O 45: Electronic structure I

Time: Wednesday 10:30–12:45 Location: H33

O 45.1 Wed 10:30 H33

Electronic structure and photoemission of ferromagnetic 3d-metals and related binary alloys — •J. Braun[1], J. Minar[1], H. Ebert[1], H.A. Dürr[2], J. Fink[2], T. Allmers[3], and M. Donath[3] — [1]Dept. Chemie und Biochemie, LMU Universität München, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]Physikalisches Institut, Universität Münster, Germany

We compare calculated spectral features of bcc Fe(110), fcc Co(100) and hcp Co(0001) for in-plane and out-of-plane configurations of the magnetization. Furthermore, it will be shown that life-time effects can be quantitatively explained in terms of electron-hole pair interactions. The influence of chemical disoder on the spectroscopical data is analysed, as an example, for the binary intermetallic Co_xCu_{1-x} alloy. The spectral distributions will be compared with corresponding experimental data. The calculations have been performed in the framework of the fully relativistic version of the one-step model of photoemission that is part of the upgraded version of the Munich SPR-KKR program package [1]. The electronic structure input is calculated self-consistently for ordered and disordered materials using the LSDA+DMFT approach in combination with the Coherent Potential Approximation (CPA) alloy theory. To guarantee for a quantitative description of the surface-sensitive spectral features special attention is payed to the image-potential behavior of the surface barrier, which is included as an additional layer in the photoemission formalism.

1. H. Ebert et al., The Munich SPR-KKR package, version 3.6, http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR (2008).

O 45.2 Wed 10:45 H33

Valence band photoemission Ni_xPd_{1-x} alloy films on $Cu_3Au(100)$ — •Matthias Gulik[1,2], Lukasz Plucinski[1], and Claus M. Schneider[1] — [1]Forschungszentrum Jülich GmbH, Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [2]Technische Universität Dortmund, Maria-Goeppert-Mayer- Str. 2, D-44221 Dortmund, Germany

Spin and angle-resolved photoemission are important experimental methods to investigate the electronic band structure of crystalline materials. Spin-integrated measurements can be performed relatively fast with a high energy and momentum resolution, whereas spin-resolved measurements reveal further information about the band structure.

On the compound of $Ni_xPd_{1-x}/Cu_3Au(100)$ we will investigate the electronic and magnetic properties with regard to the thickness and the composition of the ultrathin Ni_xPd_{1-x} layer. The composition differences should be reflected in an inverse spin-reorientation transition. Furthermore we will compare the measured spectra to the theoretical calculations of the band structure.

The measurement takes place at Beamline 5 at DELTA, Dortmund, with an unique detector setup. We can acquire 2-dimensional angle resolved data for band mapping and spin resolved one-dimensional data quasi-simultaneously. This will provide us with high resolution band structure spectra and images as well as spin resolved valence band spectra. Our samples are prepared in-situ by e-beam evaporation and characterized by LEED and Auger spectroscopy.

O 45.3 Wed 11:00 H33

Fermi-surface mapping of graphene/Ni(111) and Ni/graphene/Ni(111) — Martin Weser[1], Alexander Generalov[1,2], Carsten Enderlein[1], Stefan Böttcher[1], Karsten Horn[1], Mikhail Fonin[3], and •Yuriy Dedkov[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]St.-Petersburg State University, Russia — [3]Universität Konstanz, Germany

Recent ab initio spin-dependent transport calculations have suggested an application of graphene/graphite as a perfect spin filter in ferromagnet/graphene/ferromagnet sandwich-like structures. Due to the overlapping of the electronic structures of graphene layers and the ferromagnetic material for the minority spin only, one can expect a preferential transport of electrons of one kind of spins through this trilayer system. The Ni(111)/graphene/Ni(111) sandwich can be considered as a model system, due to the extremely small lattice mismatch, permitting to study in detail the effects of growth and interactions at interfaces without detrimental effects such as grain boundaries or the formation of Moiré patterns. Here, we present results of LEED, STM, and photoemission studies of the morphology and electronic structure of the graphene/Ni(111) and Ni/graphene/Ni(111) systems. We focus on the investigation of electronic structure of these systems in the vicinity of the Fermi level. These results are presented and discussed in the light of the available band structure calculations. The perspectives of these graphene/ferromagnet interfaces for future spintronics devices are debated.

