Two-photon photoemission of image-potential resonances in front of the Si(100) surface — Jens Kopprasch, Christian Eckhoff, Irina Ostapenko, Cornelius Gahl, and Martin Wehner
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We have investigated the dangling-bond states and image-potential resonances on the Si(100) 2 × 1 surface by means of bichromatic two-photon photoemission. Optical parametric amplification generates 70 fs ultraviolet pulses with tunable photon energies between 4.5 and 5.5 eV. These allow us to populate unoccupied states up to the Si(100) vacuum level. In the combined model, 1) the kinetics of fast non-equilibrium between free carriers and phonons are accounted for in the continuum part by means of free carrier dynamics model.

Potential Energy Surface of Laser-Excited InSb — Jessica Walkenhurst, Ewue S. Zulistr, and Martin E. Garcia — Theoretische Physik, Fachbereich Naturwissenschaften, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

A recent experiment [A. M. Lindenberg et al., Science 308, 392 (2005)] performed on InSb suggests that ultrafast laser-induced nonthermal melting occurs due to a flattening of interatomic potentials. This study was based on the Debye-Waller theory, applied in the time-domain and for nonequilibrium processes. We analyzed the nonthermal melting of InSb by using (i) first-principles electronic structure calculations for the interatomic potentials (ii) dynamical models to find the structure factors under different nonequilibrium conditions. Our calculations show that no dramatic flattening of the potential energy surface occurs. Instead, the softening of the transverse acoustic phonons at the X point suffices to explain the measured Gaussian x-ray intensity decay.

Ultrafast electron dynamics in Pb/Si(111) investigated by two-photon photoemission — Patrick S. Kirchmann, Martin Wolf, and Uwe Bovensiepen — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin-Dahlem

We studied the ultrafast electron dynamics of hot electrons in quantum well states (QWS) in ultrathin epitaxial Pb films on Si(111) [1] by femtosecond time-resolved two-photon photoemission spectroscopy.

Combining density functional and density matrix theory: Optical excitation and electron relaxation at the Si(001) 2 × 1 surface — Norbert Bücking, Peter Kratzer, Matthias Scheffler, and Andreas Knorr — 1 Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany — 2 Fachbereich Physik, 47048 Duisburg, Germany — 3 Fritz-Haber-Institut der MPG, 14195 Berlin, Germany

A theoretical two-step approach to investigate the optical excitation and subsequent phonon-assisted relaxation dynamics at semiconductor surfaces is presented and applied to the Si(001) 2 × 1 surface. In the first step, the electronic band structure and the Kohn-Sham wave functions are calculated by density-functional theory (DFT) within the LDA. In the second step, dynamical equations are derived from density-matrix theory (DMT), whereby an optical field is considered via A · p-coupling and phonon induced relaxation by a deformation potential coupling term. Into these equations, the numerical results of the DFT calculation (Kohn-Sham eigenvalues and wave functions) enter as coupling matrix elements. By numerically solving the dynamical equations, the time-resolved population of the excited states can be evaluated. The results for the Si(001) surface correspond to vacuum level, no bias, and at a fixed wavelength of 795 nm. Besides the occupied dangling-bond state D, we resolve the first two image-potential states with binding energies of E = 0.62 eV and E = 0.18 eV with respect to the vacuum level. Using these energies we obtain a surface dielectric constant of ε = 11.2 which is close to the silicon bulk-value of ε = 11.94.

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Up to four unoccupied QWSs are identified, which exhibit a biexponential decay of the hot electron population. The slower decay is assigned to a delayed decay of the metallic QWS in the Pb adlayer by scattering from electronic states of the optically excited Si(111) substrate. The faster decay is assigned to e-e scattering within the Pb film. The overall trend of the extracted decay rates is governed by Fermi liquid theory. However, a detailed analysis reveals a well resolved dip in the decay rate which occurs precisely at the binding energy of the band bottom of the first unoccupied QWS. This local minimum of the decay rate is assigned to intra-subband scattering within the Pb film.

Thus, for a comprehensive description of the electron decay in a two-dimensional metal film not only the electron density and screening parameters as in Fermi liquid theory have to be considered. Here, we show that also the electron-electron scattering processes in the quantized band structure have to be taken explicitly into account.

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The understanding of fundamental mechanisms behind the sub-wavelength length surface modification on semiconductors is of a great importance for Information Technologies. However, strong laser-induced phase perturbations, occurring under conditions of nonequilibrium between free laser-generated carriers and phonons, make the experimental and theoretical study of short pulse laser nanostructuring on semiconductors difficult. Previously, the atomistic-continuum approach for modeling of short-pulse laser interactions with metals have been proven as an efficient tool when studying processes of laser melting, ablation, and nanostructuring on metals. In present work, a computational technique that combines the advantages of different approaches into the atomistic-continuum model for semiconductors is developed on the example of Si. In the combined model, 1) the kinetics of fast non-equilibrium phase transformations is treated at atomic level with Molecular Dynamics method, and 2) the description of laser light absorption by free carriers, their transport dynamics, and strong laser-induced non-equilibrium between free carriers and phonons are accounted for in the continuum part by means of free carrier dynamics model.
discrepancy is attributed to the limited time-resolution of the experiment. However, the Pb/Si(111) is an ideal system to quantify the experimental temporal resolution and to test methods for improving the time-resolution.