Thin metal films on metal surfaces are of great interest as model systems for materials with reduced dimensionality. For ultra-thin Pb films on Cu(111) it was demonstrated that the HAS inelastic intensities provide a direct measurement of mode-selected electron-phonon (e- ph) coupling strengths for individual surface and sub-surface phonons (mode-lambda spectroscopy) [1], thus allowing to assess which phonons are actually relevant in superconductivity. For a correct description of the distribution of the phonon density of states in the film, it is important to take into account the emerging structure of the interface and the interaction between the film atoms and the atoms of the first substrate layer. The calculations presented here are based on the embedded atom method (EAM) and include the dynamics of the substrate (Fig.1). Besides leading to a detailed interpretation of the HAS experimental data, the present results are compared with a density-functional perturbation theory study on a rigid substrate. The comparison reveals the role played by the substrate dynamics at the smallest thicknesses, despite the large mass and stiffness differences between Pb and Cu.

The EAM structure analysis also reveals a considerable corrugation of the film surface and of the substrate atomic layers. A dynamically stable structure is formed with a low-energy stretching mode which results from a strong coupling of the monolayer phonons with the low-energy shear-vertical vibrations of the top substrate atoms.

**Keywords:** Superconducting films, interfaces and surfaces

**References**