SYNF 1: Ferroic materials and novel functionalities I

Time: Tuesday 10:30–13:15 Location: A 151

SYNF 1.1 Tue 10:30 A 151

Characterization of ultra thin epitaxial $BaTiO_3$ films on Pt(111): A LEED, STM and XPS study — •Stefan Förster and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle

Ultra thin epitaxial $BaTiO_3$ films have been grown on a Pt(111) single crystal substrate by r.f. magnetron sputtering and characterized by LEED, STM and XPS. The $BaTiO_3$ films were deposited at room temperature under a pressure of about $2.5{\cdot}10^{-3}$ mbar of Argon (80 %) and Oxygen (20 %) gas mixture and subsequently annealed in UHV. The magnetron sputtered films exhibit a high reproducibility of film thickness and composition. XPS spectra of the films are in good agreement with spectra of a $BaTiO_3$(111) single crystal, indicating that the films grow with $BaTiO_3$ stoichiometry. The weakening of the XPS signal from the Pt substrate was used to estimate the film thickness in the range up to several nm. Annealing to temperatures above 900 K leads to highly ordered films which are stable up to 1250 K. Their LEED pattern show several different structures depending on the preparation conditions which includes the $(\sqrt{3} \times \sqrt{3})$ structure known from the $BaTiO_3$(111) single crystal surface. Atomically resolved STM images confirm the $\sqrt{3}$ structure. Additionally, they show the growth of extended flat islands with diameters up to 200 nm separated by steps of multiple unit cell heights. These $BaTiO_3$ films might be ideal playground for future investigations of multiferroic systems.

SYNF 1.2 Tue 10:45 A 151

Exchange bias coupling in La0.7Sr0.3MnO3/BiFeO3 heterostructures — •Mark Huijben, Ying-Hao Chu, Lane W. Martin, Jan Seidel, Nina Balke, Martin Gajek, Chan-Ho Yang, Pu Yu, Micky Holcomb, and Ramamoorthy Ramesh — Department of Physics & Department of Materials Science and Engineering, University of California, Berkeley, USA

Heterostructures based on perovskite transition-metal oxides have attracted much attention because of the possibility of tuning the magnetic and electronic properties of thin films through interface effects such as exchange interactions, charge transfer, and epitaxial strain. The development and understanding of multiferroic materials such as BiFeO3, have piqued the interest with the promise of coupling between order parameters such as ferroelectricity and antiferromagnetism. In this study we investigate the magnetic properties in ferromagnetic-antiferromagnetic multiferroic heterostructures by using atomic scale controlled growth through laser-MBE in combination with real-time RHEED monitoring. We will show the controlled coupling at the interfaces in La0.7Sr0.3MnO3/BiFeO3 heterostructures. This coupling behavior is investigated by structural measurements, such as x-ray reciprocal space mapping to clarify strained states, and magnetic measurements to gain a deeper fundamental understanding of the interactions at these interfaces. The interface coupling displays a strong enhancement in the coercivity of the La0.7Sr0.3MnO3 layer and a large shift in the magnetization hysteresis loops, indicating the existence of exchange bias coupling.

SYNF 1.3 Tue 11:00 A 151

electronic structure induced reconstruction and magnetic ordering at the LaAlO3/SrTiO3 interface — •zhingcheng zhong and paul kelly — Faculty of Science and Technology and MESA+ institute for Nanotechnology, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

The finding of a high mobility electron gas at the interface between two large band gap insulators LaAlO3 and SrTiO3 led to the observation of interface magnetic ordering and, more recently superconductivity. We study this interface using density functional theory (LDA and LDA+U), taking into account the possibility of interface structural relaxation, charge and spin ordering. We find that charge, orbital and magnetic ordering can occur in a quarter-filled band system. The lowest energy configuration is a charge-ordered antiferromagnetic insulator. At a slightly higher energy, we find a charge-ordered ferromagnetic insulator with a smaller band gap. We discuss various scenarios for explaining the experimental observations.

SYNF 1.4 Tue 11:15 A 151

Influence of polarization on the surface relaxation of perovskite ferroelectrics — •Michael Fechner, Ostanin Sergey, and Ingrid Mertig — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany

Ferroelectric materials exhibit a electric polarization which is spontaneous and switchable by an electric field. These materials become important due to their possible application in multiferroic materials. In our study we investigate clean (001) surfaces of FE perovskites from first principles. We consider three different systems which are $SrTiO_3$, BaTiO3, and PbTiO3. These compounds differ in their size of spontaneous polarization from zero ($SrTiO_3$) to moderate ($BaTiO_3$) to high values ($PbTiO_3$). Due to this we could investigate the surface relaxation and electronic properties with respect to the size and the direction of the spontaneous polarization. Latter is done by considering the cases of a polarization direction parallel and antiparallel to the surface normal. In our study it turns out that the direction of polarization at the surface is independently of the polarization in the lower lying layers and the considered material. The results of our study are in good agreement with recent experimental findings [1].

