O 89: Surface Dynamics II

Time: Friday 10:30–13:15 Location: H33

O 89.1 Fri 10:30 H33

Spin polarized photoemission of gold surfaces coated with bacteriorhodopsin — •Matthias Kettner[1], Benjamin Göhler[1], Tal Z. Markus[2], Volker Hamelbeck[1], Georg F. Hanne[1], Ron Naaman[2], and Helmut Zacharias[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Chemical Physics, Weizmann Institute, Rehovot, Israel

Electron spin polarization has been measured for photoelectrons emitted from a gold substrate and transmitted through physisorbed layers of the chiral membrane protein bacteriorhodopsin. Samples are irradiated by circularly as well as linearly polarized 213 nm laser radiation, exciting photoelectrons within the gold substrate which are transmitted through the proteins. Photoelectrons are analyzed by a time-of-flight detector yielding an "unstructured" spectrum up to 1.5 eV; an electron dichroism of up to 1.4 % is measured independent on the kinetic energy. Furthermore, a Mott polarimeter is used for spin analysis. In the present experiment electron spin polarization values of up to 15 % are obtained independent of the polarization of the incident light, similar to earlier work on ordered layers of double-stranded oligo-DNA [1]. The measured electron spin polarization shows a dependence on the preparation of the samples.

[1] B. Göhler, et al., Science 331, 894 (2011)

O 89.2 Fri 10:45 H33

Tight-binding spin dynamics and tight-binding Monte Carlo: a study on BCC iron — •Siebe Rossen[1,2], Phivos Mavropoulos[1], Timo Schena[1], Stefan Blügel[1], and Theo Rasing[2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Radboud Universiteit Nijmegen, Institute for Molecules and Materials, 6525AJ Nijmegen, The Netherlands

Recent laser pulse excitation experiments on metallic films [1] show remarkable magnetisation dynamics which call for a theoretical explanation on an atomistic scale. So far the computational approach to this problem has been primarily based on a Heisenberg Hamiltonian at best, the validity of which becomes questionable in strongly non-collinear magnetic states. Therefore, we developed a code based on a calculation of the time-dependent electronic structure within the tight-binding and adiabatic approximation, in which the torque acting on the individual moments can be obtained in any spin configuration outside equilibrium. Such a method, for which the underlying principles are given in [2], is not only powerful because of the accurate description of the dynamics of magnetic materials based on the integration of the equation of motion [3], but it can also provide insights in thermodynamic properties of magnetic systems when incorporated into a Monte Carlo scheme. We will show results for BCC iron. The authors thank the Fantomas project for funding. [1] A. Kirilyuk *et al.*, RMP **82**, 2731 (2010). [2] M.V. You and V. Heine, JPF: Met. Phys. **12**, 177 (1982). [3] P. Ma and S.L. Dudarev, PRB **86**, 054416 (2012).

O 89.3 Fri 11:00 H33

Emission of correlated positron-electron pairs from surfaces — •Iuri Stefani Brandt[1], Zheng Wei[1], Frank Oliver Schumann[1], and Jürgen Kirschner[1,2] — [1]Max-PlanckInstitut für Mikrostrukturphysik, Halle, Germany — [2]Martin-LutherUniversität, Halle, Germany

The electron correlation is due to the combined action of the Pauli principle and Coulomb interaction. Electron pair emission is a powerful tool to study the aspects of the electron correlation. One way to disentangle the Pauli principle from the Coulomb interaction is to explore correlated positron-electron pair emission upon primary positron impact. This process of positron-electron pair emission is detectable and motivated a theoretical study [1,2]. We developed a dedicated laboratory positron source employing a Na22 isotope which provides a flux of $4x10^4$ e^+/s for kinetic energies in the range of 40-70 eV. We employ a symmetric geometry in which the incoming positrons hit the target along the surface normal. The emitted particles are measured in coincidence via a pair of energy dispersive spectrometers. We investigated NiO/Ag(100) and Ag(100) surfaces. In the case of electron pair emission upon primary electron impact we observe a symmetric two-dimensional energy distribution, because electrons are not distinguishable. Contrary to this electrons and positrons are distinguishable leading to an asymmetric two-dimensional energy distribution.

