O 58: Electronic Structure of Surfaces II

Time: Wednesday 15:00–18:00 Location: MA 041

O 58.1 Wed 15:00 MA 041

Two-band superconductivity of lead probed by scanning tunneling spectroscopy — •Michael Ruby[1], Benjamin W. Heinrich[1], Jose I. Pascual[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]CIC nanoGUNE and Ikerbasque, Basque Foundation for Science, Tolosa Hiribidea 78, Donostia-San Sebastian 20018, Spain

The type I superconductor lead (Pb) has been theoretically predicted to be a two-band superconductor [1]. We use scanning tunneling spectroscopy to resolve two superconducting gaps with an energy difference of 130 μeV. Tunneling into Pb(111), Pb(110) and Pb(100) crystals reveals a strong dependence of the two coherence peak intensities on the crystal orientation. We show that this is the result of a selective tunneling into the two bands at the energy of the two coherence peaks. This is further sustained by the observation of signatures of the Fermi sheets in differential conductance maps around subsurface defects.

[1] A. Floris *et al.*, *Phys. Rev. B* **75**, 054508, (2007)

O 58.2 Wed 15:15 MA 041

Core-resonant double photoemission studies of S-overlayers — •Gianluca Di Filippo[1], Frank Oliver Schumann[1], Mario Italo Trioni[2], Guido Fratesi[3], Zheng Wei[1], Chang-Hui Li[1], Lucie Behnke[1], Swapnil Patil[1], Giovanni Stefani[4], and Jürgen Kirschner[1,5] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]CNR, ISTM, Milano, Italy — [3]Università degli Studi di Milano Bicocca, Mlano, Italy — [4]Università degli Studi Roma Tre, Roma, Italy — [5]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

The power of core-resonant double photoemission (DPE), i.e. Auger decay, in determining the strength of electronic correlations in the valence band of solids is well established [1,2]. We employed this technique to investigate the properties of sulfur overlayers on metal substrates. We exposed a Cu(100), a oxygen passivated Cu(100) and a Ni(100) surface to H_2S gas. This caused the formation of S overlayers with nominal coverages of 0.25, 0.48 and 0.5 ML. We focused on the process in which the de-excitation of the S 2p level results in a doubly-ionized final state with two vacancies in the S/metal surface states. The measured DPE line shapes show small differences which are mainly ascribable to the variation of the density of states at the different surfaces. We determined the strength of the electron-electron interaction energy, which is hardly affected by coverage or substrate variations.

[1] M. Cini, Solid State Comm. **24**, 681 (1977)
[2] G.A. Sawatzky, Phys. Rev. Lett., **39**, 504 (1977)

O 58.3 Wed 15:30 MA 041

Dynamic screening probed by core-resonant double photoemission from surfaces — •Frank O. Schumann[1], Zheng Wei[1], Changhui Li[1], Lucie Behnke[1], Gianluca Di Fillippo[1], Giovanni Stefani[2], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik,06120 Halle, Germany — [2]CNISM and Dipartimento di Fisica, Università Roma Tre, I-00146 Rome, Italy

The universal response of an electronic system upon a suddenly created core hole is predicted to occur on an attosecond time scale, but lacks an experimental demonstration. A core hole switches on a local potential and triggers a series of dynamic electron screening processes, such as the shake-up of the outer-shell electrons, plasmon excitations and the emission of Auger electrons.

It is a well-known experimental fact that the 4p photoelectron lines for the elements ranging from Ag to Xe are exceptionally broad. This can be explained by a dynamic fluctuation between a continuous and discrete electron configuration.

With coincidence spectroscopy, we demonstrate an extensive energy sharing between the Ag 4p photoelectron and the NVV Auger electron exceeding 10 eV. This energy width provides access to the time scale of the emission process. We convert this to a timescale of 60 as over which the fluctuations takes place. This value is fair agreement with the theoretical calculation of the timescale to fill an exchange-correlation hole. This shows that core-resonant double photoemission is a powerful tool to probe the ultra-fast dynamic screening processes in the very beginning of the photoemission process on an attosecond timescale.

