O 79: Oxide Surfaces III

Time: Thursday 16:00–18:30 Location: H45

O 79.1 Thu 16:00 H45

Identification of the surface phonons of $BaTiO_3$(100) and ultrathin films of $BaTiO_3$ on metal substrates — •Florian Schumann[1], Klaus Meinel[1], Andreas Trützschler[1], Konrad Gillmeister[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle

Phonons and their softening are key elements for the understanding of the long range coupling in ferroelectric and multiferroic materials which causes, e.g., the paraelectric to ferroelectric phase transition. In thin films these ferroelectric properties are often controlled by strain from the underlying substrate or heterostructure. Here we study the surface phonons of a $BaTiO_3$(100) single-crystal and of $BaTiO_3$(100) thin films grown by MBE and magnetron sputtering on Pt(100) and Au(100). HREELS spectra for all cases are dominated by three well-developed phonon peaks at about 220, 460, and 650 cm^{-1}. The latter two are identified as A(TO) surface modes. For thin films on Pt(100) and on Au(100) shifts of the surface phonons are observed due to misfit strain of +2% and -2%, respectively, as compared to the single crystal. Changes of the vibrational properties due to film thickness and temperature will be discussed.

O 79.2 Thu 16:15 H45

In-situ PFM characterization of ferroelectric domain properties of epitaxially $BaTiO_3$(100) ultrathin films on Pt(100) — •Andreas Trützschler[1], Maik Christl[1], Stefan Förster[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle

The combination of ferroelectric and ferromagnetic oxides in heterostructures can lead to new multiferroic materials. For this concept the surface and interface properties are crucial and might deviate from bulk properties [1]. So far nearly all ferroelectric characterizations for thin films of the ferroelectric $BaTiO_3$ have been carried out ex-situ under ambient conditions [2]. In contrast, we present here an in-situ PFM characterization of UHV-prepared $BaTiO_3$(100) thin films which have been grown on Pt(100). Due to the lattice mismatch the film is compressed by 2 % which causes a c-domain configuration [3]. The resulting domain pattern has been locally controlled by applying a DC voltage via the AFM tip. For ultrathin films the ferroelectric properties, especially the local hysteresis curve, indicate an inequivalence of outward and inward polarized c domains.

[1] A. Höfer et al., PRL 108, 087602 (2012).
[2] A. Gruverman et al., Nano Letters 9, 3539 (2009).
[3] S. Förster et al., JCP 135, 104701 (2011).

O 79.3 Thu 16:30 H45

Stress measurements during growth of $BaTiO_3$ and $SrTiO_3$ films on Pt(001) — •Jörg Premper, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

The measurement of film stress by the cantilever deflection technique is well established to study the correlation between stress and physical properties with monolayer sensitivity for metal-on-metal epitaxy [1]. The epitaxy of functional oxides such as $BaTiO_3$ (BTO) and $SrTiO_3$ (STO) requires experimental conditions, which deviate sharply [2] from that of metal epitaxy. A high substrate temperature (700°C) and a substantial oxygen partial pressure (1×10^{-4} mbar) during film growth by pulsed laser deposition (PLD) are necessary for good epitaxial growth, but challenging for stress measurements in view of thermal drift and oxidation of the sample holder. An experimental setup is described, which allows quantitive stress measurements under these conditions. We present the first stress measurements during PLD of epitaxial BTO and STO monolayers on Pt(001). We find that the deposition of 20 ML BTO on Pt(001) (misfit = -1.9%) leads to a compressive film stress of -4.2 GPa, whereas the deposition of STO (misfit = +0.4%) induces a tensile stress of +1.2 GPa. The measured film stress is for both systems in good agreement with calculated misfit-induced stress.

[1] J. Premper, D. Sander, and J. Kirschner, Rev. Sci. Instr. **83**, 073904 (2012)
[2] J. Schwarzkopf, R. Fornari, Prog. Cryst. Growth Charact. **52**, 159-212 (2006)

O 79.4 Thu 16:45 H45

Density functional theory study of the $SrTiO_3$+TiO_x (110) surface — •Marcel Hieckel[1], Florian Mittendorfer[1], Josef Redinger[1], Raimund Podloucky[2], Michael Weinert[3], and Laurence Marks[4] — [1]Institute of Applied Physics, Vienna University of Technology, Austria — [2]Institute for Physical Chemistry, University of Vienna, Austria — [3]Department of Physics, University of Wisconsin - Milwaukee, USA — [4]Department of Materials Science and Engineering, Northwestern University, USA

Surfaces of oxide perovskites are of interest because of their intriguing physical properties. In partiuclar, growing transition metal oxid layers is of interest to design new catalysists.

