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Self-Teaching Kinetic Monte-Carlo Scheme For Small Cluster Diffusion on Cu(111)[1] PETR VIKULOV, OLEG TRUSHIN, VICTOR NAUMOV, Institute of Microelectronics and Informatics, Russian Academy of Sciences, Yaroslavl Russia, ALTAF KARIM, ABDELKADER KARA, TALAT S. RAHMAN, Department of Physics, Kansas State University — We have developed a new version of Self-Teaching Kinetic Monte Carlo technique (ST-KMC) for simulations of processes relevant to growth on fcc(111). In this method, adsorbed atoms may occupy fcc or hcp sites for 2D cases. Additionally, adatoms may occupy "top" sites in the case of 3D simulations. The environment of any diffusing adatom is mapped using a 211-site template mimicking the layer stacking on fcc surfaces. We applied this new approach to the diffusion of small copper adatom clusters with size from 1 to 7 atoms on a Cu(111) surface. Activation energies for all mechanisms were calculated using the drag method, for saddle points search, and Embedded Atom Method (EAM) for interaction potentials. With this new approach, it was possible to incorporate multi-atom concerted motion involving the occupancy of fcc and hcp sites, which has been suggested by experimental findings and MD simulations of small clusters diffusion on fcc(111). Diffusion coefficients and their scaling with size and temperature will be presented and contrasted with MD and KMC results.

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