O 45.4 Wed 11:15 H33

Ni/GaAs(001): Looking for a bcc signature with spin-resolved inverse photoemission — •Christian Eibl, Manuel Prätorius, André Berken, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

To understand the interplay between crystal structure, electronic states, and magnetism, it is worthwhile to compare the different ferromagnetic elements. Unfortunately, at room temperature the thermodynamically stable crystal structures of Ni, Fe, and Co are face-centered cubic (fcc), body-centered cubic (bcc), and hexagonal close-packed (hcp), respectively. Thus, a direct comparison is hampered and scientists endeavor to crystallize Fe, Co, and Ni in a non-native structure.

Recently, it was shown by Tian et al. that Ni can be stabilized in the bcc structure on a GaAs(001) substrate. In contrast to the fcc structure, it was found that bcc Ni exhibits different magnetic properties, e.g., Curie temperature and magnetic anisotropy [1].

A crystallographic change from fcc to bcc is known to be reflected in the electronic structure [2]. Therefore we used a spin-resolved inverse photoemission experiment to look for characteristic bcc type fingerprints. Furthermore, we compared our results with measurements taken on (bcc-)Fe/Pd(001) and (fcc-)Ni/Cu(001).

[1] C.S. Tian et *al.*, Phys. Rev. Lett. **94**, 137210 (2005)
[2] Donath et *al.*, J. Phys.: Condens. Matter **21**, 134004 (2009)

O 45.5 Wed 11:30 H33

Temperature dependent quasiparticle renormalization in nickel and iron. — •Ruslan Ovsyannikov, Setti Thirupathaiah, Jaime Sánchez-Barriga, Jörg Fink, and Hermann Dürr — Helmholtz Zentrum Berlin, BESSY II, Albert-Einstein-Strasse 15, D-12489 Berlin, Germany

One of the fundamental consequences of electron correlation effects is that the bare particles in solids become 'dressed' with an excitation cloud resulting in quasiparticles. Such a quasiparticle will carry the same spin and charge as the original particle, but will have a renormalized mass and a finite lifetime. The properties of many-body interactions are described with a complex function called self energy which is directly accessible to modern high-resolution angle resolved photoemission spectroscopy (ARPES). Ferromagnetic metals like nickel or iron offers the exciting possibility to study the spin dependence of quasiparticle coupling to bosonic modes. Utilizing the exchange split band structure as an intrinsic 'spin detector' it is possible to distinguish between electron-phonon and electron-magnon coupling phenomena. In this contribution we will report a systematic investigation of the $\boldsymbol{k}$– and temperature dependence of the electron-boson coupling in nickel and iron metals as well as discuss origin of earlier observed anomalous lifetime broadening of majority spin states of nickel at Fermi level.

O 45.6 Wed 11:45 H33

Cobalt/nickel mixed oxides - cathode materials for Li-Ion-Batteries — •Stephan Schmidt and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Konrad-Wachsmann-Allee 17, 03046 Cottbus

Replacing Co by large amounts of Ni is considered to reduce costs in Li-Ion-Batteries while maintaining their performance. We are interested in whether this replacement causes changes in the valence band (VB) and conduction band (CB) states or not.
Samples were prepared as thin films from nitrate solutions on metal substrates and annealed in air and UHV. The Co to Ni ratio was varied from 50/50 over 40/60 and 30/70 up to 20/80. The results are compared to the pure Co-oxide. Experiments were carried out at the

U49/2 beamline at BESSYII, Berlin.
XPS of the TM2p states reveals the existence of charge transfer ground states and different oxidation states. NEXAS at the Co2p, Ni2p and O1s edges projects the density of unoccupied states while resonant PES at these edges provides the related partial density of states (pDOS) and thus can be used to distinguish between the different contributions of TM3d and O2p states in the valence band region.
We find systematic variation of the VB structure, the valence band maximum and a shift at the O1s absorption edge while the TM2p XPS and absorption spectra do not seem to be affected by the mixing.

