O 29: Topological Insulators

Time: Tuesday 10:30–13:15 Location: GER 38

O 29.1 Tue 10:30 GER 38

Topological Insulator goes Elemental: α-Sn on InSb — •M. R. Scholz[1], A. Barfuss[1], L. Dudy[1], A. Fleszar[2], G. Bihlmayer[3], D. Wortmann[3], J. H. Dil[4], G. Landolt[4], M. Radovic[4], G. Li[2], R. Claessen[1], and J. Schäfer[1] — [1]Phys. Inst. and RCCM, Univ. Würzburg — [2]Inst. f. Theo. Physik u. Astronomie, Univ. Würzburg — [3]Peter Grünberg Inst. a. Inst. f. Advanced Simulation, FZ Jülich — [4]Swiss Light Source, Paul-Scherrer-Institut Villigen

We report on the topological insulator phase of epitaxially grown α-Sn on InSb substrates where compressive strain is induced by a slight lattice mismatch. The topological surface state (TSS) forms in the presence of an unusual band order not based on direct spin-orbit coupling, as shown in DFT and GW slab-layer calculations. Angle-resolved photoemission probes how the TSS emerges from the second highest bulk valence band. By means of spin-resolved photoemission we show that the surface state is highly spin-polarized with a counter-clockwise helicity below the Dirac point. The band situation in α-Sn closely resembles that of strained HgTe. Quantum well films of HgTe sandwiched between CdTe are a system where the topological properties have been successfully probed in DC transport [1]. The similarities to HgTe make α-Sn a promising candidate to exhibit the quantum spin Hall effect as well, if the film thickness is reduced to the 2D limit. Particularly, as a nontoxic elemental system, α-Sn is easier to fabricate which opens various pathways to access and manipulate the topological surface state. As a first step, we demonstrate the precise control of the Fermi level by dopants. [1] M. König et al., Science 318, 766 (2007).

O 29.2 Tue 10:45 GER 38

Temperature effects in soft and hard x-ray photoemission from topological insulators — •Jürgen Braun, Jan Minar, and Hubert Ebert — Dept. Chemie, LMU Universität München, Germany

A brief introduction to the theory of temperature-dependent soft and hard x-ray angle-resolved photo electron spectroscopy (SARPES, HARPES) of solid materials is given with an emphasis on the so-called one-step-model of photoemission. The main aspects of the theory [1,2] and its implementation within the Munich SPR-KKR program package [3] will be reviewed. Our method, which is based on the Coherent Potential Approximation (CPA) alloy theory (alloy analogy model), goes well beyond the simple, but standard Debye-Waller approach to photoemission by including in particular the temperature dependence of the effective photoemission matrix elements as well. This allows among others to reproduce the so called XPS- or density of states limit in angle-resolved photoemission which occurs for high photon energies and/or high temperatures due to a full Brillouin zone averaging caused by phonon scattering. First examples of soft- and hard x-ray ARPES calculations at finite temperature for W(110), Sb_2Te_3 and Bi_2Se_3 will be presented.

1. A. Gray, J. Minár, J. Braun, H. Ebert, C. S. Fadley et al., Nature Materials, **10**, 759 (2011) and Nature Materials **11**, 957 (2012) 2. J. Braun, J. Minár, H. Ebert et al. Phys. Rev. B **88** 005400 (2013) 3. H. Ebert et al., The Munich SPR-KKR package, version 6.3, http://olymp.cup.uni-muenchen.de/ak/ebert/

O 29.3 Tue 11:00 GER 38

Reorganization of a Topologically Protected Surface State: Theory for Au-Covered Bi_2Te_3(111) — Francisco Muñoz[1,2], •Jürgen Henk[2], and Ingrid Mertig[2] — [1]Facultad de Ciencias, Universidad de Chile, Chile — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

The electronic structure of Au-covered Bi_2Te_3 is investigated by first-principles calculations. The Dirac surface state of the topological insulator Bi_2Te_3 hybridizes with the Au sp states, which gives rise to strong reorganization of the surface electronic structure. Striking features of the modified Dirac surface state are (i) the introduction of new Dirac points within the fundamental band gap of Bi_2Te_3, (ii) an extremely weak dispersion, and (iii) an anisotropic number of conducting channels in the fundamental band gap of Bi_2Te_3 which leads to a complicated Fermi surface. Our findings have impact for spin-dependent surface transport.

