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Self-Diffusion of small Ag and Ni islands on Ag(111) and Ni(111) using the self-learning kinetic Monte Carlo method[1] SYED ISLAMUDDIN SHAH, GIRIDHAR NANDIPATI, ABDELKADER KARA, TALAT S. RAHMAN, University of Central Florida — We have applied a modified Self-Learning Kinetic Monte Carlo (SLKMC) method [1] to examine the self-diffusion of small Ag and Ni islands, containing up to 10 atom, on the (111) surface of the respective metal. The pattern recognition scheme in this new SLKMC method allows occupancy of the fcc, hcp and top sites on the fcc(111) surface and employs them to identify the local neighborhood around a central atom. Molecular static calculations with semi empirical interatomic potential and reliable techniques for saddle point search revealed several new diffusion mechanisms that contribute to the diffusion of small islands. For comparison we have also evaluated the diffusion characteristics of Cu clusters on Cu(111) and compared results with previous findings [2]. Our results show a linear increase in effective energy barriers scaling almost as 0.043, 0.051 and 0.064 eV/atom for the Cu/Cu(111), Ag/Ag(111), and Ni/Ni(111) systems, respectively. For all three systems, diffusion of small islands proceeds mainly through concerted motion, although several multiple and single atom processes also contribute. [1] Oleg Trushin et al. Phys. Rev. B 72, 115401 (2005) [2] Altaf Karim et al. Phys. Rev. B 73, 165411 (2006)

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