O 100: Electronic Structure of Surfaces II

Time: Thursday 10:30–13:00 Location: REC C 213

O 100.1 Thu 10:30 REC C 213

Scanning tunneling spectroscopy on Be(0001) — •Hermann Osterhage, Roland Wiesendanger, and Stefan Krause — Department of Physics, University of Hamburg, Germany

Beryllium is an alkaline earth metal with peculiar electronic properties. The bulk material behaves similar to a semiconductor with a partial bandgap around the Fermi energy. In contrast, on the Be(0001) surface there is a delocalized electron system contributing substantially to the electronic density of states (DOS) at the Fermi energy.[1] Large amplitudes of Friedel oscillations seen in STM near the Fermi level disagree with a nearly free electron model.[2] A charge density wave and electron-phonon coupling were proposed as possible explanations for this deviation. More recently, the presence of Dirac node lines of surface bands in alkaline earth metals was identified as another possible cause for the unusually large amplitude observed in STM.[3]

While the surface bands of Be(0001) have been studied in angle resolved photoemission spectroscopy,[4] investigations using scanning tunneling spectroscopy have been lacking so far. We recorded tunneling spectra on a clean Be(0001) surface and mapped the charge oscillations at cryogenic temperatures. The energy dependence of the charge oscillations' wave vector will be compared to the surface state dispersion derived from previous photoemission studies.

[1] P. J. Feibelmann *et al.*, Phys. Rev. B **50**, 17480 (1994).
[2] P. T. Sprunger *et al.*, Science **275**, 1764 (1997).
[3] R. Li *et al.*, Phys. Rev. Lett. **117**, 096401 (2016).
[4] K. B. Ray *et al.*, Surf. Sci. **285**, 66 (1993).

O 100.2 Thu 10:45 REC C 213

Measuring the scattering phase shifts of single non-magnetic impurity atoms buried in Cu by STM — •Thomas Kotzott[1], Mohammed Bouhassoune[2], Henning Prüser[1], Samir Lounis[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Germany

Scattering in a solid due to impurity atoms and other crystal imperfections has been subject of research for decades because of its fundamental significance for our understanding of matter and its application in technology. Various experimental approaches have been used to access bulk scattering properties, especially the phase shift, which can be determined by transport properties or the de Haas-van Alphen effect. Here, we use a UHV-low temperature scanning tunneling microscope (STM) to measure the effective scattering phase shift of a single, non-magnetic impurity buried below a Cu(100) surface. We compare silver and germanium atoms by their LDOS surface signature which is created by standing electron waves in the crystal due to electron focusing. We reproduce the experimental topographies accurately with a simple tight-binding model that we use to determine the phase shift. The experimental values match for both species with calculations based on density functional theory. Furthermore, in energy-dependent data we find that the simple model of a Lorentzian scatterer has to be extended to characterize a non-magnetic atom on the local scale. This work was supported by DFG projects LO 1659/5-1 and WE 1889/8-1.

O 100.3 Thu 11:00 REC C 213

Observation of anisotropic vortices on clean superconducting Nb(110) — •Felix Friedrich, Artem B. Odobesko, Robin Boshuis, Stefan Wilfert, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The quest for Majorana zero modes in solid state systems requires the possibility to distinguish between true zero energy modes and the variety of other, trivial, modes that can occur inside the superconducting gap. Large values of the gap facilitate the analysis of these in-gap states. We suggest the clean Nb(110) surface that we obtain by electron beam heating [1] as a suitable platform for future investigations of possible topological states due to its large superconducting gap $\Delta_{\mathrm{Nb}} \approx 1.53\,\mathrm{meV}$. We use low-temperature STM/STS to examine the response of the Nb(110) surface to an external magnetic field. As a type-II superconductor, Nb(110) develops an Abrikosov lattice of vortices. Spectroscopy measurements at the vortex core reveal conductance peaks around zero bias, which we attribute to Caroli-de Gennes-Matricon states. Intriguingly, $\mathrm{d}I/\mathrm{d}U$ maps recorded at bias voltages corresponding to energies inside the superconducting gap uncover an anisotropic shape of the vortices. We explain this observation with the pronounced nesting of the Fermi surface of Nb(110).

[1] A. B. Odobesko *et al.*, Phys. Rev. B **99**, 115437 (2019).

