

1057-74-314

Tim P. Schulze* (schulze@math.utk.edu), Department of Mathematics, University of Tennessee, 104 Aconda Court · 1534 Cumberland Avenue, Knoxville, TN 37996-0614, and **Peter Smereka**. *Efficient Computational Methods for the Simulation of Heteroepitaxial Growth using Kinetic Monte Carlo*.

Heteroepitaxial growth is a process where one atomic species is deposited upon a substrate of another. If the natural atomic spacing of the two species is different, then elastic effects can become important. In particular the film can lower its elastic energy by forming three dimensional islands. Therefore, layer-by-layer growth can be destabilized by elastic effects. It has been suggested that new materials with interesting electronic properties could be developed by exploiting this instability.

One modeling approach is based on a discrete solid-on-solid model. The elastic effects are incorporated using a ball and spring type model and the system is evolved using kinetic Monte Carlo. This talk introduces several new ideas which allow a very efficient implementation of the method. Results for simulations in both two and three dimensions will be presented. (Received January 25, 2010)