

Abstract Submitted
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Low-temperature Ag/Ag(100) growth revisited¹ JACQUES G. AMAR, YUNSIC SHIM, University of Toledo — Recent experiments on Ag/Ag(100) growth indicate that the surface roughness exhibits a non-monotonic temperature-dependence - with peaks at approximately $T = 90$ K and 200 K. While the high-temperature peak has been previously explained the low-temperature peak has not. Here we present the results of hybrid molecular-dynamics/kinetic Monte Carlo simulations - with activation barriers obtained from recent parallel-temperature accelerated dynamics simulations - which were carried out in order to understand the growth behavior over the temperature range $T = 55 - 180$ K. Our simulations indicate that even at high temperature the surface roughness depends sensitively on a competition between a variety of low-barrier processes including downward funneling of depositing atoms, island relaxation via edge-zipping and edge-diffusion, atom-attraction, and concerted interlayer diffusion at kinks, while the short-range attraction of depositing atoms to microprotrusions also plays a crucial role. By taking these processes into account in our simulations, good agreement with experiment is obtained over the entire temperature range. A comparison between DFT calculations and EAM predictions for certain key barriers will also be presented.

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