Abstract Submitted
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Kinectic Monte Carlo Simulation of Strained Heteroepitaxial Growth[1] PETER SMEREKA, University of Michigan, TIM SCHULZE, University of Tennessee — An efficient algorithm for the simulation of strained heteroepitaxial growth with intermixing in 2+1 dimensions is presented. The talk will first describe a KMC solid-on-solid model that has been modified to incorporate elastic interaction. The simulation of such models is computationally difficult due to the need to repeatedly update the elastic displacement field. This hurdle can be overcome by using local updates of the displacement field combined with a multigrid approach for global updates (when needed). The validity of this technique can be theoretically justified. This algorithm is efficient enough to allow the simulation of heteropitaxy on macroscopic time scales. Simulations will have 100 million to 10 billion atomistic moves. Results will be presented showing how various parameters (e.g. temperature, misfit, and deposition rate) effect the morphology of growing films. Annealing simulations of a single 3d island reveal something akin to the pyramid to dome transition observed for Ge islands on Si. Simulations of stacked quantum dots will be presented, these simulations show the capping layer can erode the dots and the alignment of the dots is somewhat different than is often proposed in the literature.

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