Quantum-mechanical simulation of attosecond streaked photoemission from Mg-covered W(110) surfaces

2015 J. Phys.: Conf. Ser. 635 102002

(http://iopscience.iop.org/1742-6596/635/10/102002)

Quantum-mechanical simulation of attosecond streaked photoemission from Mg-covered W(110) surfaces

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Synopsis We apply a quantum-mechanical model to simulate infrared-streaked photoelectron emission by an ultrashort extreme ultraviolet pulse from adsorbate-covered metal surfaces. Incorporating effects of energy-dependent electron mean-free paths, the properties of initial states, photoelectron energy dispersion, and the screening of the streaking field, this model is able to reproduce recently measured photoelectron spectrograms and adsorbate-thickness-dependent photoemission time delays.

Attosecond streaking, using an isolated attosecond extreme ultraviolet (XUV) pump pulse and a delayed few-cycle infrared (IR) streaking pulse, is able to time-resolve electron photoemission from atoms and condensed matter systems on an attosecond time scale [1]. A recent streaked photoemission experiment with ultrathin Mg adsorbate films on a W(110) substrate [2] reveals a monotonic dependence of the relative photoemission time delay $\Delta\tau_{4f-2p}$ between W($4f$) and Mg($2p$) core-level (CL) photoelectrons and a non-monotonic dependence of the relative photoemission time delay $\Delta\tau_{CB-2p}$ between conduction band (CB) and Mg($2p$) CL photoelectrons on the adsorbate thickness.

In order to interpret the measured relative photoemission time delays from the Mg/W(110) systems, we apply a quantum-mechanical model [3, 4]. By taking the energy-dependent electron mean-free path (MFP), the properties of initial states (including band-structure and wave-function-localization effects), energy dispersion, and the screening of IR streaking field at the surface into account, our numerical results [5] reproduce measured [2] streaked photoemission spectra and relative photoemission time delays as a function of the Mg-film thickness (Fig. 1).

As input for our numerical simulation, we only employ measured and calculated MFPs and an IR skin depth of 2 Å [2, 3]. In addition, we describe the dispersion of released CB electrons inside the W substrate based on an adjusted effective electron mass (0.86 a.u.). We assume free-electron propagation of CB electrons in the Mg adsorbate film and for electrons that are released from Mg($2p$) and W($4f$) CLs, to match the relative photoemission delay between CB and W($4f$) photoelectrons for the adsorbate-free W(110) surface. Our quantum-mechanical results also agree with classical free-electron calculations [2] for $\Delta\tau_{4f-2p}$.

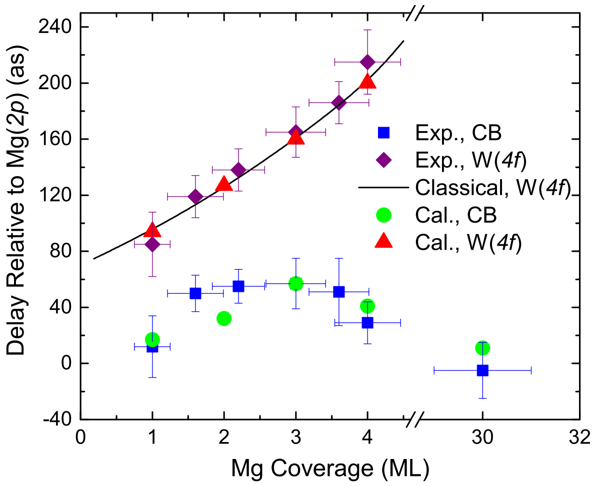

Figure 1. Measured [2] and classically [2] and quantum-mechanically [5] calculated streaking time delays relative to Mg($2p$) emission for CB and W($4f$) photoelectrons as a function of the Mg coverage on a W(110) substrate. The central XUV photon energy is 118 eV.

This work was supported by NSF Grant PHY 1068752 and the Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, Office of Science, U.S. DOE.

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