O 100.4 Thu 11:15 REC C 213

Scanning Tunneling Microscopy of Sub-Surface Atomic Structure of the Phase Change Material $GeSb_2Te4$ **Enabled via Surface Antiresonances** — •Philipp Küppers[1], Peter Schmitz[2], Marcus Liebmann[1], Albert Ratajczak[3], Hilde Hardtdegen[4], Detlev Grützmacher[3], Riccardo Mazzarello[2], and Markus Morgenstern[1] — [1]II. Inst. Phys. B and JARA-FIT, RWTH Aachen University — [2]Institut für Theoretische Festkörperphysik, RWTH Aachen University — [3]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI 9) — [4]Forschungszentrum Jülich GmbH, Ernst Ruska Centre for Microscopy and Spectroscopy with Electrons (ERC-2)

The detailed atomic structure of phase change materials including its disorder is crucial for the understanding of many of its key features. A detailed mapping of the atomic disorder is challenging by standard approaches such as transmission electron microscopy, atom probe tomography or scanning tunneling microscopy. The latter suffers from the fact that the surface is covered by the well ordered Te layer. Here, we show by comparison of scanning tunneling spectroscopy and density functional theory data that details of the subsurface layer consisting of Ge, Sb and vacancies can be mapped by exploiting states that are suppressed towards the surface, so-called surface antiresonances. Probing such states becomes apparent as a honeycomb structure consisting of the Te layer and a significant contribution from the subsurface arrangement.

O 100.5 Thu 11:30 REC C 213

Layer thickness dependence of the electronic correlation in the surface alloy $CeAg_x$ **on Ag(111)** — •Katharina Kissner, Hendrik Bostelmann-Arp, and Friedrich T. Reinert — Experimentelle Phyik VII, Universität Würzburg

Ce-based compounds present a role model for the investigation of electronic correlation. At low temperatures the local interaction of conduction band electrons with the single *4f*-electron provided by Ce leads to distinct features in the electronic structure in $CeAg_x$ on Ag(111). These features appear in the valence band electronic structure in terms of the Kondo resonance, its spin orbit partner and the *4f*-ionization peak, as well as in the Ce *3d*-core levels. The appearance of Kondo physics strongly depends on the local environment of the Ce ion in the lattice and can therefore be modified by varying the alloy film thickness or by doping with different adatoms [1, 2].

In this study we investigate the electronic structure and stoichiometry of different surface alloy film thicknesses of $CeAg_x$ on Ag(111) by means of Angle Resolved and X-Ray Photoelectron Spectroscopy (ARPES and XPS). Furthermore we study the surface lattice structure by Low Energy Electron Diffraction and Scanning Tunneling Microscopy (LEED and STM). This provides us with the opportunity to tune the strength of the electronic correlation in $CeAg_x$ on Ag(111).

[1] H. Schwab, Phys. Rev. B, 85, 2012; [2] C. Praetorius et al., Phys. Rev. B 92, 045116, (2015)

O 100.6 Thu 11:45 REC C 213

Multiple scattering x-ray photoelectron diffraction study on the Ni-doped SrTiO3 (100) films — •Fatima Alarab[1,2], Sylvain Tricot[3], Berengar Leikert[4], Matthias Muntwiler[5], Karol Hricovini[2], Didier Sébilleau[3], and Ján Minár[1] — [1]NTC, University of West Bohemia, Pilsen, Czech Republic — [2]LPMS, Université de Paris Seine, Neuville sur-Oise, France — [3]IPR, Université de Rennes, Rennes, France — [4]RCCM, Universität Würzburg, Würzburg, Germany — [5]PSI, Villigen, Switzerland

The atomic surface structure of Ni-doped SrTiO3(100) films grown by pulsed laser deposition (PLD) method with (Ni=6 at% and 12 at%) was investigated by x-ray photoelectron diffraction (XPD) at the PEARL beamline of the Swiss-Light-Source. The main goal is to define Ni impurity locations (Substitutional and/or interstitial positions) in the hosting lattice. The results have been compared to similar XPD

measurements on pure SrTiO3(100) films. Ekin of all recorded spectra was chosen to be in the range of 190-198 eV. In this interval of energy, the photoelectron diffraction peaks are assigned by considering not only the forward scattering of photoelectrons by the atomic potential near the emitter atom, but also the backward scattering effects. This makes XPD more sensitive on an atomic scale and useful for local atomic structure analysis down to the monolayer and surface relaxation. With the large number of elastic scattering events, it was necessary to use the multiple scattering package for spectroscopies (MsSpec) in which same experimental conditions used for the XPD data acquisition were applied for the multiple scattering calculations.

O 100.7 Thu 12:00 REC C 213

In operando angle-resolved photoemission on a graphene device — •Davide Curcio[1], Alfred Jones[1], Jyoti Katoch[2], Klara Volckaert[1], Deepnarayan Biswas[1], Ryan Muzzio[2], Charlotte E. Sanders[3], Pavel Dudin[4], Cephise Cacho[4], Jill A. Miwa[1], Søren Ulstrup[1], and Philip Hofmann[1] — [1]Aarhus University, Denmark — [2]Carnegie Mellon University, USA — [3]Central Laser Facility, STFC Rutherford Appleton Laboratory, UK — [4]Diamond Light Source, UK

The electronic structure and properties of two-dimensional (2D) materials are widely tuneable via the choice of substrate, vertical electric fields or subtle structural features, and surprising new properties such as gate-switchable superconductivity have been observed in transport experiments. The directly accessible surface of 2D materials permits, at least in principle, a simultaneous study of transport properties and electronic structure using in-operando angle-resolved photoemission spectroscopy (ARPES). So far, this has been achieved for applied gating voltages but not in presence of a steady state current through the device, mainly because a large voltage drop within the area of the UV light spot proves detrimental to the energy resolution of the experiment. Here, using a graphene device as a model system, we show that this restriction can be overcome with a nano-scale light spot. We demonstrate non-invasive nanoARPES spectroscopy of the spectral function in a graphene device for current densities of up to $10^7 \mathrm{Acm}^{-2}$, mapping properties such as the local doping, many-body effects, conductivity, and carrier mobility.