O 29.4 Tue 11:15 GER 38

Barrier-free sub-surface incorporation of magnetic impurities into the Bi(111) surface: Manipulation of the protected surface state - Experiment — •C. Klein[1], P. Zahl[2], N. Vollmers[3], U. Gerstmann[3], D. Lückermann[4], G. Jnawali[1], H. Pfnür[4], C. Tegenkamp[4], W.-G. Schmidt[3], P. Sutter[2], and M. Horn-von Hoegen[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, DE — [2]Center for Functional Nanomaterials, Brookhaven National Laboratory, New York, USA — [3]Department of Physics, University of Paderborn, DE — [4]Institut for Solid State Physics, University of Hannover, DE

Due to the large spin orbit coupling, electron backscattering within the Bi(111) surface states is strongly suppressed. In order to identify possible scattering mechanisms we performed low temperature scanning tunneling microscopy (LT-STM) measurements in which submonolayer amounts of 3d-metals (Fe, Co, Ni, Cu) were deposited at 5K. The metal atoms become immediately embedded in a sub-surface site, as they are not present in STM topography. They only become apparent in STS at tunneling conditions close to the Fermi-energy, as they are surrounded by a pronounced anisotropic threefold electronic scattering pattern with lateral dimensions of more than 10 nm. DFT calculations indeed confirm a barrier free incorporation of the 3d-metal impurities into the first Bi-Bilayer even at such low temperatures. This incorporation effect is limited to 3d-metals, as screening effects of the s- and p- orbitals are of great importance and leads to an effective reduction of the free surface energy of about 5 eV.

O 29.5 Tue 11:30 GER 38

Efficient full-relativistic DFT calculations for large systems: Application to Bi-related surface states — •Uwe Gerstmann[1], Nora Jenny Vollmers[1], Wolf Gero Schmidt[1], Claudius Klein[2], Michael Horn-von Hoegen[2], Philipp Kröger[3], Daniel Lückermann[3], Herbert Pfnür[3], and Christoph Tegenkamp[3] — [1]Department of Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn — [2]Center for Nanointegration CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg — [3]Institut for Solid State Physics, University of Hannover, Appelstr. 2, 30167 Hannover

Spin-orbit coupling is well-known to be the driving force behind ferromagnetism and can be used to control the functionality of electronic devices in spintronics. In asymmetric quantum wells and at surfaces spin-split electron gases may form and give rise to the Rashba-effect. In some cases, e.g. Bi(111) bilayers, the bandstructures are furthermore affected by k-point dependent shifts in the order of several eV. This effect may become crucial if adatoms are incorporated or adsorbed at the surface, strongly influencing the occupancy of the adatom-induced states and by this the magnetic moments and further magneto-transport properties of the resulting structures. In this work, we present an efficient pseudopotential-based method that allows a full-relativistic description of large systems containing several hundreds of atoms. The approach is used to describe the incorporation of a wide range of atomic species (3d-transition, coin-metal as well as rare-earth ions) into Bi(111) surfaces, where supercells with more than 200 atoms are needed to describe the resulting extended magnetic structures correctly.

O 29.6 Tue 11:45 GER 38

Magnetic impurities on Bi thin films - Conductivity and surface diffusion — •Philipp Kröger[1], Daniel Lükermann[1], Sergii Sologub[2], Nora Vollmers[3], Uwe Gerstmann[3], Wolf Gero Schmidt[3], Herbert Pfnür[1], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Inst. für FKP, Appelstr. 2, 30167 Hannover — [2]Inst. of Ph., Nat. Acad. of Sc., Nauky Av. 46, 03028 Kyiv, Ukraine — [3]Universität Paderborn, Theoretische Physik, 33098 Paderborn

