DFT investigations of ultrathin Pb films

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We report on the investigations of the charge transport in ultrathin Pb(111) slabs. Specific for ultrathin films is lack of translational invariance in the direction perpendicular to the film. This influences the electron bandstructure, each bulk band splits into a set of discrete sub-bands. Using the DFT as implemented in the WIEN2k code we calculated the electron bandstructure, the Fermi lines, the Fermi velocities and the effective masses of all sub-bands in 1 - 8 monolayers thin Pb(111) slabs. With the Botzmann transport equation we then calculated the electrical and Hall conductivities and the Hall coefficient. The results are compared with the experiments on Pb/Si(111) films. The main mechanism limiting the conductivities at low temperatures is the diffuse scattering on the surface roughness which leads to a linear thickness dependence of the electrical conductivity, like in the Fuchs-Sondheimer theory. The films show strong quantum-size effects; the Hall coefficient, e.g., oscillates in sign as the film thickness is varied.