Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Kinetic Monte Carlo simulations of Ag(111) island coarsening[1]
GIRIDHAR NANDIPATI, YUNSIC SHIM, JACQUES AMAR, University of Toledo, ALTAF KARIM, University of Delaware, ABDELKADER KARA, TALAT RAHMAN, University of Central Florida — The results of parallel kinetic Monte Carlo simulations of submonolayer island coarsening on the Ag(111) surface are presented. Our simulations are carried out using a large database of activation barriers which has been generated from previous self-learning kinetic Monte Carlo simulations of small and medium-size clusters. In this database, which includes both single-atom and multi-atom concerted moves, interactions between a central atom and all other adatoms within the first two nearest-neighbor rings are taken into account, while the symmetry of the (111) surface is also used. In order to reach extended time and length-scales we have implemented a novel parallel kinetic Monte Carlo scheme in which processor domains are dynamically assigned in order to minimize boundary events. Preliminary results using an open database corresponding to a true self-learning kinetic Monte Carlo simulation will also be presented.

[1]Supported by NSF through grant CCF-042882622

Jacques Amar
University of Toledo

Date submitted: 20 Nov 2006 Electronic form version 1.4