O 100: Electronic Structure of Surfaces: Spectroscopy, Surface States II

Time: Thursday 16:00–18:30 Location: WIL C307

O 100.1 Thu 16:00 WIL C307

Existence of Topological Nontrivial Surface States in Strained Transition Metals: W, Ta, Mo, and Nb — Danny Thonig[1], Tomáš Rauch[2], Hossein Mirhosseini[3], •Jürgen Henk[2], Ingrid Mertig[2,3], Henry Wortelen[4], Bernd Engelkamp[4], Anke B. Schmidt[4], and Markus Donath[4] — [1]University Uppsala, Sweden — [2]Martin Luther University Halle-Wittenberg — [3]Max Planck Institute of Microstructure Physics, Halle — [4]Westfälische Wilhelms-Universität, Münster

We show that a series of transition metals with strained body-centered cubic lattice—W, Ta, Nb, and Mo—hosts surface states that are topologically protected by mirror symmetry and, thus, exhibits nonzero topological invariants. These findings, reported in [1], extend the class of topologically nontrivial systems by topological crystalline transition metals. The investigation is based on calculations of the electronic structures and of topological invariants. The signatures of a Dirac-type surface state in W(110), e. g., the linear dispersion and the spin texture, are verified. To further support our prediction, we investigate Ta(110) both theoretically and experimentally by spin-resolved inverse photoemission: unoccupied topologically nontrivial surface states are observed.

[1] D. Thonig *et al.*, Phys. Rev. B **94** (2016) 155132.

O 100.2 Thu 16:15 WIL C307

Asymmetric Rashba band topology of Fe films — •Sanjoy Kr Mahatha[1], Paolo Moras[1], Gustav Bihlmayer[2], Polina M Sheverdyaeva[1], and Carlo Carbone[1] — [1]Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, 34149 Trieste, Italy — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The control and manipulation of the electron spin in a two-dimensional system without the need to apply an external magnetic field is a key topic in condensed matter research aiming at future spintronic devices. In this regard, heterostructures where heavy metal and ferromagnetic layers brought in contact, are attracting increasing interest since the Rashba effect and exchange interaction can together control the electron transport. Electronic spin bands in ferromagnetic metal exhibit exchange energy splitting, while the Rashba spin-orbit effect shifts the spin-polarized bands in k||. The combination of these effects has been realized at the interface of a Fe thin film grown on a W(110) substrate. We find an asymmetry in the band dispersion of Fe quantum well states along structurally equivalent directions, resulting from exchange and spin-orbit effects at the interface and propagating in the whole film.

O 100.3 Thu 16:30 WIL C307

One and two-photon photoemission from the giant Rashba system Bi/Ag(111) — •Philipp Rosenzweig, Sebastian Otto, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Time- and angle-resolved, mono- and bichromatic two-photon photoemission (2PPE) with different photon energies $h\nu$ ranging from 1.51 eV to 4.89 eV is used to study the electronic structure of the $(\sqrt{3}\times\sqrt{3})R30°$ substitutional surface alloy Bi/Ag(111). Various unoccupied band structure features are found, such as a surface state dispersing downwards from around 1.1 eV above the Fermi level as well as two image-potential states with binding energies of 0.69 eV and 0.18 eV. The spin-split sp_z surface state [1] is also identified as an initial state in 2PPE and in one-photon photoemission at $h\nu = 6.2$ eV. In addition, circular dichroism is employed as an indirect probe of the unconventional spin structure [2] of this giant Rashba system.

[1] C. R. Ast et al., Phys. Rev. Lett. **98**, 186807 (2007).
[2] S. N. P. Wissing et al., Phys. Rev. Lett. **113**, 116402 (2014).

O 100.4 Thu 16:45 WIL C307

Multiple Dirac cones at the surface of the topological metal LaBi — •Jayita Nayak[1], Shu-Chun Wu[1], Nitesh Kumar[1], Chandra Shekhar[1], Sanjay Singh[1], Jörg Fink[1,2], Emile E. D. Rienks[2,3], Gerhard H. Fecher[1], Stuart S. P. Parkin[4], Binghai Yan[1,5], and Claudia Felser[1] — [1]Max Planck Institut CPFS, Dresden, Germany — [2]Leibniz Institut fur Festkorper- und Werkstoffforschung IFW Dresden, Dresden, Germany — [3]Institute of Solid State Physics, Dresden University of Technology, Dresden, Germany — [4]Max Planck Institute for Microstructure Physics, Halle, Germany — [5]Max Planck Institute for Physics of Complex Systems, Dresden, Germany

