

Abstract Submitted
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Off-lattice self-learning kinetic Monte Carlo: application to 3D island decay on fcc(100) surface¹ GIRIDHAR NANDIPATI, ABDELKADER KARA, SYED ISLAMUDDIN SHAH, TALAT S. RAHMAN, University of Central Florida — We report the development of an off-lattice kinetic Monte Carlo (KMC) method with a new three-dimensional (3D) pattern recognition scheme to better identify the local environment and processes involving 3D motion which was not possible in the earlier approach [1]. In the present scheme, to uniquely identify the 3D neighborhood around the central atom or leading atom we split it into 3D rectangular boxes whose dimensions dictate the accuracy with which the motion of the diffusing entity to be accounted. This technique combines the idea of self-learning KMC (SLKMC) [2] method with the new pattern-recognition scheme fitted to an off-lattice model. We present application of this off-lattice SLKMC to 3D island decay on fcc (100) surface and compare the results and computational efficiency to that available in the literature.

[1] A. Kara et al, J. Phys.: Condens. Matter, 21 (2009)

[2] O. Trushin et al, Phys. Rev. B, 72, 115401 (2005)

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