Diffusion kinetics of small islands of Ni on Cu (111) and Cu on Ni (111) using the self-learning kinetic Monte Carlo (II) simulations and rationale for variation based on first-principles calculation[1] SHREE RAM ACHARYA, TALAT S. RAHMAN, University of Central Florida — We elucidate the diffusion kinetics of two dimensional small islands (upto 8 atoms) of Ni on Cu(111) and Cu on Ni(111) 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. In this method, the activation energy barriers for various possible single-atoms, multi-atoms and concerted processes are calculated using semi-empirical embedded-atom method potential on the fly and stores them in a database. The rationale for the variation of activation energy barriers on those systems is presented based on first principle calculations. We present the rate limiting processes for diffusion of islands of various sizes and their energetics: concerted processes on Ni/Cu(111) and various competing single atom or multi-atom and concerted processes on Cu/Ni(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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