Self-Diffusion of Small Ag, Cu, and Ni Islands on fcc(111) Surfaces: An Application of SLKMC-II

S. I. Shah, G. Nandipati, A. Kara, and T. S. Rahman

Department of Physics, University of Central Florida, FL, USA.

A few years ago, our group proposed a self-learning kinetic Monte Carlo (SLKMC) scheme [1] in which inclusion of a pattern recognition scheme and on-the-fly calculation of activation energy barriers allowed the creation of a data base of possible diffusion processes for adatom islands, containing up to 30 atoms. While this addressed the issue of lack of completeness of diffusion mechanisms in standard KMC simulations, the scheme was limited to adatom occupancy of only the fcc sites. Here we report the development of a new pattern-recognition scheme that takes into account both fcc and hcp adsorption sites in performing self-learning kinetic Monte Carlo (SLKMC-II) simulations on fcc(111) surfaces. In this scheme, the local environment of each under-coordinated atom is uniquely identified by grouping the fcc and hcp sites and the top-layer substrate atoms around it into hexagonal rings. As simulation progresses, all possible processes—including shearing, reptation and concerted gliding, which may involve fcc-fcc, hcp-hcp and/or fcc-hcp moves are automatically found, and their energetics calculated on the fly. We present results of application of this new pattern-recognition scheme to the self-diffusion of (Mg) on M(111), where M = Cu, Ag or Ni.

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[1] O. Trushin, A. Karim, A. Kara , and T. S. Rahman, Phys. Rev. B **72**, 115401 (2005).

Contact: islamuddin@knights.ucf.edu