O 5: Spin-Orbit Interaction at Surfaces I

Time: Monday 11:15–12:45 Location: WIL B321

O 5.1 Mon 11:15 WIL B321

Topologically trivial and non-trivial states at the surface of Bi_2Se_3 — •Hadj Mohamed Benia, Klaus Kern, and Christian R. Ast — Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

Angle Resolved Photon Emission Spectroscopy (ARPES) measurements at the surface of Bi_2Se_3 single crystals show the existence of Rashba spin-split quantum-well states (QWS) together with the known topological surface state around the Γ point. Up to three QWS with different Rashba-splitting are observed between the Fermi level and the Dirac point. The origin of the QWS is traced back to a formation of a 2D electron gas at the crystal surface as a result to downward bending of the conduction band. A shift to higher binding energies of the QWS accompanied with a change in the Rashba splitting is observed as function of time and temperature. A triangular potential is used to model the band bending, fit the QWS levels, and extract the corresponding potential asymmetry at the surface for various measurement conditions.

O 5.2 Mon 11:30 WIL B321

Spin-resolved electronic structure of the surface Rashba-system Bi/Cu(111) — •Hendrik Bentmann[1], Takuya Kuzumaki[2], Gustav Bihlmayer[3], Kazuyuki Sakamoto[2], and Friedrich Reinert[1] — [1]Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg, Germany — [2]Graduate School of Advanced Integration Science, Chiba University, Chiba 263-8522, Japan — [3]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

Recently several surface adsorbate systems on metal and semiconductor substrates have been identified whose electronic structure is heavily influenced by the spin-orbit interaction. The spin orientation of the polarized electronic states in these systems can show quite unexpected effects including sign changes within a single band or even a complete rotation out of the plane [1,2]. Here we report spin- and angle-resolved photoemission experiments on the surface alloy Bi-Cu(111)$(\sqrt{3} \times \sqrt{3})R30°$. The results directly demonstrate that the Bi-induced surface state bands of sp_z orbital character are split in energy by the spin-orbit interaction. The spin orientation is found to be in accordance with the Rashba model within the probed energy window. Another surface state of p_xp_y character shows no spin polarization suggesting that this state consists of two unresolvable components of opposite spin orientation. First-principles calculations of the spin orientation vectors are in line with the experimental observations.

[1] H. Mirhosseini *et al.*, Phys. Rev. B **79**, 245428 (2009).
[2] K. Sakamoto *et al.*, Phys. Rev. Lett **103**, 156801 (2009).

O 5.3 Mon 11:45 WIL B321

Strong effect of substrate termination on Rashba spin-orbit splitting: Bi on $BaTiO_3(001)$ from first principles — •Samir Abdelouahed and Jürgen Henk — Max Planck Institute of Microstructure Physics, Halle, Germany

A sizable Rashba splitting of surface states requires a number of ingredients: a strong atomic spin-orbit coupling, a steep surface-potential barrier, and a large in-plane potential gradient. We demonstrate by first-principles calculations that a suitable substrate termination is another prerequisite.

Our calculations for a Bi adlayer on $BaTiO_3(001)$ show that the Rashba spin-orbit splitting in the Bi-6p states is strongly affected by the substrate termination. For the TiO_2 termination the absolute splitting is very large (about $0.23\,Å^{-1}$) and can be mildly affected by the orientation of the electric polarization in the ferroelectric substrate [1]. In striking contrast, the splitting becomes strongly reduced for the BaO termination (less than $0.07\,Å^{-1}$). Our findings are explained by the termination-dependent hybridization of the Bi surface states with electronic states in the substrate. It turns out that a strongly asymmetric charge density at the site of the heavy element (here: Bi) is a signature of a large Rashba splitting.

[1] H. Mirhosseini et al, Phys. Rev. B **81** (2010) 073406.

O 5.4 Mon 12:00 WIL B321

Local structure of the mixed surface alloy $Bi_xPb_{1-x}/Ag(111)$ measured with scanning tunneling microscopy — •Fabian Zinser, Maximilian Assig, Klaus Kern, and Christian R. Ast — Max Planck Institute for Solid State Research, Stuttgart, Germany

The mixed surface alloy $Bi_xPb_{1-x}/Ag(111)$ is part of a class of surface alloys that exhibit a 2D electronic structure with an extremely large spin-splitting [1]. In this surface alloy, changing the concentration ratio x allows the continuous tuning of the spin splitting as well as the band occupation [2]. With the ability of scanning tunneling microscopy (STM) to discern single bismuth and lead atoms from each other, new insight into the local structure of these systems is possible. Here we present our studies of the local structure for different compositions of the mixed surface alloy $Bi_xPb_{1-x}/Ag(111)$.

[1] C. R. Ast *et al.*, Phys. Rev. B **75**, 201401(R) (2007)
[2] C. R. Ast *et al.*, Phys. Rev. B **77**, 081407(R) (2008)

O 5.5 Mon 12:15 WIL B321

Spin-resolved measurements of the Rashba-split surface state on Au(111) above the Fermi level — Sune N. P. Wissing[1], •Anna Zumbülte[1], Christian Eibl[1], Anke B. Schmidt[1], Jürgen Braun[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfaelische Wilhelms-Universitaet, Wilhelm-Klemm-Str. 10, 48149 Muenster, Germany — [2]Dept. Chemie und Biochemie, LMU München, Germany

We report on the first spin-resolved measurement of an unoccupied Rashba-split surface state via inverse photoemission.

Since the discovery of the spin-orbit splitting on a Au(111) surface by LaShell *et al.* [1] in 1996, many different systems have been investigated for a better understanding of Rashba-type phenomena. Yet it was not possible to expand the present information by spin-resolved measurements above the Fermi level.

Spin and angle-resolved inverse photoemission is a powerful tool to determine the unoccupied electronic structure of solid surfaces and thin films. In order to demonstrate the potential of this method for investigating interesting Rashba phenomena, we present measurements of the prototype Rashba system: the Au(111) surface. We were able to confirm the Rashba splitting of the surface state as it continues above the Fermi level. Moreover, we investigated its behaviour when the surface state becomes degenerate with bulk states.

[1] S. LaShell *et al.*: Phys. Rev. Lett. **77**, 3419 (1996)

O 5.6 Mon 12:30 WIL B321

Anisotropic Scattering of Bi(111) Surface State Electrons at a Point Defect Visualized by Low Temperature Scanning Tunneling Microscopy and Spectroscopy — •Maren Cottin[1], Christian Bobisch[1], Johannes Schaffert[1], Andreas Sonntag[1], Giriraj Jnawali[1], Gustav Bihlmayer[2], and Rolf Möller[1] — [1]Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

The semimetal bismuth (Bi) has recently attracted a lot of attention due to its interesting transport properties. The metallic surface states which occur on various of its surfaces underlie a large spin orbit splitting. We use scanning tunneling microscopy to analyze the lateral variation in the local density of states in the vicinity of a point defect on a Bi(111)-surface. The observed pattern in the dI/dV-images visualizes the scattering of surface state electrons. At energies close to the Fermi level, the pattern is highly anisotropic and shows a threefold symmetry. Using the calculated Fermi surface of Bi(111) the scattering processes are ascribed to spin-conserving transitions between two spin orbit split surface states. The scattering pattern can be simulated by the superposition of three monochromatic waves where the phase with respect to the scattering center has a significant impact on the appearance and the symmetry of the pattern.