Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Comparative studies of Pb films on different substrates by first-principles calculations[1] YU JIA, Zhengzhou University, China & ORNL, BIAO BU, Inst. of Phys. CAS, China, H.H. WEITERING, The University of Tennessee & ORNL, ZHENYU ZHANG, ORNL & The University of Tennessee — Quantum growth of ultrathin Pb on Ge(111) and Cu(111) substrates up to more than 25 monolayers are studied using total energy calculations within density functional theory. Our studies show that the surface energy, work function, and lattice relaxation of these films all oscillate strongly with the film thickness. The oscillation pattern is always even-odd with interruptions by crossovers, in good agreement with experimental observations. However, the positions of the crossovers and the separation between the crossovers depend on which substrate is used. These results are rationalized based on the interplay between Friedel oscillations, quantum size effects, and charge transfer effects.

[1]Supported by US DOE, US NSF, & NSF of China.

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Date submitted: 06 Dec 2005 Electronic form version 1.4