A Kinetic Monte Carlo Study of the Morphology of Si Thin Films Deposited On Si(100) at Varying Angles of Incidence

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Two- and three-dimensional Kinetic Monte Carlo simulations are used to model the deposition of a hyperthermal molecular beam at varying angles of incidence. The simulations incorporate incident atom - substrate interactions, many layer growth and, for the three-dimensional model, mimic deposition and growth of Si on a Si(100) substrate. At high angles of incidence, the formation of porous columnar structures seen in the 2-D simulations transform into "flakes"' in the three-dimensional model. While the growth angles of the columns and flakes follow the same general trends as previous ballistic deposition simulations with respect to the formation of porous films, current theories do not quantitatively reflect the simulation results. In the 2D model, the incorporation of an additional step-edge reflection barrier increases porosity in deposited films demonstrating columnar growth. Increasing the substrate temperature increases the widths of the columns and flakes in the direction perpendicular to the path of the beam. Higher substrate temperatures also allow the grown film to remain defect-free for longer times before columnar structure begins.