O 58.4 Wed 15:45 MA 041

Photon-energy dependent double photoemission spectroscopy from transition metal oxides — •Andreas Trützschler[1,2], Cheng-Tien Chiang[1,2], Michael Huth[1], Frank O. Schumann[1], Jürgen Kirschner[1,2], and Wolf Widdra[2,1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120, Halle(Saale), Germany — [2]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120, Halle(Saale), Germany

In the double photoemission (DPE) process, the excitation by a single photon leads to the emission of a pair of photoelectrons. The corresponding transition probability is closely related to the strength of electron correlation in the material [1]. In this contribution we report on DPE experiments on weakly correlated Ag(100) and strong correlated NiO(100) and CoO(100) surfaces [2]. By using a high-order harmonic generation light source at MHz repetition rates in combination with two time-of-flight spectrometers, we are able to compare single and double photoemission propabilities for these materials at different photon energies from 15 to 30 eV. At all photon energies, the ratio between single and double photoemission probability is significantly higher for NiO(100) and CoO(100) as compared to Ag(100), reaching about a factor of 4 at 30 eV photon energy.

[1] Berakdar, Phys. Rev. B 58, 9808 (1998)
[2] Huth, Chiang, Trützschler, Schumann, Kirschner, Widdra, Appl. Phys. Lett. 104, 061602 (2014)

O 58.5 Wed 16:00 MA 041

Simultaneous ARPES and transport measurements — •Lukasz Plucinski[1,2], Ewa Mlynczak[1], Markus Eschbach[1], and Claus M. Schneider[1,2] — [1]PGI-6, FZ Jülich, 52425 Jülich, Germany — [2]Universität Duisburg-Essen, 47048 Duisburg, Germany

It is an open secret, that from the perspective of materials science, angle-resolved photoemission (ARPES) measurements are typically interpreted having in mind transport properties. Electrons measured in high resolution ARPES have kinetic energies for which the inelastic mean free path inside the crystal is in order of few atomic layers, therefore in practice ARPES probes at most a nanometer or two of the surface region of the sample. Spectral contribution from electronic states deeper inside the crystal is negligible. Yet, in "volume" samples, with each dimension larger than (to provide some number) 10 nm, it is the volume of the sample that typically has the dominant contribution to its transport properties. I will present first results of simultaneous ARPES and transport measurements on ultrathin, conducting films grown on insulating substrates and electrically contacted *in situ* under UHV. Furthermore, I will provide an overview of new exciting scientific avenues which will be opened up by this new approach.

O 58.6 Wed 16:15 MA 041

Anomalous d-like Surface Resonance on Mo(110) Analyzed by Time-of-Flight Momentum Microscopy — •Sergey Chernov[1], Katerina Medjanik[1], Christian Tusche[2], Dmytro Kutnyakhov[1], Sergej Nepijko[1], Andreas Oelsner[3], Jürgen Braun[4], Jan Minár[4,5], Stephan Borek[4], Hubert Ebert[4], Hans Joachim Elmers[1], Jürgen Kirschner[2], and Gerd Schönhense[1] — [1]Johannes Gutenberg-Universität, D-55128 Mainz — [2]Max Planck Institut für Mikrostrukturphysik, D-06120 Halle — [3]Surface Concept GmbH, D-55124 Mainz — [4]Ludwig-Maximilians-Universität, D-81377 München — [5]University of West Bohemia, 306 14 Pilsen, Czech Republic

The d-like surface resonances on Mo(110) have been investigated by the novel technique of Time-of-Flight (ToF) momentum microscopy at BESSY (single-bunch). Regions of 3.4 $\AA^{-1}$ dia. in k-space and 4 eV binding energy range were detected simultaneously. 3D (k_x, k_y, E_B) maps of the electronic bands in the full surface Brillouin zone were acquired with high efficiency. Photoemission calculations were performed by means of the one-step model in its density matrix formulation. Band symmetries were probed by linear dichroism. It will be shown that close to the midpoint between $\bar{\Gamma}$ and $\bar{N}$ an anomalous band crosses the symmetry center of a band gap at E_B=0.8 eV. The anomalous band has linear dispersion in a very large energy range and

shows much analogy to a similar state previously found on W(110) [Miyamoto et al., PRL 108, 066808 (2012)]. The project is funded by BMBF (05K12UM2, 05K12EF1, 05K13WMA) and COST.

