O 15: Spin-Orbit Interaction at Surfaces II

Time: Monday 15:00–17:15 Location: H38

O 15.1 Mon 15:00 H38

Graphene with strong extrinsic spin-orbit effects: an ab-initio study — •Gustav Bihlmayer and Stefan Blügel — Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Recent experimental investigations of Au-intercalated graphene on Ni(111) reported strong spin-orbit (SO) induced splittings in the spectrum near the $\overline{K}$-point [1]. Theoretical studies of a model Hamiltonian for graphene with extrinsic SO coupling predict an unusual spectrum and spin-orientation pattern for this case [2].

We present first principles calculations of this system, basically confirming the scenario developed in [2], but including effects from the realistic materials, e.g. modifications due to the substrate. Our calculations show quantitative agreement with the experimental results [1]. Moreover, the complex interplay of the nickel's exchange field and Rashba-type SO-fields (induced by the intercalated Au monolayer) is analysed and compared to other cases, e.g. the Rashba-split surface state of the Gd(0001) surface [3].

[1] A. Varykhalov et al., Phys. Rev. Lett. **101**, 157601 (2008)
[2] E. I. Rashba, Phys. Rev. B **79**, 161409(R) (2009)
[3] O. Krupin et al., Phys. Rev. B **71**, 201403(R) (2005)

O 15.2 Mon 15:15 H38

Spin-orbit coupling and Rashba effect in graphene: *Ab initio* model studies — •Samir Abdelouahed[1], Hossein Mirhosseini[1], Igor V. Maznichenko[2], Arthur Ernst[1], and Jürgen Henk[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

Significant spin-orbit effects have been found experimentally in graphene, e. g. Rashba-type splittings at the Dirac point. Because the atomic spin-orbit coupling of carbon is very weak, additional mechanisms must come into question to explain these splittings. Theoretical studies already addressed these mechanisms but sometimes relied on empirical methods.

Here, we report on a first-principles investigation of spin-orbit coupling in graphene, in which various ingredients of Rashba-type effects are systematically considered. Besides a potential gradient normal to the carbon sheet which gives rise to the conventional Rashba effect, an in-plane potential gradient and corrugation effects are discussed.

O 15.3 Mon 15:30 H38

Structural Influence on the Rashba-type Spin-Splitting in Surface Alloys — •Christian R. Ast[1], Isabella Gierz[1], Benjamin Stadtmüller[1,2], Johannes Vuorinen[3], Matti Lindroos[3], Hugo Dil[4], Fabian Meier[4], and Klaus Kern[1] — [1]MPI für Festkörperforschung, Stuttgart — [2]Exp. Physik II, Universität Würzburg — [3]Tampere University of Technology, Dept. of Physics, Tampere, Finland — [4]PSI, SLS, Villigen, Switzerland

The Rashba-Bychkov (RB) model has been remarkably successful in describing the spin splitting of two-dimensional (2D) electron systems with a structural inversion asymmetry (SIA). It explains how the spin-degeneracy is lifted by an electric field perpendicular to a 2D free electron system. Looking in more detail, different contributions to a strong spin-splitting at surfaces include a strong atomic spin-orbit interaction, orbital character, a SIA as well as other structural modifications. For surface states, the RB effect can only serve as a qualitative model, because it only accounts for an effective electric field. A number of surface alloys (Bi/Ag(111), Pb/Ag(111), etc.) have been identified with an extremely large spin-split surface state. Interestingly, only a fraction of the atoms at the surface feature a sizeable atomic spin-orbit coupling so that the source of the large spin-splitting must be sought in the structure. We present a systematic study of the alloy atom relaxation in different Ag(111) surface alloys using quantitative low-energy electron diffraction (IV-LEED) measurements and calculations. We relate the alloy atom relaxation to the size of the spin-splitting and discuss possible scenarios of the underlying mechanism.

O 15.4 Mon 15:45 H38

Tuneable Hybridization between Rashba-split Surface States in $BiAg_2$/Ag/Au(111) Trilayer Systems — •Hendrik Bentmann[1], Frank Forster[1], and Friedrich Reinert[1,2] — [1]Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg, Germany — [2]Forschungszentrum Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

We have studied the surface states of a $BiAg_2$ surface alloy grown on thin Ag films on Au(111) by angle-resolved photoelectron spectroscopy. In contrast to the case of the bulk Ag(111) substrate we find the sp_z-type and the p_xp_y-type surface state to be separated by a hybridization gap that is accompanied by a pronounced kink in the dispersion of the p_xp_y-type state. The size of the gap is tunable via the Ag film thickness, whereas the gap closes for higher coverages. Our observations are attributed to slight variations in the protrusion height of the Bi atom. We propose that these variations are induced by thickness-dependent partial charge densities of the Ag quantum well states in the topmost layer. According to previous calculations we anticipate an unconventional sign change of the spin polarization at the hybridization kink of the p_xp_y-type state [1,2].

[1] H. Mirhosseini, J. Henk, A. Ernst, S. Ostanin, C.T. Chiang, P. Yu,
A. Winkelmann, and J. Kirschner, Phys. Rev. B **79**, 245428 (2009).
[2] G. Bihlmayer, S. Blügel, and E. V. Chulkov, Phys. Rev. B **75**, 195414 (2007).