The rare-earth monopnictide LaBi, LaSb exhibits very large, unusual magnetoresistance which stimulates the interest in directly observing any topological surface states. Although band inversions have been postulated to induce a topological phase in LaBi but there were no experimental evidence for topological surface states in this compound. By using angle-resolved photoemission spectroscopy (ARPES) and ab initio calculations, we have revealed the existence of topological surface states of LaBi through the observation of three Dirac cones: two coexist at the corners and one appears at the center of the Brillouin zone. The odd number of surface Dirac cones is a direct proof of the topological nature of LaBi compound. Our results afford insight of the topological surface states of LaBi and semi-metallicity and related magneto-transport properties.

O 100.5 Thu 17:00 WIL C307

Reconstruction-induced trefoil knot Fermi contour of Au(111) — •Maciej Dendzik, Marco Bianchi, Matteo Michiardi, Charlotte Sanders, and Philip Hofmann — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark

Using angle-resolved photoemission spectroscopy (ARPES), we study the effect of the so-called herringbone reconstruction of Au(111) on the dispersion of the free electron-like surface state [1]. While earlier ARPES investigations have only reported a minor interplay of the surface state dispersion and the underlying reconstruction, we show that the uniaxial lattice distortion and the thereby changed reciprocal lattice for the first atomic layer leads to distinct surface state dispersions around the first order reciprocal lattice points of the three domains, creating a constant energy surface resembling a trefoil knot. The findings resolve the long-standing discrepancy between, on one hand, the reconstruction-induced surface state modifications reported in scanning tunnelling microscopy and first principle calculations and, on the other hand, their conspicuous absence in photoemission.

[1] M. Dendzik *et al.*, Phys. Rev. B (Rapid Communication) **94**, 201401 (2016).

O 100.6 Thu 17:15 WIL C307

Strain–induced surface state shift on Ag(111) and Ag/Fe(110) — •Schmitt Martin, Kemmer Jeannette, and Bode Matthias — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The surface electronic properties of both, pristine Ag(111) as well as Ag films grown on various substrates, are well studied. Especially the spectroscopic fingerprint of the *L*-gap Shockley-type surface state (SS) is commonly used for calibration purposes. While the SS onset is energetically located at $E_{SS} = -65$ meV on pristine Ag(111), a depopulation was observed on strongly miscut Ag(111) crystals [1]. Furthermore, thin Ag films grown on Si(111) indicated that the SS onset may also be influenced by strain that occurs around dislocation lines [2,3].

We have investigated in the electronic properties of Ag(111) around screw dislocations found on a pristine single crystal by low temperature scanning tunneling spectroscopy. While the expected electronic properties are confirmed on terraces, strain–induced spatial variations of the SS onset are observed at certain locations around screw dislocations. The structure–electronic property relationship identified on Ag(111) will be used to qualitatively explain the SS pinning of the Ag/Fe(110) epitaxial system.

[1] K. Morgenstern *et al.*, Phys. Rev. Lett. **89**, 226801 (2002).
[2] Neuhold and Horn, Phys. Rev. Lett. **78**, 1327 (1997).
[3] K. Sawa *et al.*, Phys. Rev. Lett. **104**, 016806 (2010).

O 100.7 Thu 17:30 WIL C307

Manipulation of two-dimensional states at the $XTiO_3$ surface (X=Sr, Ba, Ca) — •Stefan Muff[1,2], Mauro Fanciulli[1,2], Nicolas Pilet[2], Andrew Weber[1,2], Zoran Ristic[2], Zhiming Wang[2], Nicholas Plumb[2], Milan Radovic[2,3], and Hugo Dil[1,2]

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The discovery of a two dimensional electron gas (2DEG) at the surfaces of clean $SrTiO_3$ and $KTaO_3$ triggered research into possibilities to manipulate its characteristics in a controlled manner, using the wide range of physical properties as ferroelectricity, superconductivity, and giant magneto resistance observed in this class of materials. A more direct way to influence the properties of the 2DEG is by chemical or lattice strain and by changes of the atomic structure of the sample surface. In this work we grow films of different perovskites by the help of pulsed laser deposition and studied the formation and properties of the 2DEG by UV ARPES.