O 58.7 Wed 16:30 MA 041

Electronic band structure of thin Fe films epitaxially grown on Au(001) and MgO(001) — •Ewa Mlynczak[1,2], Markus Eschbach[1], Pika Gospodaric[1], Vitaliy Feyer[1], Giovanni Zamborlini[1], Lukasz Plucinski[1,3], and Claus M. Schneider[1,3] — [1]Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, al. Mickiewicza 30, 30-059 Kraków, Poland — [3]Fakultät für Physik and Center for Nanointegration Duisburg-Essen (CeNIDE), 47048 Duisburg, Germany

Detailed knowledge of the electronic band structure of thin ferromagnetic films is a first step towards the proper understanding of the spin-based phenomena important for future spintronics such as tunneling anisotropic magnetoresistance or spin-orbit torque. In this contribution, we will present results of comprehensive angular resolved photoemission (ARPES) studies of the electronic band structure of thin Fe(001) films grown on Au(001) and MgO(001). In both cases, Fe shows high crystalline quality providing perfect model systems for these fundamental investigations. The studies conducted using a laboratory based high resolution ARPES apparatus operated with an unpolarized discharge source were complemented by the k-space microscopy (NanoESCA) performed at Elettra light source (Trieste, Italy). The experimentally obtained electronic band structures will be confronted with the results of the DFT calculations.

O 58.8 Wed 16:45 MA 041

Probing the magnetic properties of Cr atoms adsorbed on copper nitride — •Zsolt Majzik[1], Roberto Robles[2], Carmen Rubio-Verdú[1], Martina Corso[3,4], Nicolás Lorente[2], and Nacho Pascual[1,3] — [1]CIC nanoGUNE, Donostia-San Sebastián, Spain — [2]Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Spain — [3]Ikerbasque, Basque Foundation for Science, Bilbao, Spain — [4]Materials Physics Center, EHU, Donostia-San Sebastián, Spain

In the last decade it has been shown that magnetic properties of a single atom can be probed by inelastic electron tunneling spectroscopy. In addition, magnetic nanostructures have been routinely assembled via atomic manipulation. Spin excitation is induced if the bias voltage exceeds the threshold energy for excitation. This process allows inelastic tunneling that leads to a characteristic change in the conductance. Here we aimed to study the magnetic properties of isolated Cr atoms adsorbed on Cu_2N/Cu(100) surface. Different inelastic tunneling spectra were observed over Cr atoms adsorbed on N sites than on Cu sites. In the first case we interpret our spectra as interplay between spin excitation and Kondo screening effect, which appears here at larger biases. However, if Cr atom adsorbs on the Cu site, the Kondo effect does not appear in the spectra, only a spin excitation has a contribution near the Fermi level. Our results suggest that the spin configuration of the Cr atom varies among different adsorption positions. We have performed DFT calculations to better understand the change in spin configuration as well as in the magnetic anisotropy.

O 58.9 Wed 17:00 MA 041

Fermi surface tomography of the ferromagnetic transition metals Co and Ni by momentum microscopy — •Martin Ellguth[1], Christian Tusche[1], Alexander Krasyuk[1], Vitaliy Feyer[2], Carsten Wiemann[2], Claus Michael Schneider[2], and Jürgen Kirschner[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle — [2]Peter-Grünberg-Institut, Forschungszentrum Jülich — [3]Institut für Physik, Martin-Luther-Universität, Halle

