O 49 Electronic structure IV

Time: Friday 11:15–13:00 Room: WIL B321

O 49.1 Fri 11:15 WIL B321

Self-energy and many-body effects in graphite — •S. Bengiò[1], T. K. Kim[1], Ph. Hofmann[1], A. Leonardo[2], and E. V. Chulkov[2] — [1]Institute for Storage Ring Facilities and iNano Center, University of Aarhus, 8000 Aarhus C, Denmark — [2]Donostia International Physics Center (DIPC), 20018 San Sebastián / Donostia, Basque Country, Spain

Graphite is a semimetal, a prototype of layered crystals and the parent compound for carbon nanotubes. Despite of its great importance, detailed studies of many body effects by angle-resolved photoemission (ARPES) are rare, mostly caused by the lack of high-quality samples. Here we present an ARPES study on high-quality graphite films grown on a SiC substrate. The temperature dependence of the self energy was determined by a systematic linewidth analysis for the Fermi surface states close to the $\bar{K}$ point of the surface Brillouin zone. The Fermi surface crossing is sharp in momentum space (of the order of 0.07 $Å^{-1}$) and its full width at half maximum is almost constant for temperatures between 70 and 600 K. The experimental results for the self-energy are compared to first principles calculations for one layer of graphene.

O 49.2 Fri 11:30 WIL B321

Fermi Surface of Be(0001) — •Ivana Vobornik[1], Jun Fujii[1], Mattia Mulazzi[1,2], Giancarlo Panaccione[1], Michael Hochstrasser[3], and Giorgio Rossi[1,2] — [1]TASC National Laboratory, INFM-CNR, S.S. 14, km 163.5, I-34012 Trieste — [2]Dipartimento di Fisica, Universita di Modena e Reggio Emilia, Via Campi 213/A, I-41100 Modena — [3]Laboratorium für Festkörperphysik, Wolfgang-Pauli-Str. 16, ETH Hönggerberg, CH-8093 Zürich

We used angle-resolved photoemission (ARPES) to determine the Fermi surface of Be(0001). The Fermi surface cuts that were measured for more than twenty different photon energies enabled us to reconstruct the three-dimensional Fermi surface. We find that the Fermi surface obtained from the ARPES data differs significantly from the Fermi surface of bulk beryllium determined by de Haas - van Alphen oscillations. The so-called cigar features appear to be significantly shorter, while the coronet is enlarged. Furthermore, new states appear in the gap between the two subsequent cigars. This change of the Fermi surface topology is the consequence of the surface relaxation in Be(0001) and the ARPES surface sensitivity (mean free pass in the photon energy range used in our experiment is only 2-3 Å). Our data are relevant for any theory aiming to describe the considerable surface relaxation in Be(0001).

O 49.3 Fri 11:45 WIL B321

Surface electronic structure of Cr(001) — •Michael Budke[1], Tobias Allmers[1], Matthias Bode[2], Georgi Rangelov[1], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, D-48159 Münster — [2]Institute of Applied Physics and Microstructure Research Center, Jungiusstr. 11, D-20355 Hamburg

There is an ongoing controversy whether a sharp peak close to the Fermi level E_F which appears in scanning tunneling spectroscopy (STS) measurements on the Cr(001) surface is related to a d_{z^2}-like surface state [1] or to an orbital Kondo resonance [2]. A recent variable-temperature STS study was not able to bring about a decision which of the two interpretations is correct [3]. We have performed photoemission and inverse photoemission measurements on the Cr(001) surface to reveal the nature of the electronic states just below and above E_F. Surface- and bulk-like contributions are identified by their sensitivity to adsorbates. In agreement with previous STS data, we found a surface sensitive feature in our IPE measurements just above E_F. The results are dicussed in terms of their compatibility to the surface state and Kondo resonance model.

[1] J. A. Stroscio *et al.*, Phys. Rev. Lett. **75**, 2960 (1995).
[2] O. Y. Kolesnychenko *et al.*, Nature **415**, 507 (2002).
[3] T. Hänke *et al.*, Phys. Rev. B **72**, 085453 (2005).

