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Rapid Diffusion of Magic-Size Islands by Combined Glide and Vacancy Mechanisms

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Monolayers of Ag on Cu(001) are well known to reconstruct forming a (10x2) reconstruction with Ag atoms packed hexagonally on the four-fold Cu(001) surface [1]. We have investigated the surface diffusion of hexagonally-packed Ag monolayer islands of various sizes on Cu(001) using computer simulation techniques. Our examination reveals a novel cooperative diffusion mechanism consisting of core glide coupled with the migration of edge vacancies. It should be noted that island diffusion is completely one-dimensional with the direction determined by the orientation of the (10x2) reconstruction for the diffusing island. In other words, rows of the hexagonal Ag lattice move along the hollow and bridge sites of the Cu substrate in a {110} type direction. In addition, we have observed magic-sized islands for which diffusion occurs much more rapidly as a result of their reduced diffusion barrier. In particular for a 169-atom hexagonal island, the activation energy for diffusion is smaller than the barrier for a single Ag atom hop. For this island size, diffusion occurs rapidly at temperatures as low as 200K. Molecular dynamics simulations suggest that the surface diffusion process displays non-Arrhenius behavior possibly resulting from the temperature-dependent lattice mismatch. Our findings should provide insight to future experimental research on the size distribution and shapes observed during the growth of thin films in similar systems.

References:

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