O 45.7 Wed 12:00 H33

Neutral Excitations of Physisorbed Helium — •Sarah Kossler[1], Reinhold Schneider[1], Peter Feulner[1], and Jean Pierre Gauyacq[2] — [1]TU München, Garching, Germany — [2]UMR CNRS-Université Paris Sud, Orsay, France

We study neutral excitations of He mono- and bilayers on Pt(111), Ru(001), Ag(111) and Cu(111) surfaces, and sandwich layers of He on well ordered Ne and Ar monolayers on these substrates. We apply narrow bandwidth undulator radiation of variable polarization (BESSY, UE-112-PGM-1) in combination with a Time-Of-Flight technique that enables us to detect electrons, ions, metastable atoms and fluorescence photons. Therewith we obtain comprehensive data sets on excitation and decay processes below the 1s ionization edges of these layers. Compared to the isolated atom, strong inter- and intralayer coupling is found that is well reproduced by calculations. We observe hybridization of s and p final states, and for higher principal quantum numbers also admixture of d states. We demonstrate that the comparison of data from different samples as indicated above is indispensable for a complete understanding of these processes.

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O 45.8 Wed 12:15 H33

Rashba Type Spin-Splitting in the Two-Dimensional Electron System Au/Ge(111) Studied by Angle-Resolved Photoemission — •Philipp Höpfner[1], Jörg Schäfer[1], Sebastian Meyer[1], Christian Blumenstein[1], Andrzej Fleszar[2], Xiaoyu Cui[3], Luc Patthey[3], Werner Hanke[2], and Ralph Claessen[1] — [1]Exp. Physik 4, Universität Würzburg — [2]Theor. Physik 1, Universität Würzburg — [3]Swiss Light Source, PSI, Villigen, Switzerland

The confinement of electrons in a single atomic adsorbate layer on a semiconductor surface presents an excellent playground for the study of electronic correlations in low dimensions. In this way, several intriguing two-dimensional electron systems (2DES) have been realized experimentally, such as e.g. the $\sqrt{3}$-reconstructions on (111) surfaces of Si and Ge. These systems are candidates for a spin-orbit splitting, due to the strong potential gradient at the surface, being in particular of the Rashba type.

In choosing heavy elements as adatoms, the spin-orbit interaction may play a significant role and one may ask what will happen to the Rashba splitting. We present results from angle-resolved photoelectron spectroscopy using synchrotron light of the metallic $\sqrt{3}$-Au/Ge(111) system. Two sets of metallic surface bands are observed, each of which appears to be split in pairs, originating from a Rashba type spin-splitting, as assigned by density functional theory calculations. Interestingly, the in-plane spin component varies across the Fermi surface. This metallic monolayer 2DES may represent a novel approach for spin injection into a semiconductor from a monolayer only.

O 45.9 Wed 12:30 H33

Structure and Energetics of Si(111)5×2−Au Atomic Chains — •Ingo Barke[1], Steven C. Erwin[2], and F. J. Himpsel[3] — [1]Universität Rostock, Germany — [2]Naval Research Laboratory, Washington, DC — [3]University of Wisconsin-Madison, WI

We propose a structural model for the Si(111)5x2-Au reconstruction [1]. The model incorporates a revised experimental value of 0.6 monolayer for the coverage of gold atoms, equivalent to six gold atoms per 5×2 cell [2]. Results obtained from first-principles total-energy calculations are in excellent agreement with experimental observations: (1) In the presence of silicon adatoms the periodicity of the gold rows spontaneously doubles. (2) The dependence of the surface energy on the adatom coverage indicates that a uniformly covered phase is unstable and will phase separate into empty and covered regions. (3) High-resolution scanning tunneling microscopy images are precisely reproduced by theory. (4) The calculated band structure is consistent with angle-resolved photoemission spectra. (5) The calculated activation barrier for diffusion of silicon adatoms along the row direction is in excellent agreement with the experimentally measured barrier [3].
[1] S. C. Erwin et al., Phys. Rev. B 80, 155409 (2009)
[2] I. Barke et al., Phys. Rev. B 79, 155301 (2009)
[3] E. Bussmann et al., Phys. Rev. Lett. 101, 266101 (2008)