O 21 Elektronische Struktur II

Zeit: Samstag 10:45–13:00 Raum: TU EB107

O 21.1 Sa 10:45 TU EB107

Contribution of electron-magnon scattering to the lifetimes of lanthanide-metal surface states studied by scanning tunneling spectroscopy — •Daniel Wegner, Andreas Bauer, and Günter Kaindl — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin-Dahlem

While electron dynamics at surfaces of noble metals is well understood by now, we still have a rather poor knowledge of electron dynamics at transition-metal surfaces, in particular for magnetic systems where electron-magnon scattering has to be taken into account. A better understanding would be of particular importance for spin electronics.

We have systematically studied lifetime broadening of exchange-split (0001)-surface states for all trivalent lanthanide metals by low-temperature scanning tunneling spectroscopy (STS) at 10 K. Since those states are highly spin-polarized, they allow for a separate analysis of majority (spin-up) and minority (spin-down) states. The results give evidence for strong electron-magnon scattering of the minority states, while for the majority states, electron-electron and electron-phonon scattering seem to be dominant.

O 21.2 Sa 11:00 TU EB107

Surface state scattering by atomic–scale clusters on noble metals — •S. Lounis, Ph. Mavropoulos, S. Blügel, and P. H. Dederichs — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

When surface state electrons scatter at perturbations, such as magnetic or nonmagnetic adatoms or clusters on surfaces, an electronic resonance can develop at the bottom of the surface state band for both spin channels. In the case of adatoms, these states have been found very recently in scanning tunneling spectroscopy experiments of the group of R. Berndt (University of Kiel). Motivated by these experiments, we carried out a systematic theoretical investigation of the electronic structure of these surface states in the presence of magnetic and non-magnetic 3d atoms on Cu(111) and Ag(111) surfaces. The calculations are performed using the full-potential scalar–relativistic Korringa-Kohn-Rostoker Green–function method extended to treat noncollinear magnetic nanostructures on surfaces.

We extended this investigation to dimers and trimers, and investigate how the resonance state depends on cluster size and complexity of the magnetic configuration.

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O 21.3 Sa 11:15 TU EB107

Spin Filtering at a Ferromagnetic-Paramagnetic Interface Observed by Spin-Polarized Standing Waves — •Jörg Schäfer[1], Markus Hoinkis[1], Eli Rotenberg[2], and Ralph Claessen[1] — [1]Institut für Physik, Universität Augsburg — [2]Advanced Light Source, Berkeley, USA

For thin Fe films the spin-selective transmission of electrons near the Fermi level across a ferromagnetic-paramagnetic interface is investigated. The majority and minority Fermi surface sheets of the Fe film are probed for standing wave formation by angle-resolved photoemission. Knowledge of the exchange-split Fermi surface from density functional calculations allows straightforward assignment of the spin character. Reflection at the interface is expected to lead to quantum well states. However, using a W(110) substrate, these are observed only for majority states, which is attributed to a strongly spin-dependent transmission through the Fe/W interface. This can be traced back to the Fermi surface topologies of the connecting solids, and the choice of the Fe/W-interface for this reason produces a particularly strong effect.

O 21.4 Sa 11:30 TU EB107

Role of the spin in quasiparticle interference — •Ph. Hofmann[1], J. I. Pascual[2,3], G. Bihlmayer[4], Yu. M. Koroteev[5,6], H.-P. Rust[3], G. Ceballos[3], M. Hansmann[3], K. Horn[3], E.V. Chulkov[5], S. Blügel[4], and P.M. Echenique[5] — [1]Institute for Storage Ring Facilities, University of Aarhus, Denmark — [2]Institut für Experimentalphysik, Freie Universität Berlin — [3]Fritz-Haber-Institut der MPG, Berlin — [4]Institut für Festkörperforschung, Forschungszentrum Jülich — [5]Donostia International Physics Center (DIPC), Basque Country, Spain — [6]Institute of Strength Physics and Materials Science, Tomsk, Russia

Defects on metal surfaces are screened by the surrounding electron gas, leading to the formation of standing electron waves or, more correctly, quasiparticle interference patterns. These patterns can be observed by scanning tunneling microscopy, either for a very small tunneling voltage or in conductance images. A Fourier transformation of conductance images can therefore give valuable information about the electronic structure and Fermi surface of quasi two-dimensional systems. Here we show that even in non-magnetic systems the spin of the quasiparticles can have a profound effect on the interference patterns. On Bi(110), where the surface state bands are not spin-degenerate, the patterns are not related to the dispersion of the electronic states in a simple way. In fact, the features which are expected for the spin-independent situation are absent and the observed interference patterns can only be interpreted by taking spin-conserving scattering events into account.