We present results of density functional theory (DFT) calculations for the adsorption of TiO_x layers on $SrTiO_3$ (110) which were performed by VASP. For the exchange-correlation functional the generalized gradient approximation of Perdew-Burke-Ernzerhof [1] was used.

The thermodynamically stable surface structures for varying TiO_x compositions were studied to determine the phase diagram as a function of the TiO_x concentration by making use of the chemical potentials of oxygen and titanium. Scanning tunneling microscopy (STM) images are simulated within the Tersoff-Hamann approximation [2] which are compared to very recent low temperature STM experiments. Work supported by the Austrian FWF, project Nr. F4511-N16.

[1] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865(1966). [2] J. Tersoff and D. R. Hamann, Phys. Rev. B 31, 805 (1985).

O 79.5 Thu 17:00 H45

Post deposition annealing of ceria *films on Si(111) — •Henrik Wilkens[1], Robert Oelke[1], Olga Schuckmann[1], Reinhard Olbrich[1], Marvin H. Zoellner[2], Thomas Schroeder[2], Michael Reichling[1], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — [2]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

A 250 nm cub-CeO_2(111) film grown on hex-Pr_2O_3/Si(111) is annealed under UHV conditions. Atomic force microscopy (AFM) and spot profile low energy electron diffraction (SPA-LEED) were used to resolve the surface morphology. The chemical composition was studied by photoelectron spectroscopy (XPS). In addition, the changes of the bulk structure were probed by in-situ x-ray diffraction (XRD) measurements.

The surface exhibit triangular shaped facets as shown by AFM which vanish at higher temperatures. Moreover, several superstructures appear in the LEED pattern due to ordered oxygen vacancy formation. Also the XPS data shows that the surface reduces continuously at higher annealing temperatures.

The XRD measurements reveal that not the whole film is reduced since a diffraction signal of cub-CeO_2(111) is still visible at elevated temperatures. Furthermore, it is shown that above a critical temperature the hex-Pr(0001) buffer layer is destroyed and silicon diffuses into the ceria film.

O 79.6 Thu 17:15 H45

Characterization of thin cerium oxide films on Cl/Si(111) studied by GIXRD and XPS — •Jan Höcker[1], Björn Kaemena[1], Florian Bertram[2], Jan Ingo Flege[1], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen — [2]Hamburger Synchrotronstrahlungslabor am Deutschen Elektronensynchrotron, 22607 Hamburg

Cerium oxide is of strong interest in today's research because of its catalytic properties as well as its potential application in microelectronics, e.g., as an epitaxial high-k gate oxide on Si. As known from previous studies of ultrathin cerium oxide films on Si(111) (cf. Flege et al., PRB **84**, 2011), Cl-passivation facilitates epitaxial growth of the sesquioxide Ce_2O_3 phase and suppresses amorphous interface formation.

We have investigated the structural and chemical composition of 3 - 18 nm thin cerium oxide films grown by reactive MBE on either clean or Cl-passivated Si(111) by ex-situ grazing-incidence x-ray diffraction (GIXRD) and x-ray photoelectron spectroscopy (XPS). Only for Cl-passivated substrates reciprocal space mapping reveals well

ordered oxide films. Capped samples show a dioxide fluorite (Ce^{4+}) as well as a sesquioxide bixbyite (Ce^{3+}) phase in contrast to uncapped samples, which only show a dioxide phase. XPS confirms a larger Ce^{4+} proportion for passivated substrates after exposure to ambient conditions whereas a mixture of Ce^{3+} and Ce^{4+} in the non-passivated case is observable. We conclude that only on passivated Si(111) a metastable Ce_2O_3 film crystallizes, which is converted into a well ordered dioxide phase under ambient conditions.

O 79.7 Thu 17:30 H45

Preparation and characterization of electrochemically deposited cerium oxide films — •Marc Sauerbrey[1], Jan Ingo Flege[1], Robert Rettew[2], Faisal Alamgir[2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen, Germany — [2]School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332, USA

Cerium oxide has been under intensive investigation over the last decades due to its interesting structural (oxygen storage capacity) and electronic properties (unfilled 4f shell). These properties result in a pronounced chemical reactivity as well as an enhancing effect on the reactivity of catalytically active metals like Pt, Au, and Rh.
In contrast to ultrahigh-vacuum methods, electrochemical preparation approaches are scalable, less complex and less expensive and thus are a promising alternative for industrial production purposes. In this contribution we present our results on the electrochemical growth and modification of cerium oxide films on Au and high-surface-area carbon substrates. A combined XPS (X-ray photoelectron spectroscopy) and SEM (scanning electron microscopy) analysis of as-prepared films shows predominantly fully oxidized cerium oxide with a rough morphology. Based on the analysis of Ce3d and O1s XPS data, annealing in oxygen atmosphere converts cerium oxide in predominantly CeO_2 (ceria). Furthermore, the influence of the ceria support on the oxidation state of post-deposited Pt will be discussed. First results indicate a ceria-promoted platinum oxidation, leading to the formation of PtO_2 particles.

