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Self-Learning Off-Lattice Kinetic Monte Carlo method as applied to growth on metal surfaces[1] OLEG TRUSHIN, Institute of Microelectronics and Informatics RAS, Yaroslavl, Russia, ABDELKADER KARA, TALAT RAHMAN, University of Central Florida — We propose a new development in the Self-Learning Kinetic Monte Carlo (SLKMC) method with the goal of improving the accuracy with which atomic mechanisms controlling diffusive processes on metal surfaces may be identified. This is important for diffusion of small clusters (2 - 20 atoms) in which atoms may occupy Off-Lattice positions. Such a procedure is also necessary for consideration of heteroepitaxial growth. The new technique combines an earlier version of SLKMC [1] with the inclusion of off-lattice occupancy. This allows us to include arbitrary positions of adatoms in the modeling and makes the simulations more realistic and reliable. We have tested this new approach for the case of the diffusion of small 2D Cu clusters diffusion on Cu(111) and found good performance and satisfactory agreement with results obtained from previous version of SLKMC. The new method also helped reveal a novel atomic mechanism contributing to cluster migration. We have also applied this method to study the diffusion of Cu clusters on Ag(111), and find that Cu atoms generally prefer to occupy off-lattice sites. [1] O. Trushin, A. Kara, A. Karim, T.S. Rahman Phys. Rev B 2005

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