

Abstract Submitted
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Langevin Equation for the Morphological Evolution of Strained Epitaxial Films¹ DIMITRI VVEDENSKY, Imperial College London, CHRISTOPH HASELWANDTER, Imperial College London — A stochastic partial differential equation for the morphological evolution of strained epitaxial films is derived from an atomistic master equation. The transition rules in this master equation are based on previous kinetic Monte Carlo (KMC) simulations of a model that incorporates the effects of strain through local environment-dependent energy barriers to adatom detachment from step edges. The morphological consequences of these rules are seen in the transition from layer-by-layer growth to the appearance of three-dimensional islands with increasing strain. The regularization of the exact Langevin description of these rules yields a continuum equation whose lowest-order terms provide a coarse-grained theory of this model. The coefficients in this equation are expressed in terms of the parameters of the original lattice model, so a direct comparison between the morphologies produced by KMC simulations and this Langevin equation are meaningful. Comparisons with previous approaches are made to provide an atomistic interpretation of a similar equation derived by Golovin *et al.* based on classical elasticity.

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