O 26: Oxides and insulators: Clean surfaces

Time: Tuesday 10:30–12:45 Location: H40

O 26.1 Tue 10:30 H40

Improved atomic scale contrast via bimodal dynamic force microscopy — Shigeki Kawai, Thilo Glatzel, •Sascha Koch, Bartosz Such, Alexis Baratoff, and Ernst Meyer — Department of Physics, University of Basel, Klingelbergstr. 82, CH-4056 Basel, Switzerland

We implemented a multi-frequency technique into atomically resolved frequency-modulation dynamic force microscopy for a further improvement of force sensitivity in ultra-high vacuum [1]. The first and second flexural resonance modes of a commercially available Si cantilever are simultaneously excited by controlled amplitudes, while the resonance frequency shifts (Δf_1st and Δf_2nd) are demodulated by two phase-locked loop circuits (Nanonis: Dual-OC4). The combination of sub-angstrom amplitude oscillation A_2nd at the second resonance with the commonly used large amplitude oscillation A_1st at the first resonance enables a high force sensitivity at Δf_2nd while avoiding atomic jump-to-contact instabilities caused by controlling the tip sample distance with Δf_1st [2-4].

Simultaneously in quasi-constant height mode recorded Δf_1st and Δf_2nd maps of KBr(001) show that the Δf_2nd signal has a higher tip-sample distance dependence. With A_1st=16 nm and A_2nd=50 pm at different tip-sample distances in the attractive region the signal-to-noise of Df2nd was higher than that of Δf_1st especially at close tip-sample distances. This high-sensitive detection of the short-range interaction clearly revealed tip/sample deformations.

O 26.2 Tue 10:45 H40

The valence band structure of $\beta - Ga_2O_3$ single crystals — •Mansour Mohamed[1], Christoph Janowitz[1], Zbigniew Galazka[2], Reinhard Uecker[2], Roberto Fornari[2], and Recardo Manzke[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

The valence band structure of the (100) surface of high-quality $\beta - Ga_2O_3$ single crystals grown by the Czochralski method has been investigated by angle-resolved photoelectron spectroscopy utilizing He I and synchrotron radiation along the symmetry directions of the surface Brillouin zone. The surface of $\beta - Ga_2O_3$ single crystal was characterized by different techniques (LEED, Laue, and STM). From the ultraviolet photoemission spectra measured along the parallel directions of the Brillouin zone, it is found that the valence bands along (k_b) and (k_c) do not show so much dispersion. On the other hand, the measurements performed with synchrotron radiation to probe the direction normal to the surface (k_a) indicate much stronger dispersion of the valence bands. The experimental valence band structure of $\beta - Ga_2O_3$ single crystals will be discussed and compared with theoretical results.

O 26.3 Tue 11:00 H40

Interaction potential for fast atoms in front of KCl(001) surface — •Uwe Specht[1], Marco Busch[1], Konrad Gärtner[2], and Helmut Winter[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, D-12489 Berlin, Germany — [2]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Max-Wien-Platz 1, D-07743 Jena, Germany

Fast He, Ne, Ar and N atoms with energies from 1 kev up to 60 keV are scattered under grazing angles of incidence ($\leq 2^\circ$) from a clean and flat KCl(001) surface. For scattering along low-index directions (axial surface channeling), we observe pronounced peaks in the angular distribution of the scattered projectiles. This can be attributed to rainbow-scattering caused by the corrugated interaction potential. On the basis of classical trajectory calculations, we derive from comparison with the experimental data the effective interaction potential of He, Ne, Ar and N atoms in front of a KCl(001) surface. Fair agreement is found for individual pair potentials calculated from Hartree-Fock wave functions, where the charge state of K and Cl ions located at lattice sites of the ionic crystal is taken into account. For the generalized ZBL (Ziegler, Biersack and Littmark) and OCB (O'Connor and Biersack) potentials, the agreement for interaction energies below 20 eV is found to be poor.

O 26.4 Tue 11:15 H40

3D force spectroscopy on KBr(001) by tuning fork based nc-AFM at low temperatures — Bartosz Such[1], •Sweetlana Fremy[2], Shigeki Kawai[2], Sascha Koch[2], Thilo Glatzel[2], and Ernst Meyer[2] — [1]Research Center for Nanometer-Scale Science and Advanced Materials (NANOSAM), Faculty of Physics, Astronomy, and Applied Computer Science, Jagiellonian University, Reymonta 4, 30-059 Krakow, Poland — [2]University of Basel, Klingelbergstrasse 82, 4056 Basel

We will present 3D dynamic force spectroscopy measurements on KBr(001) by tuning fork based nc-AFM [1] at low temperatures. The high stiffness of a tuning fork enables high-sensitive measurements of the short-range interaction with small oscillation amplitudes [2]. We performed the topographic method to collect 3D frequency shift and energy dissipation maps while keeping an amplitude of 200 pm [3]. The results suggest that significant tip relaxation is present at the smallest tip-sample separations. Analyzing the shape of force vs. distance curves and the cross sections of the 3D frequency shift dataset allows the identification of chemical identity of the tip apex as K+ ion.

[1] F.J. Giessibl, Appl. Phys. Lett. 76, 1470 (2000). [2] S. Hembacher and F. J. Giessibl and J. Mannhart, Science 305, 380 (2004). [3] B. J. Albers, T. C. Schwendemann, M. Z. Baykara, N. Pilet, M. Liebmann, E. I. Altman, U. D. Schwarz, Nature Nano. 4, 307 (2009).

