

Abstract Submitted  
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**Diffusion of small Ni and Cu clusters on Ni (111): Application of SLKMC-II\***<sup>1</sup> SYED ISLAMUDDIN SHAH, Department Of Physics, University Of Central Florida, GIRIDHAR NANDIPATI, Pacific Northwest National Laboratory, TALAT S. RAHMAN, Department Of Physics, University Of Central Florida — We have examined the diffusion of small Ni and Cu islands (consisting of up to 10 atoms) on the Ni(111) surface using a self-learning kinetic Monte Carlo (SLKMC-II) [1] method with an improved pattern-recognition scheme that allows inclusion of both fcc and hcp sites in the simulations. In an SLKMC simulation [2] a database holds information about the local neighborhood of an atom and associated processes that is accumulated on-the-fly, as the simulation proceeds. The activation energy barriers for the identified diffusion processes were calculated using semi-empirical interaction potential based on the embedded-atom method. Although a variety of concerted, multi-atom and single-atom processes were automatically revealed in our simulations, we found that these small islands diffuse primarily via concerted motion. We report diffusion coefficients for each island size at several temperatures, and from the Arrhenius plot extract the size-dependent effective diffusion barrier for these islands. Our evaluation of the occurrence frequency of processes most responsible for the diffusion of island of a specific size reveal several that are not accessible in SLKMC-I [2] or in short time-scale MD simulations. We also provide results of extending SLKMC-II to examine epitaxial growth in these systems. [1] S. Islamuddin Shah, et al., J. Phys.: Condens. Matter 24, 354004 (2012). [2] O. Trushin, et al., Phys. Rev. B 72, 115401 (2005).

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