin films — •Yao Shuai[1], Wenbo Luo[1], Chuangui Wu[1], Wanli Zhang[1], Oliver G. Schmidt[2,3], and Heidemarie Schmidt[2] — [1]State Key Laboratory of Electronic Thin Films and Integrated Devices, UESTC, China — [2]University of Technology Chemnitz, Faculty of Electrical Engineering and Information Technology, 09107 Chemnitz, Germany — [3]Institute for Integrative Nanosciences, IFW Dresden, 01069 Dresden, Germany

Nonvolatile [1], bipolar, and multilevel [2] resistive switching has been observed in ca. 500 nm thick polycrystalline BiFeO3 thin films with rectifying, circular Au top electrodes and a nonrectifying Pt bottom electrode. The diameter of the Au top electrodes amounts to ca. 0.5 mm. By scanning a positionable top contact with a diameter of only 10 nm over polycrystalline BiFeO3 thin films under a constant applied dc voltage, the high and low resistance state can be locally written and afterwards read. It has been observed that for thinner polycrystalline BiFeO3 films with a thickness below 300 nm, no resistive switching can be observed either with large or with small scale top contacts. Bipolar resistive switching can also be realized in ca. 50 nm thick epitaxial BiFeO3 films on SrRuO3/SrTiO3 with a positionable top contact. This resistance is mainly determined by the ferroelectric polarization and the barrier height of the top and bottom contact. For thicker epitaxial BiFeO3 films the unique relation between ferroelectric polarization and resistance state is diminished. [1] Y. Shuai et al., J. Appl. Phys. 109 (2011). [2] Y. Shuai et al., IEEE Device Letters (2012) in press.

KR 7.11 Fri 12:15 H32

An electronic implementation of amoeba anticipation — •Mirko Hansen[1], Karlheinz Ochs[2], Martin Ziegler[1], and Hermann Kohlstedt[1] — [1]Faculty of Engineering, Christian-Albrechts-Universität zu Kiel, 24143 Kiel, Germany — [2]Ruhr-Universität Bochum, 44780 Bochum, Germany

In nature, the capability to memorize environmental changes can already be observed in unicellular organisms like amoebas[1]. An amoeba changes its locomotive speed when it is exposed to unfavorable conditions. If a series of unfavorable conditions is applied, the amoeba later on behaves similarly on a single incident. Pershin et al.[2] are able to emulate this behavior using a simple resistive switching circuit model consisting of an inductor, a capacitor and a resistive switching device. We experimentally implement this model using a resistive switching device. A theoretical analysis of the circuit is presented to gain further insight into the functionality of this model and to give advice for the implementation of resistive switching devices in LC-circuits.

[1] T. Saigusa, A. Tero, T. Nakagaki, Y. Kuramoto, Phys. Rev. Lett. **100**, (2008) 018101

[2] Y. V. Pershin, S. La Fontaine, M. Di Ventra, Phys. Rev. E **80**, (2009) 021926

KR 7.12 Fri 12:30 H32

Lattice dynamics in Sb- and Te-based phase-change materials — •Ronnie Ernst Simon[1,2], Ilya Sergueev[3], and Raphaël Pierre Hermann[1,2] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, Jara-FIT Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — [2]Faculté des Sciences, Univer- sité de Liège, B-4000 Liège, Belgium — [3]Deutsches Elektronen- Syn- chrotron, D-22607 Hamburg, Germany

Phase-change materials exhibit a significant change of the optical reflectivity and electrical resistivity upon crystallization which renders these materials applicable for optical storage devices and non-volatile electronic memories. In order to understand the switching kinetics between the amorphous and the metastable crystalline states a detailed

knowledge of the lattice dynamics of the different phases is crucial. A suitable technique for the investigation of lattice dynamics is nuclear inelastic scattering (NIS) which gives access to the element specific density of phonon states (DPS). We performed NIS measurements in Sb- and Te-based phase-change materials in the amorphous and crystalline phases. We have recently extended the experimental possibilities by demonstrating the feasibility of high pressure NIS measurements, up to 75 GPa, in Sb_2Te_3 . The ESRF is acknowledged for the provision of synchrotron radiation beamtime at ID18.