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Diffusion of small Cu islands on the Ni(111) surface: Results of the self learning kinetic Monte Carlo(II) simulations[1] SHREE RAM ACHARYA, SYED ISLAMUDDIN SHAH, TALAT S. RAHMAN, University of Central Florida — We have examined the diffusion of two dimensional Cu islands (up to 10 atoms) on the Ni(111) surface using Self-Learning Kinetic Monte Carlo (SLKMC-II)[1] method which allows occupancy of both fcc and hcp sites on the fcc(111) surface for the identification of local neighborhood of a diffusing atom.The SLKMC-II reveals various single-atom , multi-atoms and concerted processes on the fly and stores them in a database. Energy barriers for these processes are calculated using semi-empirical embedded-atom method potential. Here we discuss some of the novel processes and their energy barriers found during the simulations and compare them with those found for the diffusion of Cu islands on Cu(111). We also report temperature dependence of the diffusion constants and frequency of occurrence of single-atom, multi-atom and concerted processes for these islands. The size dependence of effective energy barriers derived from the Arrhenius plots is also discussed. [1].S.I.Shah, et al., J.Phys.: Condens. Matter 24(2012)354004

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