O 48: Focused Session: Spin-Orbit Interaction at Surfafces: From the Rashba Effect to Topological States of Matter I

Time: Thursday 10:30–13:00 Location: HSZ 02

Topical Talk O 48.1 Thu 10:30 HSZ 02

The Rashba and quantum size effects in ultrathin Bi films — •Toru Hirahara — Department of Physics, University of Tokyo, Japan

Semimetal bismuth (Bi) is one of the most extensively studied elements in solid state because of its extreme physical properties. For example, Bi has been employed to examine the quantum size effect (QSE) in thin films or nanowires due to its extraordinary large Fermi wavelength. An oscillation in the conductivity or the Hall coefficient with film thickness due to the QSE was predicted theoretically [1]. Furthermore since Bi is a very heavy element, spin-orbit coupling (SOC) effects play a dominant role in the electronic and transport properties, which can be found in the large atomic splitting (1.5 eV), or the anti-localization behavior in magnetotransport measurements [2].

When the system downsizes to the nanometer scale, it can be expected that the contributions from the surface states will make the system more intriguing. In this talk, I will present our recent results obtained for a well-defined ultrathin Bi film [3] utilizing the state-of-art spin- and angle- resolved photoemission spectroscopy, first-principles calculations, and surface-sensitive conductivity measurements. Particular focus will be given on the QSE and SOC effect at the surface (Rashba effect).

[1] V. B. Sandomirskii, Sov. Phys. JETP 25, 101(1967). [2] F. Komori et al., 52, 368(1983). [3] T. Nagao et al., Phys. Rev. Lett. 93, 105501 (2004).

Topical Talk O 48.2 Thu 11:00 HSZ 02

Giant Spin-Splitting on Metallic and Semiconducting Surfaces — •Christian R. Ast — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

One of the goals in the emerging field of spintronics is to manipulate the electron spin without the use of magnetic fields. This can be achieved at surfaces and interfaces where the inversion symmetry is broken so that a strong spin-orbit interaction can lift the spin-degeneracy (Rashba-Bychkov Model). Such a spin-splitting can further be enhanced by additional contributions from an in-plane inversion asymmetry as has been found for the Bi/Ag(111) surface alloy. The observed spin-splitting in this system is more than an order of magnitude stronger than in the Au(111) surface state. This introduces a new component in the mechanism of the Rashba-type spin-splitting. The strength of the splitting can be tuned by mixing different elements in the surface alloy. In particular, this concept can be transferred onto a semiconducting substrate in order to make it more interesting for the broad field of spintronics.

Topical Talk O 48.3 Thu 11:30 HSZ 02

Exploring the Rashba spin-orbit splitting by *ab initio* theory — •Gustav Bihlmayer — Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

Since the discovery of a Rashba-type spin-orbit splitting of the surface state of Au(111), many new manifestations of this effect have been discovered, e.g. on surfaces of magnetic or semimetallic elements, in surface alloys and even in quantum-well states of thin metallic films. These systems offer the possibility to study phenomena beyond the usual Rashba-type effect, leading to splittings that are no longer linear in the momentum and show complex spin-orientation patterns in surface states [1]. We also observe unconventional Fermi surface topologies [2], and will discuss new ways to tune the effect to meet specific requirements [3]. Employing first-principles calculations, the origin of these intriguing phenomena will be analyzed. In particular, I will focus on the appearance of a spin-splitting in thin Bi [4] and Pb films, which offers a view on the shape of the wavefunction of the surface- and quantum-well states in these films.

[1] G. Bihlmayer, E. V. Chulkov, and S. Blügel, Phys. Rev. B **75**, 195414 (2007)
[2] O. Krupin, G. Bihlmayer, K. Starke, S. Gorovikov et al., Phys. Rev. B **71**, 201403 (R) (2005)
[3] Yu. M. Koroteev, G. Bihlmayer, E. V. Chulkov, and S. Blügel, Phys. Rev. B **77**, 045428 (2008)
[4] T. Hirahara, T. Nagao, I. Matsuda, G. Bihlmayer et al., Phys. Rev. Lett. **97**, 146803 (2006)

O 48.4 Thu 12:00 HSZ 02

Giant Rashba spin-orbit splitting in the unoccupied quantum-well band-structure of Bi/Cu(111) — •M. Aeschlimann[1], S. Mathias[1], A. Ruffing[1], F. Deicke[1], M. Wiesenmayer[2], G. Bihlmayer[3], E.V. Chulkov[4,5], Yu.M. Koroteev[4,6], and M. Bauer[2] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]IEAP, Christian-Albrechts-Universität zu Kiel, 24908 Kiel, Germany — [3]FZ Jülich, 52425 Jülich, Germany — [4]DIPC, 20018 San Sebastián/Donostia, Spain — [5]Departamento de Fisica de Materiales, UPV/EHU, Apdo 1072, 20080 San Sebastián, Spain — [6]Institute of Strength Physics and Materials Science, RAS, 634021, Tomsk, Russia