[1] Y. Urakami Ferroelectrics, 346 (2007)

SYNF 1.5 Tue 11:30 A 151

Dynamic strain in metallic vs insulating manganite films — •Martina Cornelia Dekker, Steffen Oswald, Ludwig Schultz, and Kathrin Doerr — IFW Dresden, Germany

The use of a ferro- and piezoelectric substrate, PMN-PT (001) $(PbMg_{1/3}Nb_{2/3}O_3)_{0.72}(PbTiO_3)_{0.28}$, allows us to biaxially compress as grown epitaxial films by as much as 0.2% [1]. This reversible dynamic strain process gives a unique insight into the effect of strain on perovskite oxides, eliminating effects such as varying oxygen concentration, which may occur when several substrates with different lattice mismatch are used.

We have prepared PLCMO $(Pr_{1-x}La_x)_{0.7}Ca_{0.3}MnO_3$ films on PMN-PT substrates for a range of x values. Around $x = 0.6$, the system exhibits a transition from an insulating to a metallic ground state. We have recorded changes in magnetic moment and transition temperature upon varying x, and compared the effects of dynamic strain on transport behaviour in the metallic and insulating ground states.

[1] C. Thiele et al., Phys. Rev. B 75, 054408 (2007)

SYNF 1.6 Tue 11:45 A 151

Strain-dependent magnetism and electric transport properties of $La_{0.7}Sr_{0.3}CoO_3$ films — •Andreas Herklotz, Diana Rata, Orkidia Bilani, Ludwig Schultz, and Kathrin Dörr — IFW-Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

The electronic and magnetic properties of some perovskite-type 3d transition metal oxides are known to be sensitive to epitaxial strain. In order to investigate the influence of strain in $La_{0.7}Sr_{0.3}CoO_3$ (LSCO) compound, epitaxial films under different biaxial strain have been grown using various substrates. Additionally, piezoelectric substrates of the composition $0.72PbMg_{1/3}Nb_{2/3}O_3$-$0.28PbTiO_3$ (PMN-28%PT) were employed to control the in-plane strain dynamically by applying an electrical field. An insulator-type behaviour was observed in films grown under tensile strain, whereas compressed films show bulk, metallic properties. This drastic influence of strain was confirmed by using the PMN-PT substrates, where a reversible strain of 0.15% caused a resistance change of one order of magnitude at room temperature. On the contrary, the magnetization data revealed a rather small impact of tensile strain on the magnetic behaviour of LSCO films. We suggest that the insulator state of $La_{0.7}Sr_{0.3}CoO_3$ is caused by a stain-induced static Jahn-Teller-type deformation of the CoO_6 units, which may be efficient as a localization mechanism.

SYNF 1.7 Tue 12:00 A 151

Separation of magnetic and dielectric domains in $BiFeO_3$ and $BiCrO_3$ thin films — •Denny Köhler[1], Ulrich Zerweck[1], Christian Loppacher[3], Stephan Gepräg[2], Sebastian Gönnenwein[2], Rudolf Gross[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden — [2]Walter-Meissner Institut, Bayrische Akademie der Wissenschaften, München — [3]Laboratoire de Matériaux et Microélectronique de Provence, Universités Paul Cézanne, Marseille

In our work we present low-temperature noncontact-AFM investigations (nc-AFM) in combination with Kelvin Probe Force Microscopy (KPFM) and Magnetic Force Microscopy (MFM) to investigate the magnetic and ferroelectric properties of $BiFeO_3$ and $BiCrO_3$ thin films on the nm length scale. Samples are prepared as described in [1]. Complementary to nc-AFM measurements, Piezoresponse Force Microscopy (PFM) was used to deduce the ferroelectric polarisation of the investigated thin films.

Our experiments show that the separation of magnetic and electrostatic forces is possible by simultaneously running KPFM and MFM, but delicate due to the fact that both interactions are of long range nature. We show the separation of ferroelectric and magnetic domains on both materials and monitored a magnetic phase transition on $BiCrO_3$.

[1] S. Geprägs et al., *Phil. Mag. Lett.* **87**: 141-147 (2007)

SYNF 1.8 Tue 12:15 A 151

Contrast Mechanism for the Detection of Ferroelectric Domains on all Faces of LiNbO3 using Piezoresponse Force Microscopy — Tobias Jungk, Akos Hoffmann, and •Elisabeth Soergel — Institute of Physics, University of Bonn, Wegelerstrasse 8, 53115 Bonn, Germany

We apply piezoresponse force microscopy (PFM) to reveal the domain structures on all faces of LiNbO3 single crystals. Therefore we investigated a two-dimensionally poled sample, all faces optically polished. On the z-face the PFM contrast is known to be caused by the piezoelectrically driven thickness change of the crystal. On the x- and y- faces, however, the contrast mechanism was found to be governed by a lateral movement of the surface underneath the tip. Depending on the relative orientation of the cantilever with respect to the crystallographic axes of the sample this results in a torsion or buckling movement of the cantilever. In order to support this explanation we mounted the sample on a high-precision rotation stage. The high stability of the set-up allows to rotate the sample during data acquisition. We could therefore precisely determine the angular dependency of the movement on the tip on the crystallographic axis. The experimental results are in good agreement with the theoretically expected values.

