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KMC simulations in 3+1 dimensions and the effects of attachment probabilities and potential gradients on island morphologies CHRISTOPHER FLECK, JUDITH YANG, University of Pittsburgh, ALAN MCGAUGHEY, Carnegie Mellon University, JUN REN, University of Pittsburgh — Thin film growth and nano-oxidation have received significant attention lately, especially given the interesting nature of Cu_2O growth. Our long-term vision is for a comprehensive, fundamental understanding of a gas-surface reaction via coordinated multi-scale theoretical and in situ experimental efforts. The link between the theoretical and experimental efforts is our kinetic Monte Carlo (kMC) code that simulates general behavior of the irreversible nucleation and growth of epitaxial islands. This simulation was originally a versatile 2+1 dimensional kMC code (Thin Film Oxidation or TFOx) that considered a wide range of elementary steps, including deposition, adsorption, dissociation of gas molecules, surface diffusion, aggregation, desorption, and substrate-mediated indirect interactions between static adatoms. Recently, TFOx has been extended to a 3+1 dimensional kMC code composed of a C++ console program and Python GUI, such that parameterized testing, parallel execution, and 3D growth capabilities are feasible. Emphasis has been placed on the affects of the potential gradient, multilayer nucleation and sticking parameter on the 3D island morphology.

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