O 100.8 Thu 12:15 REC C 213

Spectroscopic evidence for a charge-density wave in monoclinic TaTe2 — •Sanjoy K Mahatha[1], Florian Diekmann[2], Sebastian Rohlf[2], Matthias Kalläne[2,3], and Kai Rossnagel[1,2,3] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [3]Ruprecht-Haensel-Labor, Christian-Albrechts-Universität zu Kiel und Deutsches Elektronen-Synchrotron DESY, 24098 Kiel und 22607 Hamburg, Germany

Layered transition-metal dichalcogenides have been a subject of intense research for the last 40 years or so as they are characterized by a plethora of interesting physical phenomena including the formation of charge-density waves (CDWs). Recently, considerable interest in the electronic properties of transition-metal ditellurides has been sparked by the discoveries of Weyl fermions and extremely large magnetoresistance in WTe2 [1]. Within the ditelluride family, however, one compound, TaTe2, has received very little attention until now. Monoclinic TaTe2 undergoes a first-order structural transition around 170 K [2] that has been suggested to originate from a CDW instability. Yet, spectroscopic signatures of the interplay between the complex lattice distortion and charge-density modulation are still missing. Here, we will give a detailed account of the experimental geometric and electronic structure of this "neglected" material.

[1] M. N. Ali, et al., Nature 514, 205 (2014). [2] J. J. Gao, et al., Phys. Rev. B 98, 224104 (2018).

O 100.9 Thu 12:30 REC C 213

Investigation of strong correlation and topological phase in Thulium monochalcogenides $\mathbf{TmSe_{1-x}Te_x}$ — •Simon Müller[1], Chul-Hee Min[2], Celso Fornari[1], Chang-Jong Kang[3], Byung Il Min[4], Yong Seung Kwon[5], and Friedrich Reinert[1] — [1]Institut für Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany. — [2]IEAP, Christian-Albrechts-Universität zu Kiel, Germany. — [3]Departement of Physics and Astronomy, Rutgers University, New Jersey, USA. — [4]PCTP, Pohang University of Science and Technology, Republic of Korea. — [5]Department of Emerging Materials Science, DGIST, Daegu, Republic of Korea.

To understand the possible interplay between strong correlation and topology it is necessary to find a compound possessing these properties. Surface states with strongly localized 4f character is a good starting point, but the Dirac point has not been clearly identifying by experiments, yet. Our investigation of $\mathrm{TmSe}_{1-x}\mathrm{Te}_x$, which belongs to a mixed valence [1] and is predicted to show a band inversion in our DFT studies, has two main focuses. On the one hand, we try to continuously tune the lattice parameter of the system to a region, which for single crystalline samples was not reachable in ambient pressure, and on the other hand, we want to investigate other facets that are not possible to achieve by cleaving single crystals. In this talk, we will present experimental results of the single crystals but also first results of the grown film. [1] H. Launois, et al., PRL 44, 1271 (1980)

O 100.10 Thu 12:45 REC C 213

Understanding chemical constrast in field ion microscopy — •Christoph Freysoldt, Shyam Katnagallu, Baptiste Gault, Michael Ashton, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40273 Düsseldorf

Field ion microscopy (FIM) was the first technique to image surfaces with atomic resolution. In FIM, rare gas atoms are ionized near the surface of a nano-sharp tip subject to a very high voltage. FIM has recently seen renewed interest as a 3D imaging technique for crystallographic features: by applying additional voltage pulses, the surface atoms can be slowly evaporated, revealing the atomic structure of the tip layer by layer. Today's machinery of automated image processing allows then for a reconstruction of the tip's atomic structure.

While the FIM imaging contrast (which strongly depends on field strength, geometrical, and electronic structure) is generally not well understood, recent combined FIM and atom-probe tomography experiments demonstrated and proved a high chemical contrast in a Ni-based model superalloy, where Re atoms are imaged much brighter than the Ni matrix. To explain this effect from a density-functional theory perspective, we exploit a hitherto unknown formal equivalence in the theory of electron tunneling between FIM and scanning tunneling microcopy (STM). The calculations show not only a significant enhancement of the local density of states above Re atoms in a Ni matrix, but also show that adsorbed rare gas atoms may act as 'tunneling lenses' that generally improve lateral contrast.