O 69: Electronic structure I

Time: Thursday 11:15–13:15 Location: WIL C107

O 69.1 Thu 11:15 WIL C107

Structural/electronic interplay in tunable dislocation networks — •Frederik Schiller[1], Zakaria Abd-el-Fattah[1], Manfred Matena[2], Javier Cordon[3], and Enrique Ortega[1,2,3] — [1]Centro de Fisica de Materiales (CFM-CSIC), Materials Physics Center (MPC), San Sebastian, Spain — [2]Donostia International Physics Center, San Sebastian, Spain — [3]Dpto. Fisica Aplicada, Universidad del Pais Vasco, San Sebastian, Spain

Moiré and strain dislocation networks arise when a monolayer or two of one material grows on a substrate with the same crystal symmetry but different atomic lattice constant. Beyond their use as growth templates, such metallic superlattices may be used as model two-dimensional metallic superstructures at which surface states scatter, thereby leading to two-dimensional superlattice band folding and gap opening. The Ag monolayer on Cu(111) system, with its characteristic free-electron-like surface state, is a prototype scenario. At low temperature, it forms a perfect coincidence lattice (Moiré), which transforms into a hexagonal array of triangular dislocations by annealing above 300 K. Such structural transition is accompanied by a deep surface state transformation, i.e., from a parabolic band in the Moiré structure to a superlattice-folded and gapped two-dimensional band structure in the dislocation network. The latter features a full 25 meV gap that can be brought below the Fermi level by lowering the temperature or by gold doping, thereby making the noble metal surface effectively semiconducting.

O 69.2 Thu 11:30 WIL C107

Localized gap states in cobalt/nickel mixed oxides — •Stephan Schmidt and Dieter Schmeisser — Brandenburg University of Technology 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 investigate the electronic structure of Co/Ni compounds because of their direct impact on battery operation. Thin Co/Ni oxide films on metal substrates were prepared by dropping/spin-coating from nitrate solutions followed by subsequent annealing in air and UHV. The following Co to Ni ratios have been investigated: 50/50, 40/60, 30/70, and 20/80. The results are compared with the pure Co-oxide and magnetron sputtered $LiCoO_2$ reference samples. Spectroscopic measurements on these samples were carried out at the U49/2 beamline at BESSYII, Berlin. XPS of the transition metal (TM) 2p states reveals the existence of charge transfer ground states and different oxidation states. NEXAFS at the Co L_3, Ni L_3 and O K edges reflects the density of unoccupied states while resonant PES at these edges provides the related partial density of states (pDOS). Therefore, these techniques can be used in order to distinguish between the different contributions of TM3d and O2p states in the valence band region. We find sharp localized features at the valence band edge and at the O K and Co L_3 absorption edges that are discussed to originate from the strong hybridization between metal and oxygen states in that region.

O 69.3 Thu 11:45 WIL C107

Surface electronic structure of clean and oxidized Fe and O/Fe films on Pd(001) — •Christian Eibl, Anke B. Schmidt, and Markus Donath — Westfälische Wilhelms-Universität Münster

Spin-polarization detectors based on exchange interaction have attracted great attention due to their rather high figure of merit and Sherman function compared with spin-orbit-interaction based detectors. Especially oxidized iron films are already in use [1,2].

Here we report on spin-resolved inverse photoemission and target current spectroscopy measurements on Fe(001) and differently prepared O/Fe(001) films. A Pd(001) crystal is used as substrate for film growth. The aim is to understand in detail the influence of oxygen on the Fe(001) surface electronic structure and thereby to improve the spin-detector efficiency in view of Sherman function and stability.

[1] A. Winkelmann *et al.*, Rev. Sci. Instrum. **79**, 083303 (2008)
[2] T. Okuda *et al.*, Rev. Sci. Instrum. **79**, 123117 (2008)

O 69.4 Thu 12:00 WIL C107

Photoelectron momentum mapping over the whole hemisphere: Experiment and theory for Cu(111), Ag(111), and Cu(001) — •Aimo Winkelmann, Christian Tusche, Martin Ellguth, A. Akin Ünal, Jürgen Henk, and Jürgen Kirschner — MPI für Mikrostrukturphysik, Halle (Saale), Germany

Knowledge of the detailed electronic structure in the entire Brillouin zone and in the whole valence-band regime is a prerequisite for understanding new effects at surfaces. This information is obtained with unprecedented efficiency by an energy- and momentum-resolving photoelectron emission microscope (momentum microscope) that detects constant-energy intensity distributions of electrons emitted into the full hemisphere.

The complete valence-band structure which is accessible by unpolarized He I radiation was mapped for the paradigmatic systems Cu(111), Ag(111), and Cu(001) using the momentum microscope.

The measurements provide simultaneous access to extended parts of the photoelectron momentum space beyond high-symmetry regions and, thus, serve as a testing ground for theoretical photoemission from bulk and surface states. For example, agreement of the experimental and theoretical intensity distributions in the entire phase space is obtained only by improving the treatment of the *d*-bands which are unsatisfactorily described within the local density approximation.