O 49.4 Fri 12:00 WIL B321

Electronic Structure of the (2×3)–N/Cu(110) Surface — •Peter Lendecke, Tobias Allmers, Georgi Rangelov, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Sputtering a Cu(110) surface with nitrogen and subsequent annealing induces a (2×3) reconstruction. The copper atoms in the topmost layer are arranged in a nearly square array formed by additional $[1\bar{1}0]$–rows. Nitrogen atoms are bonded in almost every second hollow site of this strongly corrugated pseudo–(100) layer [1].
We investigated the unoccupied electronic structure of this reconstructed surface by angle–resolved inverse photoemission. Preparation of the reconstruction was controlled by LEED and *in–situ* STM. Inverse photoemission spectra are dominated by Cu(110) bulk transitions. The reduced surface Brillouin zone along [001] is reflected by surface *umklapp* processes. Unoccupied surface states of Cu(110) are already quenched at low nitrogen doses. The reappearance of a surface resonance along $[1\bar{1}0]$ in the high–dose regime is most probably due to improved long–range order of the surface.
[1] S. Moré et al., Surf. Sci. **381**, L589 (1997)

O 49.5 Fri 12:15 WIL B321

Electronic structure of ZnO$(11\bar{2}0)$ single crystals and thin films — •Stefan Andres[1], Christian Pettenkofer[1], Wolfgang Bremsteller[1], and Leonard Broekman[2] — [1]Hahn-Meitner-Institut, Glienicker Str. 100, D-14109 Berlin, Germany — [2]Department of Physics, La Trobe University, VIC, 3086, Australia

Zinc oxide (ZnO) is a transparent semiconductor with a direct band gap of about 3.3eV. This makes ZnO an interesting candidate for future applications in transparent electronics and UV-light emission. In order to develop such devices a detailed understanding of the band structure of ZnO is neccessary.

However, until now angle resolved photoemission spectroscopy (ARPES) studies on ZnO focussed only on the highly symmetric (0001), $(000\bar{1})$ and $(10\bar{1}0)$ surfaces. We present comparative ARPES results from ZnO$(11\bar{2}0)$ single crystals and MOMBE grown thin films, recorded at the TGM7 beamline at BESSY II synchrotron light facility in Berlin. The spectra clearly show energy dispersions of the occupied valence states as a function of the wave vector both perpendicular and parallel to the surface. Our results are discussed along with band structure calculations.

O 49.6 Fri 12:30 WIL B321

Band structure of epitaxially grown $CuInS_2$ films — •Carsten Lehmann[1], Ralf Hunger[2], and Christian Pettenkofer[1] — [1]Hahn-Meitner Institut, SE6, Berlin, Germany — [2]TU Darmstadt, Oberflächenforschung, Inst. f. Materialforschung

The ternary compound semiconductor $CuInS_2$ with a direct band gap of 1.53 eV seems to be very promising as absorber material for thin film solar cells. For a better understanding of the parameters determining the properties of a junction detailed information on the electronic structure is necessary. Besides a calculation of Zunger et al [1] no experimental data on the valence electronic structure of $CuInS_2$ are available.

We report on thin epitaxial $CuInS_2$ layers prepared on sulfur passivated GaAs (100). To have a better control on the deposition process we introduced a MOMBE type deposition with an organic sulfur precursor.

Clean and well defined surfaces were obtained despite a lattice mismatch of 2%. Samples were prepared in a dedicated UHV deposition and analysis system. Precharacterized samples were transferred by an UHV box within 15min to the TGM7 beamline at BESSY and investigated by ARUPS. We will discuss the obtained band structure with respect to available theoretical data and derive the effective mass from the valence band curvature. Implications of the observed reconstruction on the band structure will be discussed.

[1] E.J. Jaffe, A. Zunger, Phys. Rev. B 28, 1983, 5822

O 49.7 Fri 12:45 WIL B321

Electronic bandstructure of the NiMnSb(001) surface below and above the Fermi energy — •Christian Eibl, Juliet Slayton Correa, Georgi Rangelov, Jürgen Braun, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

For more than 20 years the Half-Heusler alloy NiMnSb has been investigated because of its predicted 100% spin polarization at the Fermi energy E_F [1]. Together with its high Curie temperature (750 K), this material is interesting for many technological applications.

We report on surface bandstructure measurements for the (001) surface of single crystal NiMnSb. The experimental techniques used are angle resolved ultraviolet photoemission spectroscopy (ARUPS) und inverse Photoemission spectroscopy (ARIPES) to probe the bandstructure both below and above E_F. ARUPS and ARIPES are used quasi-simultaneously in a multi-chamber UHV-system to ensure well defined and equal sample preparation conditions.
We see both non-dispersive (ARIPES) and dispersive (ARUPS) structures in the spectra, which stem from d-like bulk states. Furthermore, by comparison with theoretical calculations, we have found a surface state candidate.
[1] R.A. deGroot et al., Phys. Rev. Lett. 50, 2024 (1983)