O 79.8 Thu 17:45 H45

Probing Surface and Bulk Phonons in Nickel Oxide — •Srijan Kumar Saha[1], Oleg Brovko[1], Sebastian Polzin[2], Krassimir Kostov[2], Florian Schumann[2], Wolf Widdra[2], and Valeri Stepanyuk[1] — [1]Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle/Saale, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik FG Oberflächen- und Grenzflächenphysik, Von-Danckelmann-Platz 3, 06120 Halle/Saale

Using first-principles density-functional theory, we determine the vibrational properties of bulk NiO and its N-layer films; and compare our results with experiments performed by high-resolution electron energy loss spectroscopy (HREELS) on NiO(100) films on Ag(100). Because of the strong Coulomb interaction between the 3d electrons on the transition-metal ion, here we apply the DFT+U approach for this oxide, known as a model system of Mott or charge-transfer insulators. We find that the highest frequency surface optical phonon mode is highly dispersive and exhibits a huge blueshift as a function of number of layers in the film. The underlying physics of our main results will be discussed together with the pictorial representation of the phonon modes.

O 79.9 Thu 18:00 H45

Is the $BaTiO_3$ (001)-(2x1) reconstruction magnetic ? — •Holger. L. Meyerheim[1], A. Ernst[1], K. Mohseni[1], I.V. Maznichenko[2], S. Ostanin[1], F. Klimenta[1], N. Jedrecy[3], W. Feng[1], I. Mertig[2], R. Felici[4], and J. Kirschner[1] — [1]Max-Planck-Institut f. Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Institut f. Physik, Martin-Luther-Univ. Halle-Wittenberg, D-06099 Halle, Germany — [3]Institut des Nano Sciences de Paris, UPMC-Sorbonne Univ., CNRS-UMR7588, 75005 Paris, France — [4]ESRF, B. P. 220, F-38043 Grenoble Cedex, France

Though $BaTiO_3$ is the prototype perovskite type ferroelectric and its (2x1) reconstruction has been observed more than 30 years ago [1] no detailed analysis of its atomic geometry has been reported so far. We have carried out a surface x-ray diffraction analysis of the BTO(001)-(2×1) reconstructed surface [2]. While the crystal is terminated by two TiO_2 layers similarly to $SrTiO_3$(001)-(2×1) [3], we find that one Ti-atom of the top TiO_2 layer resides in a tetragonal pyramidal oxygen environment. Ab initio calculations based on this structure model suggest that the surface is metallic and magnetic involving local magnetic moments up to $2\mu_B$ in magnitude located at surface Ti and O atoms.

References: [1] R. Courths, Phys. Status Solidi B 100, 135 (1980) [2] H. L. Meyerheim, A. Ernst, K. Mohseni, I. V. Maznichenko, S. Ostanin, F. Klimenta, N. Jedrecy, W. Feng, I. Mertig, R. Felici,, and J. Kirchner, Phys. Rev. Lett. 108, 215502 (2012) [3] N. Erdman, K.R. Poeppelmeier, M. Asta et al., Nature 419, 55 (2002)

O 79.10 Thu 18:15 H45

An Atomic-Force-Microscopy study of Cu_2N on Cu(100) — •Maximilian Schneiderbauer, Matthias Emmrich, and Franz J. Giessibl — Regensburg University, Department of Physics, Regensburg, Germany

Recently Loth et al. [1] showed a new approach to push the spatial size of stored bits to the atomic scale. They tailored a switchable antiferromagnetic nanostructure made of a (2x6) Fe atom array exhibiting large magnetic anisotropy. To magnetically decouple this stand-alone spin structure from the conducting Cu substrate they used Cu_2N.

Thorough Scanning-Tunneling-Microscopy (STM) studies revealed the incommensurability of Cu_2N monolayer islands on Cu(100) [2, 3]. Although Cu_2N was as of yet just used in (spin polarized) STM experiments it is a promising candidate for magnetic sensitive Atomic-Force-Microscopy measurements. We have shown the qPlus setup capable of imaging magnetic domains [4] and, more recently, of detecting spin contrast [5]. Therefore we are currently studying Cu_2N on Cu(100) for future work on magnetic exchange force microscopy. In this contribution we show recent results from our home-built low-temperature qPlus setup.

[1] S. Loth et al Science 335, 196-199 (2012).
[2] F.M. Leibsle et al Surf. Sci. 317, 309-320 (1994).
[3] T. Choi et al Phys. Rev. B 78, 035430 (2008).
[4] M. Schneiderbauer et al Beilstein J. Nanotechnol. 3, 174-178 (2012).
[5] F. Pielmeier et al submitted.