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Modeling of morphological evolution on Cu(111) surface: application of Self-Teaching KMC-MD method[1] OLEG TRUSHIN, VICTOR NAUMOV, Institute of Microelectronics and Informatics RAS, Yaroslavl, Russia, ABDELKADER KARA, TALAT RAHMAN, Department of Physics, Kansas State University, Manhattan, KS — We present a novel integrated approach which combines Self-Teaching kinetic Monte-Carlo (STKMC) and molecular dynamics (MD), and its application in modeling morphological evolution on Cu(111) surface at homoepitaxial growth. MD is applied for modeling adatom-surface collision event, while STKMC is used for simulation of diffusion driven kinetics between deposition events. We use semi-empirical EAM potential for estimating energetics of different diffusion processes in STKMC and interatomic forces in MD simulation. STKMC represents standard KMC algorithm on lattice gas model with constantly accumulated database of atomic diffusion processes. This approach allows to include explicitly different single and many atomic processes and accurately take into account effect of local atomic surrounding. Adatoms are deposited with thermal energies, which corresponds to physical vapor deposition conditions. Using this method we are modeling morphological evolution on the surface during thin film growth in submonolayer regime and different postdeposition phenomena.

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