

Abstract Submitted
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Crossover from concerted motion to periphery diffusion for Cu clusters on Cu(111): Application of Fine Grid On-Lattice SLKMC¹ SYED ISLAMUDDIN SHAH, GIRIDHAR NANDIPATI, University of Central Florida, ALTAF KARIM, Lawrence Berkeley National Laboratory, ABDELKADER KARA, TALAT S. RAHMAN, University of Central Florida — The “fine grid on-Lattice” Self-Learning Kinetic Monte Carlo (SLKMC) technique combines the ideas embedded in the SLKMC [1] method with a new pattern recognition scheme which incorporates both fcc and hcp sites to characterize and store configurations. Application of methods for saddle point searches have revealed several new mechanisms involving multiple atoms which contribute to cluster migration. We present results for the diffusion of 2D Cu islands on Cu(111), using semi-empirical interatomic potentials [2], at three temperatures (300K, 500K and 700K). Long time simulations show a trend in crossover from concerted motion to periphery diffusion for clusters containing more than 14 atoms. The calculated trends in effective energy barriers and diffusion constants are compared with those obtained earlier from the SLKMC Method [1] which allowed only surface fcc site occupancy.

[1] A. Karim et al. Phys. Rev. B 73, 165411 (2006)

[2] S. M. Foiles et al. Phys. Rev. B 33, 7983 (1986)

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