The Fermi surface of a metal represents its electronic structure at one particular energy: the one which separates occupied from unoccupied electronic states. These states are responsible for the electric conductivity and related properties such as the thermoelectric behaviour. As such it is both interesting from a fundamental physics viewpoint as well as for applications. In this study, we have used momentum microscopy as a highly efficient photoemission experiment to probe the Fermi surface of the elemental ferromagnets Co and Ni. The combination of this setup with synchrotron radiation in the energy range from 30 eV to 200 eV allows for scanning the two-dimensional manifold through the perpendicular axis and thus acquire for the first time a volumetric dataset showing the Fermi surface for Co and Ni as photoemission resonances. The majority-spin surface and one of the minority surface sheets of Co are most clearly observed. Our data provides a sensitive test to the energetic position of electronic bands crossing the Fermi level, and therefore to a possible renormalization induced by many-body interactions.
M.E. acknowledges support from the BMBF (05K12EF1).

O 58.10 Wed 17:15 MA 041

Investigation of the surface of binary metallic alloys using PAES, XPS and STM — •Samantha Zimnik, Christian Piochacz, Sebastian Vohburger, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany

The characterization of the elemental composition of surfaces is of high importance for the understanding of many surface-related processes such as catalysis or oxidation. However, surface segregation causes changes in the elemental constitution of the surface, which affects significantly the macroscopic properties of the system. Therefore, e.g. in the system Fe/Pt, it is of great interest to investigate the theoretically predicted surface segregation process.
Positron annihilation induced Auger Electron Spectroscopy (PAES) is a powerful technique to gather information about the elemental composition of only the topmost atomic layer of a specimen. The positron beam facility NEPOMUC delivers a high intensity positron beam of $10^9 e^+/s$ and enables measurement times of only a few minutes per PAES spectrum. Thus, time-dependent PAES became possible and enables the in-situ observation of surface segregation processes. The upgraded surface spectrometer at NEPOMUC uses the complementary techniques PAES, XPS and STM for a comprehensive surface analysis. First temperature-dependent measurements on binary alloys are presented. Financial support by the BMBF (project no. 05K13WO1) is gratefully acknowledged.

O 58.11 Wed 17:30 MA 041

Manipulating STM induced light emission by organic adlayers — •Maren C. Cottin, Ebru Ekici, Rolf Möller, and Christian A. Bobisch — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

Light emitted from the tip-sample junction of a scanning tunneling microscope (STM) carries information about energy transfer processes at surfaces. We use thin layers of bismuth (Bi) on Cu(111) as a substrate for different archetype organic layers, e.g. C_{60} and perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA). We find that the maximum photon yield may be enhanced if the tunneling tip is placed above the molecules as compared to the bare Bi/Cu(111)-substrate. In a comprehensive study of the light emission characteristics, we present laterally resolved maps of the overall photon intensity measured together with the surface structure. In addition, measurements of the overall photon intensity as a function of the bias voltage, dI/dV-data and spectra of the emitted light allow us to characterize the role of the molecules in the excitation/light emission process.

O 58.12 Wed 17:45 MA 041

Determination of charge neutrality level in TiO2 films from res-PES measurements. — •Chittaranjan Das, Massimo Tallarida, and Dieter Schmeisser — Lehrstuhl Angewandte Physik/Sensorik Brandenburgische Technische Universität, Cottbus-Senftenberg Cottbus-03046

Titanium dioxide is one of the metal oxides which have versatile application in different fields. The applications of TiO2 are in the field of cosmetics, electronics (memory resistive switching), dye, photonics and photocatalysis. In the present paper we study the resPES data of TiO2 films prepared by atomic layer deposition. The measurements are done in in-situ system at beam line U49/2-PGM2 in BESSY-II. The density of state in valence band and conduction band is obtained from the resonance photo electron spectroscopy (res-PES) of the O1s and the Ti2p edge. The data allow to determine the position of the VBM and CBM with respect to the Fermi energy. Also the existence of localized O2p and Ti2p derived states is deduced which appear in the gap. In addition we determine the charge neutrality level (CNL).The CNL is the position where the weight of the density of state from valence band and conduction band are equal. This is an important quantity for the discussion of interface properties.