## Abstract Submitted for the MAR05 Meeting of The American Physical Society

Finite size effects on multilayer relaxations ERIK HOLMSTRÖM, ANDERS NIKLASSON, NICOLAS BOCK, SVEN RUDIN, JOHN WILLS, Los Alamos National Laboratory — We calculate the out of plane layer relaxations of thin embedded metallic films as a function of film thickness. The relaxations show an oscillating behavior that is consistent with superimposed surface-induced Friedel oscillations of the charge density of the film. Additionally there is an effect on the relaxation from the interaction between the surfaces that is analogous to the change in density of states that is induced by quantum well states. The calculations are performed by means of pseudopotential, first principles calculations in the framework of the Vienna ab initio simulation package (VASP).

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