The semimetal bismuth has attracted a lot of interest because of its unique electronic properties such as a low carrier concentration and a large mobility. The surface states reveal a pronounced Rashba splitting and the conductivity can be well discriminated from bulk contributions if thin films are grown epitaxially on Si(111) substrates, making surface related effects accessible even in macroscopic conductance measurements.
In this context the adsorption of the magnetic atom Cr (4,8 μ_B) on the Bi(111) surface will be discussed. In comparison to other adsorbates

(Fe, Co, Tb) Cr exhibits the strongest scattering effect, accompanied by a transition from Weak Anti- to Weak Localization. This transition indicates strong impurity scattering, which lifts all spin-dependent selection rules. Furthermore, a significant increase of electron concentration due to hybridization effects has been found. For Tb and Cr surface diffusion of adsorbate-atoms even at T≈10 K needs to be considered.

O 29.7 Tue 12:00 GER 38

Magnetic interaction and magnetic fluctuations in topological insulators with ordered and disordered magnetic adatoms — •MAIA G. VERGIORY[1,4], LEVAN CHOTORLISHVILI[2], ARTHUR ERNST[1], VITALI DUGAEV[1], ANDREAS KOMNIK[3], MIJAIL OTROKOV[4], EVGUENI CHULKOV[4], and JAMAL BERADKAR[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Institut fr Physik, Martin-Luther-Universitat Halle-Wittenberg, Germany — [3]Institut fr Theoretische Physik, Universitt Heidelberg, Germany, — [4]Donostia International Physics Center, Donostia - San Sebastian, Spain

Using a first-principles Green's function approach we study magnetic properties of the magnetic binary topological insulators Bi2Se3, Bi2Te23 and Sb2Te3 doped with 3d transition metals. We analyze the magnetic phase for each dopant, the exchange interaction, the Curie temperature and the Bloch spectral function. Furthermore, we observe that the interaction of magnons with surface electrons essentially renormalizes the electron energy spectrum. The renormalized spectrum is nonlinear and can be characterized by a negative effective mass of electrons and holes for any k point different from 0. The electron velocity near the Dirac point depends on the electron-magnon coupling.

O 29.8 Tue 12:15 GER 38

The edge state at the dark side of the weak topological insulator $Bi_{14}Rh_3I_9$ probed by STM — •Christian Pauly[1], Bertold Rasche[2], Marcus Liebmann[1], Marco Pratzer[1], Klaus Koepernik[3], Manuel Richter[3], Michael Ruck[2], Jeroen van den Brink[3], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University and Jara Fit, Germany — [2]Departement of Chemistry and Food Chemistry, TU Dresden, Germany — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Germany

Using scanning tunneling microscopy (STM) and spectroscopy (STS) at 6 K, we probe the local atomic and electronic structure of the weak topological insulator $Bi_{14}Rh_3I_9$ [1]. In [001]-direction, the material is built from stacks of intermetallic planes with non-trivial 2D topology and spacer layers in between. Thus, the surfaces of the intermetallic planes, which are the natural cleaving planes of the material, exhibit a trivial band gap however with topologically protected states at each step edge [1]. $Bi_{14}Rh_3I_9$ is cleaved at a base pressure of 10^{-10} mbar giving rise to several hundreds of nm large terraces of the intermetallic layer interrupted by step edges. Using STS, we identified the band gap on top of the intermetallic layer, which is in agreement with ARPES data, whereas at the step edges we directly mapped the edge state. The edge state appears continuously through the band gap and exhibits a spatial distribution of 0.4 nm FWHM. The observed spatial periodicity along the step edge is in line with the atomic structure confirming the Bloch type of this state. Partially, dispersive features appear which will be discussed. [1] B. Rasche et al., Nature Mater. 12, 422 (2013)