We will show the existence of two dimensional states at the surface of of $BaTiO_3$ and $CaTiO_3$ films, whose properties are closely related, but different, to the states present on $SrTiO_3$ and $KTaO_3$. The growth of films with variable thicknesses and combinations of different perovskites, as well as the variation of surface geometry, gives us the ability to directly manipulate the properties of the two-dimensional as well as the three dimensional surface-related states.

O 100.8 Thu 17:45 WIL C307

Quantum well states and their coupling to phonons in thin multilayer Pb films on Si(111) — •Maedeh Zahedifar and Peter Kratzer — University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

The relaxation of electrons in metals far away from equilibrium constitutes a field of research that has attracted considerable attention recently. Moreover, thin metallic films on semiconductor substrates lend themselves to the study of quantum size effects in metals. In our work, we attempt to develop a sound basis for the investigation of electronic relaxation processes in atomically thin Pb layers by working with the $\sqrt{3}\times\sqrt{3}$ model for film thicknesses between 3 and 6 ML. Density functional theory calculations with the projector augmented-wave method using the software package VASP [1] are employed to obtain both the electronic and the phononic two-dimensional band structure of these films. Subsequently, the strength of the electronic-phonon coupling is investigated for some representative (either occupied or unoccupied) quantum well states in the four-layer and five-layer Pb films. The results are compared to experimental data of the energetic position, dispersion and lifetime broadening of quantum well states.

[1]G. Kresse and D. Joubert, Phys. Rev. B, 59, (1999).

O 100.9 Thu 18:00 WIL C307

Double photoemission of Pb in its normal state — Yuri Aliaev, Ilya Kostanovskiy, Jürgen Kirschner, and •Frank O. Schumann — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

We investigated double photomemission (DPE) from a polycrystalline Pb surface at room temperature. The valence consists of 6s and 6p states which are separated by an energy gap of 3.1 eV. This allows to investigate the electron-electron interaction of states with different orbital symmetry without hybridisation. The low-lying 5d core levels can be excited with a laboratory light source. Hence, core-valence-valence Auger-Photoelectron coincidences can be detected. The measured DPE intensity is dominated by the emission of 5d photoelectrons and the resulting Auger electron. The Auger electron line shape has mainly contributions due the 6p electrons rather than 6s electrons. From the sum energy spectra we find that the effective Coulomb interaction U_{eff} is to close to zero. The DPE intensity directly from the valence band is an order of magnitude smaller than the core-assisted emission. This is consistent with the small value of U_{eff}.[1,2] We discuss the experimental prospect of Cooper pair emission upon photon absorption which has been predicted theoretically.[3]

[1] B.D. Napitu and J. Berakdar, Phys. Rev. B 81, 195108 (2010).
[2] F.O. Schumann et al., Phys. Rev. B 93, 235128 (2016).
[3] K.A. Kouzakov and J. Berakdar, Phys. Rev. Lett. 91, 257007 (2003).

O 100.10 Thu 18:15 WIL C307

Double photoemission from transition metal surfaces — •Ilya Kostanovskiy, Yuri Aliaev, Gianluca Di Filippo, Jürgen Kirschner, and Frank O. Schumann — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

The evolution of the 4p photoemission spectra for the 4th group transition metals exhibits large line width. This is assigned to the breakdown of the one-electron picture and electron-electron interaction.[1] Photoemission from the 4p level is accompanied by the Auger decay resulting in the final state with two holes in the 4d level. The process of the Auger-photoelectron double photoemission (DPE) can be studies via coincidence photoemission technique. Recent studies of the DPE spectra of Pd and Ag revealed clear evidence of the attosecond dynamics of the 4p photoemission process.[2]

We studied the DPE process involving the 3d and 4p levels from Cd, In, Sn and Sb surfaces. In contrast to the Pd case, the 4d state of these materials is not part of the valence band but a core level. We measured 2D energy distributions of DPE process and plotted the sum energy shape of the Auger-photoelectron pairs. We discuss the 2D energy distributions in terms of ultrafast electron dynamics of the Auger-photoelectron pair emission. The sum energy plots of the 4p and 3d DPE spectrum are very similar despite the very different timescales.

[1] M. Ohno and G. Wendin, Solid State Commun. 39, 875 (1981).
[2] I. Kostanovskiy et al., J. Phys. Condens. Matter 28, 15601 (2016).