O 26.5 Tue 11:30 H40

Polarity healing at the local scale: MgO on Au(111) — •Philipp Myrach[1], Niklas Nilius[1], Stefania Benedetti[2], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin, Germany — [2]CNR-INFM S3, Via G. Campi 213/a, I-41125 Modena, Italy

Polar MgO films prepared on Au(111) have been investigated with scanning tunnelling microscopy and spectroscopy. The amount of oxide polarity is derived from the MgO band positions and the local surface potential. Both quantities have been measured as a function of the oxide thickness and are good indicators for the strength of the surface dipole. Whereas bi-layer MgO islands exhibit uncompensated polarity, the dipole gradually decreases in thicker films due to surface roughening. The formation of nano-pyramids and pits is hereby identified as the initial step for polarity healing. Above such structural inhomogeneities, the measured surface potential is drastically reduced with respect to flat MgO(111) patches. This effect is reproduced with simple model structures that enable an estimation of the vertical dipole strength.

O 26.6 Tue 11:45 H40

Diffraction of fast light atoms and molecules during grazing scattering from a KCl(001) surface — •Marco Busch, Uwe Specht, and Helmut Winter — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, D-12489 Berlin, Germany

Fast light atoms and molecules with energies from 200 eV up to several keV are grazingly scattered from a clean and flat KCl(001) surface. For scattering along low-indexed axial channels, we observe defined diffraction patterns in the angular distributions for scattered projectiles. The experimental results for the scattering of H, D, ^{3}He, and ^{4}He atoms as well as H_2, D_2, and HD molecules can be ascribed to atom diffraction with de Broglie wavelengths as low as about 10^{-3} Å. From the evaluation of diffraction patterns we derive the widths of axial channels and the corrugation of the interaction potential across these channels. Our analysis is based on a semiclassical model using the hard-wall approximation and individual potentials for the interaction of the atomic projectiles with the atoms of the topmost surface layer of the surface.

O 26.7 Tue 12:00 H40

Temperature stabilised surface reconstructions at polar ZnO(0001) — •Mira Todorova[1], Markus Valtiner[2], Guido Grundmeier[2,3], and Jörg Neugebauer[1] — [1]Department for Computational Materials Design, Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf — [2]Christian Doppler Laboratory for Polymer/Metal Interfaces, Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf — [3]Technical and Macromolecular Chemistry, University of Paderborn, Paderborn

Combining diffraction experiments with density-functional theory calculations and thermodynamic considerations we study the atomic

structure of the polar ZnO(0001) surfaces. We show that a large number of very different reconstructions with similar stoichiometry are energetically almost degenerate, thus surface vibrational entropy contributions significantly affect their stabilisation. The large impact of the vibrational entropy on the surface structure gives rise to a strong dependence of surface phase diagrams on temperature and enables us to consistently describe and explain the experimentally observed surface structures on polar ZnO(0001) surfaces.

M. Valtiner, M. Todorova, G. Grundmeier, and J. Neugebauer, Phys. Rev. Lett. 103, 065502 (2009).

O 26.8 Tue 12:15 H40

Relaxation and thermal vibrations at the NaF(100) surface — •Stephan Härtel, Jochen Vogt, and Helmut Weiss — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Various theoretical models predict that the (100) surfaces of ionic solids with the rocksalt structure should exhibit a surface rumpling, i. e. cations and anions in the surface layer have different vertical positions. While this type of relaxation has been measured for various alkali halides the rumpling of the NaF(100) surface is expected to be very small. We present results of an experimental determination of the relaxation of the NaF(100) surface based on low-current LEED experiments and a subsequent tensor-LEED analysis of diffraction peak intensities as a function of electron energy at various crystal temperatures. Moreover, we present experimental values of the mean amplitudes of the thermal motions of the surface ions. The experimental data are compared to the results of density functional theory (DFT) calculations using a slab model and ultrasoft pseudopotentials. According to both experiment and theory, the average vertical positions of the Na^+ and F^- ions in the topmost surface layer differ at most by 0.02Å. While the measured rumpling is smaller than the error-bars, the model calculations predict a weak inward-displacement of the Na^+ ions of 0.01Å, and an outward-shift of F^- of 0.01Å with respect to the truncated bulk geometry. The thermal motions of the ions in the topmost surface layer appear to be enhanced compared to the respective bulk mean amplitudes by a factor of 1.3 to 1.4.

O 26.9 Tue 12:30 H40

Surface termination of $NdGaO_3$(110) and $DyScO_3$(110) — •Jens Lienemann[1], Marco Busch[1], Rasuole Dirsyte[2], Jutta Scharzkopf[2], Günter Wagner[2], Helmut Winter[1], and Roberto Fornari[2] — [1]Department of Physics, Humboldt University, Newtonstraße 15, D-12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, Max Born Straße 2, D-12489 Berlin, Germany

Auger electron spectroscopy using excitation via grazing impact of protons was applied to determine the elemental composition of the topmost layer of $NdGaO_3$(110) and $DyScO_3$(110) substrates. The preparation conditions of vicinal $NdGaO_3$ and $DyScO_3$ substrates were optimized with respect to annealing temperature, time, and gas atmosphere. Well prepared surfaces show regularly arranged, smooth terraces with single-layer steps as observed by atomic force microscopy. The surfaces of $NdGaO_3$(110) were always NdO terminated with a small amount of Ga (2-4%) atoms at the surface [1]. A Ga and O depletion layer with a thickness of about 4 nm was detected at optimized preparation conditions. $DyScO_3$(110) substrates show a dependence of the termination on the annealing gas. A ScO_2 terminated surface was prepared with annealing in argon while an DyO-Termination was found after annealing in oxygen. A depletion layer of Dy and O was also detected.

[1] R. Dirsyte, J. Schwarzkopf, G. Wagner, J. Lienemann, M. Busch, H. Winter and R. Fornari, Appl. Surf. Sci. 255, 8685 (2009)