O 29.9 Tue 12:30 GER 38

Evidence for topological band inversion of the phase change material $Ge_2Sb_2Te_5$ — •Marcus Liebmann[1], Christian Pauly[1], Alessandro Giussani[2], Jens Kellner[1], Sven Just[1], Jaime Sanchez-Barriga[3], Emile Rienks[3], Oliver Rader[3], Raffaella Calarco[2], Gustav Bihlmayer[4], and Markus Morgenstern[1] — [1]II. Inst. Phys. B, RWTH Aachen University — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin — [3]Helmholtz-Zentrum für Materialien und Energie, BESSY, Berlin — [4]Peter-Grünberg-Institut and Institute für Advanced Simulation, Forschungszentrum Jülich

We present an angle-resolved photoemission study of the ternary phase change material $Ge_2Sb_2Te_5$, epitaxially grown on Si(111) in the metastable cubic phase. This material serves, e.g., in DVDs as a fast switchable material (1 ns) between the metallic cubic and an insulating amorphous phase. The observed upper bulk valence band shows a minimum at $\bar{\Gamma}$ being 0.3 eV below the Fermi level E_F and a circular Fermi contour around $\bar{\Gamma}$ with a dispersing diameter of $0.27-0.36$ Å^{-1}. This is in agreement with density functional theory calculations of the Petrov stacking sequence of the cubic phase which is topologically nontrivial. Moreover, the results are in line with all previous calculations of $Ge_2Sb_2Te_5$ exhibiting the valence band maximum at Γ for a trivial $\mathbb{Z}_2$ topology and away from Γ for a non-trivial one. Scanning tunneling spectroscopy exhibits a band gap of 0.4 eV around E_F. Our finding opens the perspective of ns-switching between a topological crystalline and an insulating amorphous phase.

O 29.10 Tue 12:45 GER 38

Step wise variation of the electrochemical potential at step edges of the Bi_2Se_3 surface — •Christian A. Bobisch, Sebastian Bauer, and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

Bi_2Se_3 is a 3D topological insulator (TI) whose surface states are protected from direct backscattering by time reversal symmetry [1]. However, step edges on a Bi_2Se_3 surface are predicted to work as an electron scatterer for other scattering angles than 180° backscattering [2]. We studied the electron transport on the surface of a 14.5 QL (quintuple layer) thick Bi_2Se_3 film grown on Si(111). By a distance dependent resistance measurement [3] in the μm range, we found a metallic character of the film with a sheet conductance of $2\times10^{-3}\Omega^{-1}$ which agrees well with recent literature [4]. By scanning tunneling potentiometry (STP) [5], we simultaneously analyzed the topography and the electrochemical potential μ_{ec} under real transport conditions. We observe on the microscopic scale a potential gradient which corresponds well the macroscopic conductance. In the vicinity of step edges we find a step-like variation of μ_{ec} which is a fingerprint of electron scattering at the step edge. For the given sample the electrical conductivity of a 1 QL step could be deduced to $3800\pm500\Omega^{-1}$cm^{-1}.

[1] M. Z. Hasan et al., Rev. Mod. Phys. 82, 3045 (2010). [2] W. Jing et al., Chin Phys. B 22, 067301 (2013). [3] P. Jaschinsky et al., J. Appl. Phys. 104, 094307 (2008). [4] A. A. Taskin et al., Phys. Rev. Lett. 109, 066803 (2012). [5] P. Muralt et al., Appl. Phys. Lett. 48, 514 (1986).

O 29.11 Tue 13:00 GER 38

Quantum phase transitions of a disordered antiferromagnetic topological insulator — •Paul Baireuther[1], Jonathan M. Edge[1], Ion C. Fulga[1], Carlo W.J. Beenakker[1], and Jakub Tworzydlo[2] — [1]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — [2]University of Warsaw, Hoza 69, 00-681 Warsaw, Poland

We have studied the effect of electrostatic disorder on the conductivity of a three-dimensional antiferromagnetic insulator (a stack of quantum anomalous Hall layers with staggered magnetization). The phase diagram contains regions where the increase of disorder first causes the appearance of surface conduction (via a topological phase transition), followed by the appearance of bulk conduction (via a metal-insulator transition). The conducting surface states are stabilized by an effective time-reversal symmetry that is broken locally by the disorder but restored on long length scales. A simple self-consistent Born approximation reliably locates the boundaries of this socalled "statistical" topological phase.