O 65: Methods: Theory and Experiment

Time: Thursday 12:00–14:45 Location: MA 141

O 65.1 Thu 12:00 MA 141

Quantum well states and Rashba-type spin-orbit splitting in ultrathin Bi films — •Gustav Bihlmayer[1], Yury M. Koroteev[2,3], Eugene V. Chulkov[3,4], and Stefan Blügel[1] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute of Strength Physics and Materials Science, RAS, 634021, Tomsk, Russia — [3]Donostia International Physics Center (DIPC), 20018 San Sebastiàn, Spain — [4]Departamento de Física de Materiales, UPV/EHU, 20080 San Sebastiàn, Spain

In this contribution a systematic study of the electronic properties of thin ($1-6$ bilayers) films of the semimetal bismuth in (111) and (110) orientation is presented, employing calculations based on density functional theory. Due to the different coordination of the atoms in these two different surfaces, a large variation of the conducting properties of the films is found, ranging from small-bandgap semiconducting to semimetallic and metallic. The evolution of the Bi(111) and Bi(110) surface states is studied as a function of the film thickness and by comparison to thicker films and simulations of the semiinfinite crystals. Interesting features arise from the strong spin-orbit effects in Bi and the resulting Rashba-type spin-splitting of the surface states. The spin-polarization of these states can be seen to change as these states transform into quantum well states at the Brillouin zone boundary. These results will be compared with recent experimental results on thin Bi films on Si substrates.

[1] T. Hirahara *et al.*, Phys. Rev. B **76**, 153305 (2007)
[2] T. Hirahara *et al.*, Phys. Rev. Lett. **97**, 146803 (2006)

O 65.2 Thu 12:15 MA 141

Efficient calculation of electronic band structure and the application to angular resolved photoemission spectroscopy experiments — •Victor Joco[1], Nikolai Mikuszeit[2], Jesús Martínez Blanco[3], and Enrique García Michel[3] — [1]Centro de Microanalisis de Materiales, Univ. Autónoma de Madrid, Spain — [2]Institute of Applied Physics, Univ. of Hamburg, Germany — [3]Dpto. Física de la Materia Condensada, Univ. Autónoma de Madrid, Spain

Angular resolved photoemission spectroscopy (ARPES) is an experiment to directly probe the valence band electronic structure of solids. Theoretical band structure calculations are of great help in understanding the ARPES data. A tight binding (TB) model interpolates the results from first-principles calculations or even experiments. This approach correctly shows all symmetry properties of the energy bands. The precision of the results are of comparable accuracy to first-principles calculations but three orders of magnitude faster.

A simulation program for comprehensive energy band and constant energy surfaces calculations has been developed. Based on the TB model the program allows precise calculation of constant energy surfaces, band structure in arbitrary surface directions and projected bulk band plots. An optimized general isosurface calculation for accurate energy surfaces as well as broadening of initial and final states have been implemented to simulate data close to ARPES experiments. The speed on a standard personal computer enables almost instant simulation during experiment. The calculations are compared to ARPES measurements on Cu(111).

O 65.3 Thu 12:30 MA 141

Anisotropic electron-phonon coupling strength at the Be(0001) surface — M. Fuglsang Jensen[1], •E. D. L. Rienks[1], T.-Y. Chien[2], I. Yu. Sklyadneva[3], A. Eiguren[3], P. M. Echenique[3], E. V. Chulkov[3], E. W. Plummer[2], and Ph. Hofmann[1] — [1]Institute for Storage Ring Facilities, University of Aarhus, Århus, Denmark — [2]Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee, USA — [3]Donostia International Physics Center, San Sebastian, Basque Country, Spain

Electronic surface states are useful model systems for understanding many-body effects in solids, such as electron-phonon coupling (EPC). Advances in angle-resolved photoemission spectroscopy not only allow one to assess the strength of the EPC, but also enable experimental determination of the Eliashberg function, that fully characterizes the electron phonon coupling in a given system.

Although the electronic structure of the Be(0001) surface is well studied, there is no agreement on the strength of the EPC at this surface. This strength is described by the mass enhancement parameter λ. An anisotropic coupling might account for this discrepancy, as these results are obtained along different crystal directions.

This study is aimed at obtaining a full description of EPC at this surface. Experimentally, the Eliashberg function (and λ) can be determined from the renomalized dispersion of the $\overline{\Gamma}$ surface state at the Fermi energy crossing. Preliminary results show that there is indeed a substantial variation of λ between the $\overline{\Gamma\mathrm{M}}$ and the $\overline{\Gamma\mathrm{K}}$ directions. The same trend is observed in a first principles study of this system.

O 65.4 Thu 12:45 MA 141

Electronic transport over single atoms — •Martyna Polok, Dmitry V. Fedorov, Peter Zahn, and Ingrid Mertig — Department of Physics, Martin Luther University Halle-Wittenberg, 06099 Halle (Saale), Germany

Scanning Tunneling Microscope (STM) experiments are important examples of the tunneling through single atoms. We try to develop a general understanding of the transport phenomena in complex structures through a case study of the STM setup.

