O 25: Oxide and Insulator Surfaces: Structure and Growth

Time: Monday 18:15–20:30 Location: Poster E

O 25.1 Mon 18:15 Poster E

Oxidation of epitaxial iron films on Ag(001) — •Jari Rodewald, Daniel Bruns, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

Ferrimagnetic magnetite Fe_3O_4 with inverse spinel structure is a promising candidate for magnetic devices like giant magneto resistance (GMR) and tunneling magneto resistance (TMR). In order to develop these devices and to select certain iron oxide phases it is important to understand the structure and growth properties of such oxide films.
Hence, this work investigates the oxidation process of crystalline iron films with respect to different annealing temperatures and oxygen pressures. Therefore, pure bcc-iron is deposited on Ag(001) substrates by molecular beam epitaxy (MBE) and the oxidation process is divided into three consecutive steps of pre-annealing, UHV-annealing and post-annealing.
Surface structure and morphology are analyzed by spot profile analysis low energy electron diffraction (SPA-LEED), while the chemical composition of the surface is investigated by Auger electron spectroscopy (AES). Additionally, grazing incidence x-ray diffraction (GIXRD) measurements are performed in order to obtain information on the bulk structure of the deposited films.
The largest amount of magnetite is generated by post-annealing at 400°C and an oxygen pressure of $1 \cdot 10^{-5}$ mbar, while higher temperatures reduce the amount of oxygen and induce a structural change at the surface.

O 25.2 Mon 18:15 Poster E

Oxygen-induced phase switch of sub-monolayer iron oxide on Ir(100) — •Christopher Sobel, Pascal Ferstl, Lutz Hammer, and M.Alexander Schneider — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

By means of STM and LEED we show that two different sub-monolayer iron oxide phases exist on the Ir(100) surface which can be converted into each other by changing the chemical potential of oxygen. In oxygen poor conditions a 3×1-phase of one-dimensional FeO_2 wires forms which covers the whole surface homogeneously. In contrast oxygen rich conditions lead to a condensation into compact islands of quasi-hexagonal FeO(111) with an incommensurate "c(8.8×2)"-structure. The remaining iridium surface is covered by a pure oxygen 2×1-O phase [1]. The energy gain when forming the latter appears to be the driving force for the switch between the extended 3×1 and the compact island iron oxide phase. The behaviour differs qualitatively from other transition metals as for example cobalt, where in oxygen rich conditions the wires change from CoO_2 to CoO_3 stoichiometry. This fact indicates a delicate energy balance between the different phases.

[1] K. Johnson *et al.*, J. Chem. Phys. **112**, 10460 (2000)

O 25.3 Mon 18:15 Poster E

***Ab initio* Raman-spectroscopic study on Ce-Zr-Oxides** — •Marcel Giar, Michael Bachmann, Limei Chen, Peter J. Klar, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-University, D-35392 Giessen, Germany

Mixed Zr-Ce-oxides may serve as oxygen-storing co-catalysts in automotive applications or as catalytically active species in oxidation reactions. Amongst these, κ-$Ce_2Zr_2O_8$ is particularly known for its excellent oxygen storage capacity (OSC). This phase may be obtained from the so-called pyrochlore phase *pyr*-$Ce_2Zr_2O_7$ by incorporating oxygen, thereby oxidizing Ce^{3+} to Ce^{4+}. The underlying structural transition form the pyrochlore to the κ-phase is the key to understanding the superb OSC. Being very sensitive to structural differences, Raman spectroscopy is a well-suited method for investigating differences between crystal phases on a structural, electronic and vibrational level. Hence, in order to understand structural as well as electronic differences of both phases we calculate Raman susceptibilities and derived spectra based on DFT calculations. With our theoretical results we aim to interpret experimental Raman spectra.

O 25.4 Mon 18:15 Poster E

Complex dielectric function of $SrTiO_3$ and $BaTiO_3$ by HREELS — •Florian Schumann[1], Klaus Meinel[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 phase transitions in ferroelectrics and multiferroics. In thin films, the phonons depend sensitively as well as the phase transition temperatures on the strain within the film. Here we report on high-resolution electron energy loss spectroscopy (HREELS) on the (001) and (111) surfaces of $BaTiO_3$ and $SrTiO_3$. HREELS reveals three dipole-active phonon polaritons, which are derived from the known transversal optical bulk phonons. In addition, it will be demonstrated that the complex dielectric function in the energy range from 4 to 1000 meV can be quantitatively extracted from the experimental loss function. This opens up the additional characterization of oxide doping levels as will be discussed for single crystal surfaces and thin films down to one unit cell thickness.

O 25.5 Mon 18:15 Poster E

Structural and magneto-optic properties of epitaxial iron films on MgO(001) — •Jannis Thien[1], Olga Kuschel[1], Timo Oberbiermann[2], Timo Kuschel[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — [2]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany

For years it is known that the linear magneto-optic Kerr effect depends on the wavelength of the applied laser. The currently outstanding question is a wavelength dependence for the quadratic magneto-optic Kerr effect as proposed by theoretical calculations for cubic crystals [1].
In order to compare the theoretical predictions with experiment, crystalline samples are needed. Thus, epitaxial iron films were grown by molecular beam epitaxy on MgO(001) at different temperatures. Each sample was capped with an amorphous silicon film at room temperature to prevent oxidation of the iron film. For the purpose of examining the purity of the evaporated iron, XPS measurements were made. The structural characterization was realised by LEED, XRR, AFM and XRD measurements. The magnetic properties were probed by MOKE experiments.
Both chemical composition and structural as well as magnetic properties of the iron film change with increasing deposition temperature. From these results the sample with the most promising characteristics was choosen for the study of wavelength dependence of the quadratic magneto-optic Kerr effect.

[1] Hamrlová et al., submitted

O 25.6 Mon 18:15 Poster E

A first step of twin polymerization to study: The self-assembly of the twin monomer Spiro at the LSI influenced by sonication and deposition substrate temperature. — •Yen D.C Nguyen[1], Ha N.T Nguyen[1], Michael Hietshold[1], Thomas Ebert[2], and Stefan Spange[2] — [1]TU-Chemnitz, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany — [2]Polymer Chemistry Group, Institute of Chemistry, TU-Chemnitz

The twin monomer 2,2*-spirobi [4H-1,3,2-benzo-dioxasiline] (SBS) consisting of building blocks bonded together covalently has been used to produce organic*inorganic nanostructured hybrid materials. The polymerization is initiated by ring opening of the 4H-1,3,2- benzodioxasilines or cleavage of the Si-O-C bonds. This way generates two structurally different homopolymers (silicon dioxide and a phenolic resin). Self-assembly of this twin monomer (SBS) at undecanol/HOPG interface investigated by STM at the liquid-solid interface (LSI) influenced by sonication and deposition substrate temperature. Firstly, by sonicating SBS/undecanol solution samples in different time periods the polymerization of spiro monomer at undecanol/HOPG has been observed without any catalyst. Secondly, the polymerization of spiro monomer can also be controlled by the substrate temperature during the deposition of the molecules out of the solution. By increasing the temperature of the pre-heated substrate, various periodic assemblies of spiro (dimer, trimer or pentamer resin) can be obtained.