[1] G.A. van Riessen et al., JPCM **20**, 442001 (2008).
[2] F. Giebels et al., JPCM **21**, 355002 (2009).

O 89.4 Fri 11:15 H33

Space-Charge Interaction in Electron Momentum Microscopy — •Gerd Schönhense[1], Katerina Medjanik[1], Marieke de Loos[2], and Bas van der Geer[2] — [1]Institut für Physik, Uni. Mainz, Germany — [2]Pulsar Physics, Eindhoven, The Netherlands

Ultrahigh-brightness sources like (X)FELs, but also table-top higher harmonics sources offer fascinating experimental possibilities. Unfortunately, electron spectroscopic methods like photo- or Auger-electron spectroscopy at such sources are facing a dramatic loss in performance due to the space-charge problem. Coulomb interaction in the beam can induce prohibitively large energy broadenings ΔE of hundreds to thousands of eV. We have considered the space-charge effect for the special situation of a momentum microscope in the hard X-ray range, based on simulations with the General Particle Tracer (GPT) code. We find that momentum microscopy offers a pathway for a certain space-charge correction since the instrument detects the $k_{||}$- distribution in a parallel-imaging microscope column. For XFEL applications in the hard X-ray range a strong immersion field of 5 MV/m (close to the limit of potential breakthrough) accelerates and widens the electron beam very rapidly, in order to reduce Coulomb repulsion. The correction makes use of the fact that the line of best-fit of the electron distribution in an energy-vs-radius plot appears tilted and can be used for a re-normalization of the measured kinetic energies. GPT calculations for different model distributions including the intense low-energy signal from the secondary cascade reveal chances of a possible space-charge correction approach. Project funded by BMBF (05K12UM2).

O 89.5 Fri 11:30 H33

Femtosecond time-resolved photoemission on 1*T*-TaS_2 in the Mott-insulating state — •Isabella Avigo[1], Simon Freutel[1], Laurenz Rettig[1], Manuel Ligges[1], Lutz Kipp[2], Kai Rossnagel[2], and Uwe Bovensiepen[1] — [1](1)*Universität Duisburg-Essen, D 47048 Duisburg — [2](2)*Christian-Albrechts-Universität zu Kiel, D 24118 Kiel

1*T*-TaS_2 is a quasi-two-dimensional transition metal dichalcogenide undergoing a metal-to-insulator transition below 180 K in which a charge density wave (CDW) coexists with a Mott insulating state. Of particular interest is the photoinduced melting of the Mott-Hubbard phase which drives the system in a crossover state [1,2] substantially different from the high temperature metallic state. Femtosecond time- and angle-resolved photoemission measurements were performed in the Mott-insulating phase at different pump fluences from 0.1 to 1 mJ/cm^2. We observe a population of states above the Fermi level (E_F) after pumping and a depletion and broadening of the lower Hubbard band (LHB) peak below E_F. Our analysis reveals a difference in the relaxation dynamics of the electron population above E_F, which decays in about 350 fs, and the intensity of the lower Hubbard band, recovering in about 900 fs. This points to a possible decoupling of populations above and below E_F and thus to an at least unconventional metallic behavior in the photoinduced state.

We acknowledge support by the DFG through BO 1823/2, /4 and the EU under grant agreement 280555 within FP7. [1] Perfetti et al., NJP 10, 053019 (2008) [2] Dean et al., PRL 106, 016401 (2011)

O 89.6 Fri 11:45 H33

Long lived electrons trapped in amorphous ice adsorbed on Cu(111) — •Daniel Wegkamp, Michael Meyer, Clemens Richter, Julia Stähler, and Martin Wolf — Fritz-Haber-Institute of the MPG, Dep. of Physical Chemistry, Berlin

