

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Patterns in strained epitaxial layers: Beyond the Frenkel-Kontorova model¹ KRISTEN FICHTHORN, Penn State University, JOSHUA HOWE, University of California at Berkeley — Although the structures of strained overlayers have been understood in terms of the classical Frenkel-Kontorova model [1], our recent work indicates that these structures can have a quantum mechanical origin. Experimental STM studies show that the second layer of Ag on Pt(111) forms a striped pattern [2]. We simulated the striped phase with a combination of DFT, to quantify Ag pair interactions up to the 53rd neighbor [3], and Monte Carlo (MC). Our MC simulations yield a striped phase with the experimental characteristics: stripes along the [112] direction that alternate between fcc and hcp sites. Although our DFT pair potential can be fit in an average way to a theoretical expression with radial symmetry [4], this fit cannot produce the striped phase, indicating that angular variations in the potential are important in producing this phase. [1] J. Frenkel and T. Kontorova, *Journal of Physics-USSR* 1, 137 (1939). [2] H. Brune, H. Roder, C. Boragno, and K. Kern, *Phys. Rev. B* 49, 2997 (1994). [3] W. Luo and K. A. Fichtorn, *Phys. Rev. B* 72, 115433 (2005). [4] P. Hyldgaard and M. Persson, *J. Phys: Cond. Matter* 12, 2981 (2000).

¹Supported by NSF DMR 0514336

Kristen Fichtorn
Penn State University

Date submitted: 20 Nov 2009

Electronic form version 1.4