Revealing Non-Adiabatic Effects on Bi(111)

P. Kraus (1), A. Tamtögl (1), M. Mayrhofer-Reinhartshuber (1), D. Campi (2), G. Benedek (2), W.E. Ernst (1)

(1) Institute of Experimental Physics, Graz University of Technology, Graz, Austria
(2) Dipartimento di Scienza die Materiali, Universitá di Milano-Bicocca, Milano, Italy

The (111) surface of the semimetal bismuth exhibits unusual electronic and vibrational behavior. Due to its large spin-orbit coupling the bands for different spin orientations are not degenerate and give rise to a very good conductivity along the surfaces [1], while the bulk stays a very poor conductor. Additionally, those unique properties of bismuth cause an unexpectedly high corrugation of the surface electron density, perfectly suited for Helium Atom Scattering experiments. Those experiments reveal a practically non-reconstructed surface layer with a sixfold symmetry [2]. Additionally to the measured scattering features, small variations in the noise as well as strong fluctuations in the specular intensity give rise to a detailed description of the He-Bi(111) interaction potential. This potential supports bound states, which furthermore can lead to elastic and inelastic surface resonances. Especially the latter can explain the rather unusual data obtained in time-of-flight measurements.
Therefore, an extensive analysis of the inelastic scattering data was performed. Using a detailed model of the bismuth crystal and comparison to the simulation of the phonon dispersion on the antimony (111) surface [3], several non-adiabatic effects were revealed that are not accessible via ordinary DFPT simulations [4].

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