In polar environments excess charges are stabilized by reorientation of the surrounding dipoles. We have studied the trapping of excess electrons and their subsequent dynamics in amorphous solid water (ASW) adsorbed on a Cu(111) surface. The electrons are excited in the metal with ultraviolet (UV) femtosecond laser pulses and injected into 20 to 35 bilayer (BL) thick ASW layers. Their stabilization and relaxation dynamics are probed by time-resolved photoemission spectroscopy. In contrast to previous studies on thin (< 7 BL) ASW layers where sub-

picosecond lifetimes have been reported [1] we observe 14 orders of magnitude longer lifetimes. These electrons reside in an excited state between 2 and 3 eV above the metal's Fermi level for tens of seconds. The binding sites of the trapped electrons are located at the ice-vacuum interface, as their spectroscopic signature is affected strongly by a co-adsorbed Xe-overlayer. Furthermore, we have studied the changes of workfunction and occupied electronic structure induced by UV irradiation and discuss possible origins.

[1] J. Stähler et al., Chem. Soc. Rev. 37 (2008) 2180

O 89.7 Fri 12:00 H33

Electron Traps at the Ice Surface — •Michel Bockstedte and Anja Michl — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudstr. 7B2, D-91058 Erlangen

Water, water clusters and ice possess the fascinating ability to solvate electrons. On the surfaces of water clusters[1] and thin crystalline ice layers deposited on a metal substrate[2] long-living solvated electron states were observed that evolve from pre-existing surface traps. The identification of initial electron traps provides important insight into the electronic structure of the water surface, ice layers on metals and the dissociative interaction of electrons with adsorbates. Theoretical models[2] based on the bilayer terminated Ih-(0001) surface related such traps to orientational defects or vacancies with dangling OH-groups.[3] So far, a conclusive microscopic model of the electron traps at the surface of water structures on metals is missing. Here we address such electron traps including also water ad-structures observed by STM[4] theoretically using hybrid density functional theory and many-body perturbation theory in the G_0W_0 approximation. We identify a hierachy of traps with increasing vertical electron affinity, ranging from water admolecules and hexagon adrows via clusters of orientational defects to vacancy-related traps.

[1] Siefermann and Abel, Angew. Chem. Int. Ed. 50, 5264 (2011).
[2] Bovensiepen et al., J. Chem. Phys. C **113**, 979 (2009).
[3] Hermann et al., J. Phys. Condens. Matter **20**, 225003 (2008).
[4] Mehlhorn and Morgenstern, Phys. Rev. Lett. **99**, 246101 (2007).

O 89.8 Fri 12:15 H33

Improving the Temporal Resolution of a Time Resolved Electron Diffraction Experiment with Tilted Laser Pulse Fronts — •Annika Kalus, Carla Streubühr, Tim Frigge, Anja Hanisch-Blicharski, Boris Krenzer, Manuel Ligges, Ping Zhou, Uwe Bovensiepen, Dietrich von der Linde, and Michael Horn-von Hoegen — Universität Duisburg-Essen, Fakultät für Physik und Center for Nanointegration Duisburg-Essen (CENIDE)

Time resolved reflection high energy electron diffraction (RHEED) is an ideal tool to study the response of the surface lattice upon femtosecond laser pulse excitation. To achieve ps time resolution a laser pulse is used in a pump probe setup to excite the sample and to generate an electron pulse via photoemission that probes the sample. The temporal resolution of the experiment is limited by the velocity mismatch between laser pump pulse and the probing electron pulse at grazing incidence. To compensate this mismatch we realized an optical setup to tilt the laser pulse front by 70° in order to achieve temporal and spatial overlap with the 30 keV electron pulse over the entire width of the sample. The tilted laser pulse was characterized by a cross-correlator based on second harmonic generation.

Using the thermal response of thin Pb films on Si(111) upon laser excitation we optimized the optical setup and determined an improved temporal resolution of less than 1.8 ps at 29 keV electron energy. Electron phonon coupling in Bi is much weaker and results in a slow down of the heating of thin Bi films: a time constant for the excitation of about 10 ps was observed.

