Quantum-size effects on vibrations and electron-phonon coupling in thin Pb(111) films

Rolf Heid

Institute for Solid State Physics, Karlsruhe Institute of Technology, Germany

Thin metal films are well known realizations of the geometrical confinement of electronic motion which manifests itself in the presence of quantum-well states and profoundly alters the electronic structure. Its influence on the electron-phonon coupling is, however, much less understood. In this context, Pb(111) films on semiconducting substrates have been studied extensively in recent years, because superconductivity was found to persist in ultrathin films, albeit with reduced transition temperature [1], and was observed even for a single monolayer [2]. This raised questions to what extend quantum-size effects modify the electron-phonon coupling directly, and what is the role of the substrate.

In this talk, I will present a comprehensive first principles investigation of electronic, vibrational, and electron-phonon coupling (EPC) properties of thin Pb(111) films in the framework of density functional perturbation theory. Similar to the findings for lead bulk [3], it was imperative to include spin-orbit interaction for a proper quantitative description of vibrational spectra and coupling strengths. Results for Fermi surface averaged couplings, relevant for superconductivity [4], as well as for EPC-induced self-energies of quantum well states for various film thicknesses are discussed in comparison with recent experiments. I will also address the influence of the substrate on these properties.

[1] Y. Guo *et al.*, Science **306**, 1915 (2004)
[2] T. Zhang *et al.*, Nat. Phys. **6**, 104 (2010)
[3] R. Heid *et al.*, Phys. Rev. B **81**, 174527 (2010)
[4] I.Yu. Sklyadneva *et al.*, Phys. Rev. B **87**, 085440 (2013)