Atomic Processes responsible for the diffusion of 2D Cu islands on Ag(111): results from self learning KMC[1] O. TRUSHIN, Institute of Microelectronics, ASR, Yaroslavl, H. YILDIRIM, A. KARA, T.S. RAHMAN, Department of Physics, University of Central Florida — Diffusion on Ag(111) of small 2D-Cu clusters (4 to 30 atoms) is examined using embedded atom method potentials, as a first step towards understanding hetero epitaxial growth. A combination of an Off-Lattice Self-Learning Kinetic Monte Carlo and spherical repulsion scheme for saddle point searches, has revealed novel diffusion mechanisms. For this size range, the diffusion of islands involve 3 classes of processes: i) collective concerted motion (gliding), found to be dominant for small sized islands (4-9); ii) processes involving shear mechanism in which some of the Cu island atoms are commensurate with the substrate and others are not (> 9 atoms), finally iii) processes involving a "breathing" mechanism in which the island "shrinks" as a whole before "relaxing" to a less compact shape with a net displacement of the whole cluster equivalent to an fcc-hcp hop (> 12 atoms). These processes were revealed during the first 100 KMC steps for each island. Diffusion coefficients as a function of temperatures, effective diffusion barriers and frequencies of the responsible events will be presented.

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