Acknowledgments: Financial support of the DFG research unit 557 and of the Deutsche Telekom AG is gratefully acknowledged.

SYNF 1.9 Tue 12:30 A 151

All-electron calculations of electronic tunneling in perovskite magnetic tunnel junctions — •Daniel Wortmann and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

Combining materials with different ferroic orders into a single multilayer transport junction offers the prospect of novel devices like 4-bit memory cells or switching schemes based on the coupling between the different ferroic configurations. However, the materials used in such junctions often exhibit extremely complex interrelations between details of their atomic, electronic and magnetic structure making the simulation of such multilayer junctions on an *ab initio* level a necessity for any realistic setup but a true challenge at the same time. We will present calculations using our all-electron, full-potential transport code [1] based on the embedding Green function method. For the model setup of a $SrRuO_3/SrTiO_3/SrRuO_3$ tunneljunction we calculate the spin-polarized electronic tunnel-current and investigate the effects of lattice distortions on the orbital character of the current carrying Bloch states in $SrRuO_3$ and the resulting changes on the spin-polarization of the current.

[1] D. Wortmann, H. Ishida, and S. Blügel, Phys. Rev. B **66**, 075113 (2002).

SYNF 1.10 Tue 12:45 A 151

Ferroelectric Tunnel Junctions — •Hermann Kohlstedt[1], Nicholay Pertsev[2], Adrian Petraru[1], Ulrich Poppe[1], and Rainer Waser[1] — [1]Institut für Festkörperforschung and CNI, Forschungszentrum Jülich, Jülich, Germany — [2]A. F. Ioffe Physico-Technical Institute, St. Petersburg, Russia

Quantum mechanical electron tunneling through nanoscale ferroelectric barriers is discussed for symmetric (identical electrodes) and asymmetric (dissimilar electrodes) junctions. It is shown that the lattice strains of piezoelectric origin modify the I-V relationship owing to strain-induced changes of the barrier thickness, electron effective mass, and position of the conduction-band edge. The effect of internal electric field caused by incomplete screening of polarization charges at the surfaces of a ferroelectric barrier is analyzed. For asymmetric junctions, this depolarizing-field effect also leads to a considerable change of the barrier resistance after the polarization reversal. The crossover between two types of hysteretic behavior is described taking into account both the strain and depolarizing-field effects. The results already obtained for these new types of tunnel junctions and the theoretical and experimental challenges existing in this area will be discussed. Experiments on the scaling properties of ultra-thin wedged BaTiO3 films will be presented. At the end we will provide an overview for the current status of the international studies of the so-called multiferroic tunnel junctions. By combing ferroelectric or multiferroic tunnel barriers with ferromagnetic and/or superconducting electrodes, a whole *zoo* of novel tunnel junctions can be proposed.

SYNF 1.11 Tue 13:00 A 151

Resistive memory switching in perovskite-derivative single crystals — •P. Müller[1], F. Chowdhury[1], V. Dremov[1], Y. Koval[1], F. Lichtenberg[2], S. Müller[3], D. Schmeisser[3], and R. Pentcheva[4] — [1]Institut für Physik der Kondensierten Materie, Universität Erlangen-Nürnberg — [2]Experimentalphysik VI, Universität Augsburg — [3]Lehrstuhl Angewandte Physik-Sensorik, BTU Cottbus — [4]Department of Earth and Environmental Sciences, LMU München

We investigated several layered perovskite derivatives of the family $A_nB_nO_{3n+2}$, such as $LaTiO_{3.41}$, $CaNbO_{3.41}$ and $SrNbO_{3.41}$, which can be considered as a stacking of blocks consisting of 5 perovskite layers. Electric transport across these layers takes place via intrinsic tunnelling. Mesa devices with a cross-sectional area of 50 to 200 μm^2 and a height between 30 and 500 nm were fabricated by electron-beam lithography and ion-beam etching. Both dc I-V characteristics and pulsed current injection have shown switching between different resistive states in these materials. The resistive states have long-term stability, which makes them interesting for memory applications. The transport experiments suggest that switching and resistive memory are controlled by trapping and release of charge carriers. Furthermore, photoelectron and NEXAFS spectroscopy of cleaved $LaTiO_{3.41}$ surfaces have been performed. The results are compared to recent correlated band theory (LDA+U) calculations.