The density functional theory (DFT) in the Korringa-Kohn-Rostoker (KKR) Green's function formulation is implemented to obtain the ground state electronic structure of the system. The transport properties are calculated in the linear response limit using the Baranger and Stone formalism.

In our ab initio investigation we consider a Cu and Co STM tip approaching a Cu (001) surface decorated with a single Cu or Co adatom. Depending on the chemical and geometrical structure of the constriction different transport channels contribute to the total conductance. Based on the spatial current distribution we can classify the open eigenchannels according to the symmetry of different angular momentum contributions i.e. the type of valence orbitals available at the Fermi energy.

The aim of this work is to demonstrate the interplay between the structure of the constriction and the electronic transport properties.

O 65.5 Thu 13:00 MA 141

Spin-orbit split two-dimensional electron gas with tunable Rashba and Fermi energy — •Christian R. Ast[1], Daniela Pacile[2], Luca Moreschini[2], Mihaela Falub[2], Marco Papagno[2], Klaus Kern[1,2], Marco Grioni[2], Jürgen Henk[3], Arthur Ernst[3], Sergey Ostanin[3], and Patrick Bruno[3] — [1]MPI für Festkörperforschung, Stuttgart, Germany — [2]EPFL, Lausanne, Switzerland — [3]MPI für Mikrostrukturphysik, Halle, Germany

In the Rashba-Bychkov-Model the strength of the spin-orbit splitting — the Rashba energy E_R — introduces a new energy scale influencing the electronic structure and competing against other energy scales, such as the Fermi energy E_F. However, in most of the known systems up to now the Rashba energy is a perturbative correction. We demonstrate that it is possible to tune the Rashba energy and the Fermi energy in a two-dimensional electron gas by a controlled change of the stoichiometry of an artificial surface alloy. In the $\mathrm{Bi}_x\mathrm{Pb}_{1-x}/\mathrm{Ag}(111)$ surface alloy the spin-orbit interaction maintains a strong influence on the band dispersion for arbitrary Bi concentration x, as is shown by angle-resolved photoelectron spectroscopy. The Rashba energy E_R and the Fermi energy E_F can be tuned to achieve values larger than one for the ratio E_R/E_F, which opens up the possibility for observing new phenomena, such as corrections to the Fermi liquid or a superconducting state. Relativistic first-principles calculations explain the experimental findings.

O 65.6 Thu 13:15 MA 141

Temperature dependence of stick-slip friction on graphite — •Lars Jansen[1,2], Harald Fuchs[1,2], and André Schirmeisen[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhlem-Klemm-Strasse 10, 48149 Münster — [2]CeNTech, Center for NanoTechnology, Heisenbergstrasse 11, 48149 Münster

The so called stick-slip phenomenon, where the tip of an atomic force microscope performs a saw-tooth like motion over a surface, is believed to be a fundamental process in atomic friction, whose investigation has become a huge challenge over the past years [1,2].

We measured atomic scale stick-slip friction on a graphite surface with an atomic force microscope under ultrahigh vacuum conditions in a temperature range from 100 K to 300 K.

In this talk, we show the results of our experiments concerning friction vs. scan-speed curves for different temperatures. Furthermore we compare our experimental results to the thermally activated Prandtl-Tomlinson-model as described by Sang et al. [3]. This allows us the direct evaluation of crucial parameters like the energy barrier and the microscopic damping coefficient, which is often assumed to be in the lower limit of aperiodic damping.

[1] Schirmeisen, Jansen, Fuchs, PRB 71, p. 245403 (2005)
[2] Evstigneev, Schirmeisen, Jansen, Fuchs, Reimann, PRL 97, p. 240601 (2006)
[3] Sang, Dubé, Grant, PRL 87, p. 174301 (2001)

O 65.7 Thu 13:30 MA 141

Temperature dependence of the energy dissipation in dynamic force microscopy — •Tino Roll, Tobias Kunstmann, Markus Fendrich, Rolf Möller, and Marika Schleberger — Universität Duisburg-Essen, Fachbereich Physik, Lotharstraße 1, D-47048, Germany

Operating an atomic force microscope under UHV conditions can be used to study energy loss processes. This can be achieved by measuring the energy necessary to maintain the amplitude of the cantilever (damping) at a given frequency shift. The dissipation of energy is usually described in terms of an adhesion hysteresis mechanism. This mechanism should become less efficient with increasing temperature. To verify this prediction we have measured topography and dissipation data with dynamic force microscopy in the temperature range from 100 K up to 300 K. We used 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) grown on KBr(001). At room temperature, the energy dissipated into the sample (or tip) is 2.5 eV/cycle for PTCDA and 1.5 eV/cycle for KBr, respectively, and is in good agreement with an adhesion hysteresis mechanism. The energy dissipation over the PTCDA surface decreases with increasing temperature yielding a negative temperature coefficient. For the KBr substrate, we find the opposite behaviour: anincrease of dissipated energy with increasing temperature. While the negative temperature coefficient in case of PTCDA agrees rather well with the adhesion hysteresis model, the positive slope found for KBr points to a hitherto unknown dissipation mechanism.