O 21.5 Sa 11:45 TU EB107

k-dependent electronic structure of NiMnSb single-crystal surfaces — •Juliet Correa, Christian Eibl, Jürgen Braun, Georgi Rangelov, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

The half-Heusler alloy NiMnSb is believed to be a half-metallic ferromagnet with 100% spin polarization at the Fermi level. This property makes it an interesting material for spintronic applications. Detailed understanding of the band structure of NiMnSb, not only in the bulk but also at surfaces and interfaces, is essential to developing spintronic applications. To date, however, the only data available are of the density of states, specifically from polycrystalline samples. We present angle-resolved photoemission results from a carefully prepared and surface-characterized NiMnSb(100) single crystal. We observed clear energy dispersion of occupied bulk states as a function of the wave vector parallel to the surface. Our results are discussed along with band structure calculations.

O 21.6 Sa 12:00 TU EB107

Electronic structure of NiO thin films on Ag(001) — •Markus Däne[1], Diemo Ködderitzsch[1], Wolfram Hergert[1], Arthur Ernst[2], Walter M. Temmerman[3], Zdzislawa Szotek[3], Christian Hagendorf[1], Henning Neddermeyer[1], and Wolf Widdra[1] — [1]Fachbereich Physik, Martin Luther Universität Halle-Wittenberg, Friedemann-Bach-Platz 6, 06108 Halle, Germany — [2]Max Planck Institute of Microstructure Physics, 06120 Halle, Germany — [3]Daresbury Laboratory, Daresbury, Warrington WA4 4AD, United Kingdom

In this work we apply the self-interaction corrected LSDA formalism, as implemented in the TB-LMTO-ASA method, to study the electronic and magnetic structure of thin transition metal oxide (TMO) films on metallic substrates. Here the properties of NiO thin films (up to 5 layers) on the Ag(001) surface are investigated. Relaxations at the Ag oxide interface are taken into account. The gap formation of the oxide thin film depending on film thickness and magnetic structure is studied. The influence of the metallic substrate is revealed by comparison with freestanding NiO films. The results can be compared to experimental data obtained by scanning tunneling microscopy and spectroscopy (STM/STS) for one to three layer thick NiO islands on Ag(001). The variation of the normalized differential conductance is discussed with respect to the calculated local density of states.

O 21.7 Sa 12:15 TU EB107

The Si(111)-(7×7) surface: a correlated electronic Hubbard system? — •Richard Schillinger, C. Bromberger, H. J. Jänsch, H. Kleine, O. Kühlert, C. Weindel, and D. Fick — Philipps-Universität, Fachbereich Physik and Zentrum für Materialwissenschaften 35032 Marburg, Germany

Li adsorption at extremely low coverages (10^{-3} ML and below) on the metallic Si(111)(7×7) surface has been studied by β-NMR experiments (measurement of T_1-times). Instead of increasing linearly with sample temperature, as expected for a metallic system, the relaxation rates $\alpha = 1/T_1$ are quite surprisingly constant in between 50 K and 300 K and rise considerably above. This temperature dependence points to an extremely localized and thus narrow band (width below 5 meV) which pins the Fermi energy. It is energetically located within an approximately 600 meV wide gap in between a lower filled and an upper empty Hubbard band. Due to its extremely narrow width it cannot be detected in photo emission experiments. In Dynamic Mean Field Theory (DMFT) based on Hubbard Hamiltonians [1,2] this kind of density of states is typical for correlated electron systems being close to a Hubbard metal-insulator transition.

[1] G. Kotliar and G. Vollard, Physics Today, March 2004
[2] Pou et al., Phys. Rev. Lett. **63** 4309 (2000)

O 21.8 Sa 12:30 TU EB107

Continuous tuning of electronic correlations by alkali adsorption on layered $1T$-TaS_2 — •Kai Rossnagel[1,2], Eli Rotenberg[2], H. Koh[2], N.V. Smith[2], and L. Kipp[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D–24098 Kiel, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Angle-resolved photoemission spectroscopy shows that a Mott-Hubbard type metal-insulator transition occurs at the Rb adsorbed surface of the layered charge-density-wave compound $1T$-TaS_2. The transition is driven by adsorption induced modifications of the charge-density wave and of the interlayer coupling, leading to an increase of the on-site Coulomb correlation energy and a narrowing of the Ta $5d$ band perpendicular to the layers, respectively. The continuous rearrangement of spectral weight is measured live during the deposition process.

The experiments were carried out at the *Electronic Structure Factory* at beamline 7 of the Advanced Light Source in Berkeley. Work at the University of Kiel is supported by DFG Forschergruppe FOR 353. K.R. gratefully acknowledges support by the Alexander von Humboldt Foundation.

O 21.9 Sa 12:45 TU EB107

Surface-state localization at adatoms — J. Kröger, L. Limot, E. Pehlke, and •R. Berndt — Institut für Experimentelle und Angewandte Physik, Institut für Theoretische und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel

Low-temperature scanning tunneling spectroscopy of magnetic and non-magnetic metal atoms on Ag(111) and on Cu(111) surfaces reveals the existence of a common electronic resonance at an energy below the binding energies of the surface states. Using an extended Newns-Anderson model, we assign this resonance to an adsorbate-induced bound state, split off from the bottom of the surface-state band, and broadened by the interaction with bulk states. A lineshape analysis of the bound state indicates that native adatoms decrease the surface-state lifetime, while a cobalt adatom causes no significant change.