O 89.9 Fri 12:30 H33

2PPE-measurement with an angle-resolving time-of-flight spectrometer — •Thomas Kunze[1,2], Dominic Lawrenz[1], Jens Kopprasch[1], Martin Teichmann[1], Thorsten U. Kampen[2], and Martin Weinelt[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]SPECS GmbH, Berlin, Germany

To increase the efficiency of electronic structure measurements we developed in cooperation with SPECS an angle-resolving time-of-flight spectrometer.

The instrument allows to measure the kinetic electron energy as a function of the two-dimensional parallel crystal momentum (E vs. $k_{x\|}$ and $k_{y\|}$) without rotating the sample. The electron lens in front of the detector allows angle or spacial resolved measurements.

While developing this new machine a number of issues had to be addressed. We developed a proper way to simulate the electron trajectories, found a method to suppress secondary electrons and established a suitable measurement procedure. The use of the instrument is not as common as measurements with a hemispherical analyzer. We will point out the advantages and disadvantages of the method.

The talk will cover the alignment of the spectrometer itself and relative to the sample and the working principle of the detector gating unit.

Finally, we will report on our two-photon photoemission studies of Cu(111) and Cu(1 1 11) which illustrate the potential of time-of-flight electron spectroscopy.

O 89.10 Fri 12:45 H33

Comparison of the electronic surface states of Si(100) and Ge(100) studied by 2PPE — Kristof Zielke, •Jens Kopprasch, Christian Eickhoff, Cornelius Gahl, and Martin Weinelt — Fachbereich Physik der Freien Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We have investigated the electronic surface states at the (100)-surfaces of Si and Ge, two of the most important semiconductor surfaces in the device industry. Si(100) and Ge(100) are ideal for a comparison, because they have the same crystal structure and surface reconstruction, but exhibit distinct bulk band structures. We discuss the binding energy, the dispersion and the lifetimes of the dangling-bond states and the image-potential resonances on both surfaces and address the excitation of these surface states and their coupling to valence and conduction band continua. Furthermore, we show that the decay of photo-excited electrons in the conduction band is significantly influenced by the surfaces states. In particular, we discuss the role of inter- and intraband electron-phonon scattering between the conduction band and the unoccupied surface state D_{down}, and back scattering to the valence band. Thereby we found significant differences in the timescale of the decay processes on Si and Ge.

O 89.11 Fri 13:00 H33

Mono-energetic target surface electron (TSE) beams produced via surface guiding and acceleration in femtosecond laser-solid interactions — •Jingyi Mao[1], Liming Chen[2], Xulei Ge[2], Lu Zhang[2], Wenchao Yan[2], Dazhang Li[3], Guoqian Liao[2], Jinglong Ma[2], Kai Huang[2], Yutong Li[2], Xin Lu[2], Quanli Dong[2], Zhiyi Wei[2], Zhengming Sheng[2], and Jie Zhang[2,4] — [1]TU Kaiserslautern and Research Center OPTIMAS, 67663 Kaiserslautern, Germany — [2]Beijing National Laboratory of Condensed Matter Physics, Institute of Physics, CAS, Beijing 100190, China — [3]Institute of High Energy Physics, CAS, Beijing 100049, China — [4]Department of Physics, Shanghai Jiao tong University, Shanghai 200240, China

Highly collimated MeV TSE guiding has been observed along the target surface following the interaction of bulk target irradiation by femtosecond laser pulses at relativistic intensities[1]. The beam quality is shown to depend critically on the laser contrast: with a ns prepulse, the generated electron beam is well concentrated and intense, while high laser contrast produces divergent electron beams. In the case of large preplasma scale lengths on the target surface, tunable guiding and acceleration of TSE is achieved by changing the laser incident angle. By expanding the preplasma scale length to several hundred micrometers, we obtained MeV monoenergetic TSE beam with 100 pC per laser pulse and divergence angles of only 3 degrees, which could be used as a stable injector for accelerators.

[1] J. Y. Mao et al., Phys. Rev. E. 85, 025401(R)(2012)