Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Super-oscillations in the Interlayer Lattice Relaxation of Quantum Pb Films.[1] YU JIA, Zhengzhou University, China, BIAO WU, Institute of Physics, CAS, China, T.L. EINSTEIN, University of Maryland, H.H. WEITERING, The University of Tennessee & ORNL, ZHENYU ZHANG, ORNL & The University of Tennessee — Using first-principles total energy calculations, we study the interlayer relaxation in lead films and observe oscillations of the interlayer lattice relaxation with layer number (distance from vacuum) and with film thickness. By analyzing the charge distribution along the direction perpendicular to the film, we show that the former oscillations of lattice relaxation are induced by Friedel oscillations in charge density that decays slowly, following a $1/r$ law rather than a $1/r^2$ law found in most metal films. The superoscillations are attributable to interference of the Friedel oscillations from the two boundaries of the film. Our results suggest that Friedel oscillations may be responsible for the quantum size effect observed in lead films.

[1]Supported by NSF of China, the DMSE program and grant No. DE-FG02-05ER46209 of US DOE, and grant Nos. DMR-0606485 and DMR-0520471 of US NSF.

Yu Jia
Zhengzhou University, China

Date submitted: 28 Nov 2007 Electronic form version 1.4