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Atomic diffusion processes in heteroepitaxial metallic systems using SLKMC-II SYED ISLAMUDDIN SHAH, ALTAF KARIM, Department of Physics, COMSATS Institute of information technology, Park Road, Tarlai Kalan, Islamabad 45550, Pakistan — We have examined the diffusion of small islands of Cu on Ag(111) surface using a self-learning kinetic Monte Carlo (SLKMC-II) [1] method with an improved pattern recognition scheme. Due to strain generated at the interface between metals with different bulk lattice constants, interesting single atom, multi-atom and concerted diffusion processes are automatically revealed in the simulations. Here we will report various processes for small islands in the case of Cu/Ag(111) system. Key processes responsible for island diffusion and their energetics together with trends in effective energy barriers as well as diffusion constants for small islands will also be provided. In addition to 2-D diffusion processes, as an application of SLKMC-II to the 3-dimensional heteroepitaxial systems, we will also report energy barriers of some of the 3-dimensional processes including down the A- and B-steps and exchange processes. [1] Syed Islamuddin Shah, et al., J. Phys.: Condens. Matter 24, 354004 (2012)

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