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Kinetic Monte Carlo Model Simulations of Nanoscale Oxidation Behavior JUDITH YANG, University of Pittsburgh, XUETIAN HAN, University of Pittsburgh, RICHARD MCAFEE[1], University of Pittsburgh — Nucleation rate theory has been successfully used to describe metal heteroepitaxy and qualitatively explained the initial stage of oxidation behavior. To further quantitative understanding of these nano-scale processes and morphological evolution, the Thin Film Oxidation (TFOx) program based on Kinetic Monte Carlo (KMC) has been developed. The TFOx model can be used to simulate the general behavior of irreversible nucleation and growth of epitaxial islands. It explicitly considers many elementary steps, including deposition, adsorption, dissociation of gas molecules (such as O_2), surface diffusion, aggregation, desorption, and substrate-mediated indirect interactions between static adatoms. The diffusion behavior of the adatoms is determined by the orthogonal and the diagonal jump probabilities, which are considered independently. Potential gradients are used to model intermediate-range interactions, such as strain, between the adatoms. The large number of possible input parameters used in this program provides a rich environment for the simulation of surface dynamics, including the oxidation behavior of thin films. The current TFOx code simulates 2-dimensional transport, nucleation and growth on a square lattice.

[1]present address: Brashear Co., Pittsburgh, PA

Judith Yang
University of Pittsburgh

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