Molecular dynamics simulations of low temperature Cu/Cu(100) growth

VALERY BOROVIKOV, YUNSIC SHIM, JACQUES G. AMAR, University of Toledo — Recent X-ray scattering studies [1] of Cu/Cu(100) growth indicate the existence of a sharp transition from epitaxial growth at high temperatures to growth with a high vacancy concentration at lower temperatures ($T < 150$ K). Here we present the results of molecular dynamics (MD) simulations carried out in order to understand the detailed mechanisms of incorporation of vacancies and voids (vacancy clusters) into the growing film during low temperature deposition. The dependence of compressive strain, vacancy concentration and vacancy-cluster size distribution in deposited thin film, as well as the surface roughness and morphology on deposition conditions, such as the growth temperature, deposition angle, and incident kinetic energy will be discussed and compared with experiments. [1] C. E. Botez, K. Li, E. D. Lu, W. C. Elliott, P. F. Miceli, E. H. Conrad, and P.W. Stephens, Appl. Phys. Lett. 81, 4718 (2002).