O 65.8 Thu 13:45 MA 141

The Surface state of Au(111) and characterization of the tunneling tip in STM — •Berndt Koslowski, Anna Tschetschetkin, Stefania C. Bobaru, and Paul Ziemann — Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm, Germany

Based on a recently developed method for recovering the electronic density of states (DOS) from Scanning Tunneling Spectroscopy (STS) data [1], we re-examine the well-known Shockley-like surface state (SS) of Au(111) at 6.2K. To do so, we employ the 3D WKB approximation for the special case of a 2-dimensional SS leading to an analytical solution for the DOS recovery. The goal of this contribution is threefold: firstly, we show why the SS does not show up as a step function in STS. Secondly it will be demonstrated, how the SS can be exploited to extract information about the tip DOS resulting in a *calibrated* tunneling sensor. Thirdly, we discuss details of the tunneling spectra such as the cross-over from 2D to 3D tunneling below the band edge of the SS.

[1] B. Koslowski, Ch. Dietrich, A. Tschetschetkin, P. Ziemann, Phys.Rev. B 75, 035421 (2007).

O 65.9 Thu 14:00 MA 141

Dynamic superlubricity on insulating and conductive surfaces — Enrico Gnecco[1], •Pascal Steiner[1], Anisoara Socoliuc[2], Sabine Maier[3], Thilo Glatzel[1], Jonas Gessler[1], Alexis Baratoff[1], and Ernst Meyer[1] — [1]Department of Physics, Klingelbergstr. 82, 4056 Basel, Switzerland — [2]Nanonis GmbH, Technoparkstr. 1, 8005 Zürich, Switzerland — [3]Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Friction between a sharp silicon tip and various atomically flat surfaces (NaCl, KBr, graphite, mica) is minimised by piezo-induced oscillations at well-defined resonance frequencies. This procedure extends an electro-capacitive way to achieve the same effect, which was recently introduced by our group and tested on insulating alkali halide crystals in ultra-high vacuum [1]. A controlled reduction of friction is observed now also on conductive surfaces like graphite, and in ambient conditions, which is quite promising for technological applications to micro-electromechanical devices. The theory previously used to interpret 'dynamic superlubricity' under general conditions is supported by new experimental observations showing that the contact between tip and sample is well maintained when the oscillations are applied.

[1] A. Socoliuc et al., Science, Vol. 313, 207 (2006).

O 65.10 Thu 14:15 MA 141

Space–Charge Effects in Photoelectron Spectroscopy at FLASH — •Martin Marczynski-Bühlow, Matthias Kalläne, Stefan Hellmann, Sabrina Lang, Claas Thede, Tim Riedel, Sönke Harm, Kai Rossnagel, and Lutz Kipp — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098

With its brilliant, ultrashort, and coherent photon pulses ranging from the VUV to the soft X–ray regime FLASH (Free–Electron Laser in Hamburg) offers the possibility to study a variety of "new physics" with novel as well as with traditional synchrotron radiation techniques. We have determined general limits for photoelectron spectroscopy experiments with these highly intense photon pulses with regard to radiation damage, space–charge effects, and FLASH machine parameters. Here we present angle–resolved as well as core–level photoelectron spectra of the transition–metal dichalcogenide $1T$–TaS_2 in the Mott insulating phase (T = 140 K). The photoelectron spectra were investigated particularly with respect to the occurrence of space–charge effects as a function of pulse intensity and compared with self-consistent N-body simulations based on the Barnes & Hut Treecode Algorithm. The measurements were carried out at the monochromator beamline PG2 of FLASH using the 3^{rd} FEL harmonic ($h\nu$ = 115.5 eV).

This work is supported by the Innovationsfond des Landes Schleswig-Holstein.

O 65.11 Thu 14:30 MA 141

Commissioning of a dedicated Soft X-Ray energy dispersive beamline for NEXAFS and other CFS/CIS studies — •D. Batchelor[1], Th. Schmidt[1], R. Follath[2], C. Jung[2], R. Fink[3], A Schöll[1], M. Knupfer[4], B. Büchner[4], and E. Umbach[1,5] — [1]Universität Würzburg, Experimentelle Physik II, Würzburg — [2]BESSY GmbH, Berlin — [3]Physikalische Chemie II, Universität Erlangen-Nürnberg — [4]IFW Dresden — [5]Forschungszentrum, Karlsruhe

We have recently published a design for a dedicated Soft X-Ray dispersive beamline (NIMA 575 (2007) 470-475) using photoelectron spectroscopy. The new dispersive technique allows not only NEXAFS without the time-consuming scanning of the photon energy but also high resolution CFS/CIS spectroscopic studies such as Auger/autoionization spectroscopy. The technique provides data with much more accuracy and detail hitherto achieved by simply stepping the photon energy. The method was originally tested using a "Pilot"setup which exploited extending the depth of focus of the monochromator by limiting the beamline angular aperture. Although very successful the decrease in angular beamline aperture obviously had drawbacks in terms of signal and also mode of operation of the monochromator (low Cff values). We will present commissioning results from the upgraded monochromator demonstrating that the new design overcomes most of these difficulties.