The unoccupied electronic structure of the Bi surfactant layer (0.5 ML coverage) on Cu(111) is investigated by angle-resolved two-photon photoemission (AR-2PPE). An unoccupied quantum-well state is observed exhibiting a large spin-orbit splitted band with a Rashba energy of $E_R \simeq$134 meV and a wave number offset of k=0.09 1/Å. This enhancement of the spin splitting is surprisingly high given the fact that the ultrathin Bi film on Cu(111) does not show surface alloying. We therefore carried out first principle calculations to unravel the origin of the large spin-splitting, potentially caused by corrugation or the influence of the interface potential onto the ultrathin Bi film, giving rise to a quantum-size induced giant spin-orbit splitting. Such a scenario would directly allow for another possibility to tailor spin-orbit splitting (next to surface alloying) by means of thin film nanofabrication.

O 48.5 Thu 12:15 HSZ 02

Electronic Structure of the Bi/Cu(111) surface alloy and its modification upon Na adsorption — •Hendrik Bentmann[1], Holger Schwab[1], Frank Forster[1], Gustav Bihlmayer[2], Luca Moreschini[3], Marco Grioni[3], and Friedrich Reinert[1,4] — [1]Universität Würzburg, Experimentelle Physik II, Am Hubland, D-97074 Würzburg, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany — [3]Ecole Polytechnique Fédérale de Lausanne (EPFL), Institut de Physique des Nanostructures, CH-1015 Lausanne, Switzerland — [4]Forschungszentrum Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

Employing angle-resolved photoelectron spectroscopy (ARPES) we have investigated the electronic structure of the long-range ordered surface alloy Bi-Cu(111)$(\sqrt{3}\times\sqrt{3})R30^\circ$ and its modification after Na adsorption. On the clean alloy we observe a spin-split surface state band with an energy maximum approximately 230 meV above the Fermi level. By doping the surface alloy with Na we are able to tune the position of Fermi level relative to the surface state continously. Our data provides direct information about electronic states above the Fermi level. This allows for an unambiguous deduction of the surface electronic structure and the Rashba parameters. The experimental findings are fully confirmed by first principles calculations.

O 48.6 Thu 12:30 HSZ 02

Rashba effect in unoccupied states: Two-photon photoemission experiments and first-principles calculations for Bi/Cu(111) — Ping Yu, Cheng-Tien Chiang, Aimo Winkelmann, Hossein Mirhosseini, Arthur Ernst, Sergey Ostanin, •Jürgen Henk, and Jürgen Kirschner — Max Planck Institute of Microstructure Physics, Halle, Germany

Surface alloys of Bi and noble metals on fcc(111) surfaces exhibit Rashba-split occupied sp_z surface states which have been thoroughly investigated by photoemission experiments and electronic-structure calculations. Their unmatched splitting is attributed to the interplay between an in-plane potential gradient and the conventional out-of-plane image-potential gradient. However, the splitting of a set of p_xp_y surface states remained unresolved so far because these unoccupied states cannot be accessed by conventional photoemission.

By angle-resolved two-photon photoemission experiments and first-principles calculations we study in detail the unoccupied p_xp_y states on $\sqrt{3}\times\sqrt{3}$R30°-Bi/Cu(111). Their experimental dispersion in the relevant energy range, band maxima (at $E_\mathrm{F} + 1.4\,\mathrm{eV}$), and momentum offset ($0.03\,\text{Å}^{-1}$) agree with the theoretical predictions. Due to their symmetry, these states are expected to be particularly responsive to an in-plane gradient. The abovementioned mechanism and its implications on dispersion and spin polarization are discussed.

O 48.7 Thu 12:45 HSZ 02

Unconventional Fermi surface spin patterns in the (Bi/Pb/Sb)/Ag(111) surface alloy — •Fabian Meier[1,2], Vladimir Petrov[3], Luc Patthey[2], Jürg Osterwalder[1], and Hugo Dil[1,2] — [1]Physik Institut Universität Zürich, CH — [2]Swiss Light Source PSI, CH — [3]Physics Institute St Petersburg, RU

By a controllable change in the stoichiometry of the long range ordered mixed surface alloy (Bi/Pb/Sb)/Ag(111) the Rashba and Fermi energy can be tuned over a wide range. We show by spin and angle-resolved photoemission spectroscopy that the spin structure of the individual surface state bands remain unaffected despite the random intermixing of the adatoms. We further report on the observation of unconventional Fermi surface spin textures. These spin textures are found when the Fermi energy lies between the crossing point and the apex of the Rashba type Kramer's pair. The results will be discussed in the context of spin transport.