O 15.5 Mon 16:00 H38

Local topography and density of states in the Bi_xPb_{1-x}/Ag(111) mixed surface alloy — •Fabian Zinser, Maximilian Assig, Klaus Kern, and Christian R. Ast — Max Planck Institute for Solid State Research, Stuttgart, Germany

The Bi/Ag(111) and Pb/Ag(111) surface alloys exhibit a 2D electronic structure with an extremely large spin-splitting [1]. Mixing the relative amounts of Bi and Pb atoms at the surface creates a mixed surface alloy where the spin-splitting as well as the band occupation can be tuned continuously [2]. We present a study of the electronic structure and local topography at the surface of the Bi_xPb_{1-x}/Ag(111) mixed surface alloy using scanning tunneling microscopy and spectroscopy (STM/STM). We discuss the local disorder of the Pb and Bi alloy atoms as well as the evolution of the local density of states as a function of relative Bi and Pb content.

[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 15.6 Mon 16:15 H38

Quantum-size induced giant spin-orbit splitting — •Andreas Ruffing[1], Stefan Mathias[1,2], Martin Wiesenmayer[3], Indranil Sarkar[1], Gustav Biehlmayer[4], Eugene V. Chulkov[5,6], Yury M. Koroteev[7], Pedro M. Echenique[5,6], Michael Bauer[3], and Martin Aeschlimann[1] — [1]Deepartment of Physics, University of Kaiserslautern, Germany — [2]JILA and Department of Physics, University of Colorado, Boulder, USA — [3]Institut für Experimentelle und Angewandte Physik, Universität Kiel, Germany — [4]Institut für Festkörperforschung und Institut for Advanced Simulation, Forschungszentrum Jülich, Germany — [5]Donostia International Physics Center (DIPC), San Sebastián/Donostia, Basque Country, Spain — [6]Departamento de Física de Materiales and Centro Mixto CSIC-UPV/EHU, San Sebastian/Donostia, Basque Country, Spain — [7]Institut of Strength Physics and Materials Science, RAS, Tomsk, Russia

We report on the observation of giant spin-orbit splitting of quantum-well states in the unoccupied electronic structure of a Bismuth monolayer on Cu(111). Up to now, Rashba-type splittings of this size have been reported exclusively for surface states in a partial bandgap. With these quantum-well states we have experimentally identified a second - and broader - class of states that show a huge spin-orbit splitting. First-principle electronic structure calculations show that the origin of the spin-orbit splitting is due to the perpendicular potential at the surface and interface of the ultrathin Bi film. This finding allows for the direct possibility to tailor spin-orbit splitting by means of thin film nanofabrication.

O 15.7 Mon 16:30 H38

Evolution of Topological Edge-States in $Bi_{1-x}Sb_x$ Films on Si(111) — •Hadj Mohamed Benia, Carola Strasser, Klaus Kern, and Christian R. Ast — Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany

Due to a semimetal-semiconductor transition in the $Bi_{1-x}Sb_x$ alloy,

Bi is transformed into a topological insulator for Sb concentrations larger than 8% [1]. So far, the evolution of the topological states with Sb concentration has only been studied theoretically [2]. We have experimentally investigated the band structure of high quality $Bi_{1-x}Sb_x$ films grown on Si(111) using angular resolved photoemission spectroscopy (ARPES). The evolution of the topological states as function of Sb concentration will be discussed.

[1] D. Hsieh et al. Nature 452, 970 (2008).
[2] L. Fu, C.L. Kane, Phys. Rev. B 76, 45302 (2007).

O 15.8 Mon 16:45 H38

Towards a ferroelectric control of Rashba spin-orbit coupling: Bi on $BaTiO_3$(001) from first principles — •Hossein Mirhosseini[1], Igor Maznichenko[2], Samir Abdelouahed[1], Sergey Ostanin[1], Arthur Ernst[1], Ingrid Mertig[1,2], and Jürgen Henk[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Institute of Physics, Martin Luther University Halle-Wittenberg, Halle, Germany

We propose a new route for controling the Rashba splitting of the electronic states of an adlayer. The Rashba spin splitting in the 6*p* states of a Bi adlayer on $BaTiO_3$(001) can be manipulated by the electric polarization in the ferroelectric substrate.

The Bi surface states display an anisotropic dispersion with an unmached splitting about 0.2 $Å^{-1}$. Switching of the intrinsic electric polarization P in $BaTiO_3$ affects the strength of the Rashba splitting in the Bi adlayer. The relative change in the splitting is about 5 %. Our findings may pave a route for new spinelectronic devices.

O 15.9 Mon 17:00 H38

Growth and characterization of $Bi_{1-x}Sb_x$ crystalline films on Si(111) — •Carola Strasser, Hadj Mohamed Benia, Klaus Kern, and Christian R. Ast — Max Planck Institute for Solid State Research, Stuttgart, Germany

Recently, the $Bi_{1-x}Sb_x$ alloys have been identified as topological insulators for Sb contents larger than 8%. While studies so far have used single crystals, we have grown $Bi_{1-x}Sb_x$ films on Si(111) with a focus on producing a particularly smooth surface.

The quality of the samples was analyzed using different techniques, such as low energy electron diffraction (LEED), secondary ion mass spectrometry (SIMS), X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS). The preparation and optimization of flat and homogenous films will be presented.