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Atomistic and Continuum Simulations of Island Coalescence EDMUND WEBB III, STEVEN SEEL, Sandia National Laboratories - Albuquerque, NM, JONATHAN ZIMMERMAN, Sandia National Laboratories - Livermore, CA — Volmer-Weber thin film growth involves nucleation of discrete islands that grow, impinge upon one another, and coalesce into a film. Coalescence has been proposed to generate stress in thin films so it is useful to study stress evolution upon coalescence. Results are presented from atomistic simulations of nanometer island coalescence. Molecular dynamics simulations are used to examine coalescence for islands with D = 2 - 200 nm in a parallel hemi-cylindrical capping geometry (D is the cylinder diameter). Atomic interactions are governed by embedded atom method potentials; the zero mismatch case of Au islands on Au(100) is modeled. Coalescence height is calculated and demonstrated to behave in accord with continuum predictions for large D but, for the smallest sizes studied, deviations are observed between atomistic and continuum results due to atomic relaxation resolved in the former but not the latter. To calculate local stress in the atomistic simulations, a spatial homogenization technique is used that permits more robust estimates of stress in small volume elements near surfaces. Stress distributions in pre and post-coalescence structures are presented to further explain observed relaxations.

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