O 69.5 Thu 12:15 WIL C107

Circular Dichroism in the Angular Distribution in Surface Alloys — •Carola Strasser, Isabella Gierz, Hadj-Mohamed Benia, Klaus Kern, and Christian R. Ast — MPI für Festkörperforschung, Stuttgart

Circular dichroism in the angular distribution (CDAD) refers to the difference of the measured photocurrent for right and left circularly polarized light. To observe this effect either the target has to be chiral or the experimental geometry has a defined handedness. The CDAD signal is dependent on the geometry of the setup, the orbital composition of the initial state and the relative phases of the partial waves in the final state.

Different surface alloys on Ag(111) and also graphene have been investigated with circularly polarized light and the CDAD signal has been measured. We compare the experimental data for the different systems to the theoretical description of CDAD by Schönhense [1] and estimate the orbital composition of the initial state.

[1] G. Schönhense, Phys. Scr., **T31**, 255, (1990)

O 69.6 Thu 12:30 WIL C107

Interplay between morphology and electronic structure of ultrathin Ni films on W(110) — •Henry Wortelen[1], Sebastian Stolwijk[1], Anke B. Schmidt[1], Kristian Döbrich[2], Martin Weinelt[2,3], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster — [2]Max-Born-Institut, 12489 Berlin — [3]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin

For Ni, a prototype band ferromagnet, measurements of the electronic structure at the phase transition suffer from dominant temperature-induced linewidth broadening. This hampers the interpretation of experimental results. An effective way to overcome this problem is to lower the Curie temperature by going from bulk samples to ultrathin films.

In this contribution, we present morphological and electronic structural changes of ultrathin Ni films grown on a W(110) substrate, as the film thickness is reduced from 10 to 1 monolayer. A combined study with scanning tunneling microscopy, low-energy electron diffraction and (inverse) photoemission shows the close relation between film thickness, quality and electronic structure. Particular attention is given to crystal-induced and image-potential surface states due to their surface sensitivity.

O 69.7 Thu 12:45 WIL C107

A Non-destructive Technique of Investigating Bulk Electronic Properties and Buried Interfaces — •Mihaela Gorgoi, Franz Schäfers, and Alexander Föhlisch — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

In the past couple of years hard x-ray high kinetic energy photoelectron spectroscopy (HAXPES) has lead to a break-through in the field of photoemission due to its non destructive way of investigating the bulk electronic properties of materials and in particular buried interfaces. In the present contribution we will report recent experiments performed at the hard x-ray HIgh Kinetic Energy (HIKE) photoelectron spectroscopy facility [1] at the Berliner synchrotron light source BESSY II of the HZB. The facility successfully combines the bending magnet source of the KMC-1 beamline [2] with a new generation electron spectrometer optimized for high kinetic energy electrons. Several topics will be detailed such as the recoil effect of high energy photoelectrons from light elements and the interface electronic properties in organic and inorganic thin films and multilayers with emphasis on the performance and abilities of the technique. [1] M. Gorgoi, S. Svensson, F. Schäfers, G. Öhrwall, M. Mertin, P. Bressler, O. Karis, H. Siegbahn, A. Sandell, H. Rensmo, W. Doherty, C. Jung, W. Braun, W. Eberhardt, Nucl. Instrum. Methods Phys. Res. A 601 (2009) 48. [2] F. Schäfers, M. Mertin, M. Gorgoi, Rev. Sci. Instrum. 78 (2007) 123102.

O 69.8 Thu 13:00 WIL C107

The electronic structure and Fermi surface of Ru(0001) and Ru(10$\bar{1}$0) surfaces measured with high resolution angle-resolved photoemission spectroscopy

— •Thanh-Nam Nguyen[1], Mattia Mulazzi[1], Sina Gusenleitner[1], Marius Ernst[1], Holger Schwab[1], Dirk Ehm[3], and Friedrich Reinert[1,2] — [1]Experimentelle Physik 7, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruhe Institute of Technology, Germany — [3]Carl Zeiss SMT AG, Rudolf-Eber-Str. 2, 73447 Oberkochen, Germany

Single-crystalline Ru surfaces are model systems for the capping of optical elements in extreme ultraviolet (EUV) lithography setups. The momentum-resolved electronic structure of these surfaces yields important information on their chemical and catalytic properties. The Fermi surface and the band structure of two ruthenium surfaces Ru(0001) and, for the first time, Ru(10$\bar{1}$0) were investigated by high-resolution angle-resolved photoemission spectroscopy (ARPES). The experimental results, though consistent with previous data, show several new features that could not be previously observed by the limited energy and angular resolution. The present results provide detailed information about the momentum-resolved electronic structure of Ruthenium that constitutes a reference to understand its chemical and catalytic properties.