

Lattice Gas Automata Simulation of Atomistic Surface Growth

R. A. Budiman¹, A. Gerisch², A. T. Lawniczak³, H. E. Ruda⁴, and H. Fuks⁵

¹Department of Mechanical and Manufacturing Engineering, University of Calgary, Canada

²Department of Mathematics and Computer Science, University of Halle, Germany

³Department of Mathematics and Statistics, University of Guelph, Canada

⁴Department of Materials Science and Engineering, University of Toronto, Canada
Department of Mathematics, Brock University, Canada

Here we describe a method based on lattice gas automata to numerically simulate atomistic surface growth processes during thin film deposition. Using a realistic approximation of surface energetics, we are able to scale our simulation time to real deposition time corresponding to individual atomic diffusion jumps. The method allows us to model adatom-adatom interaction explicitly, an important feature for investigating the effects of surface elastic forces on surface morphology. The real deposition time and the adatom-adatom interaction distinguishes our method from the more standard kinetic Monte-Carlo simulations of atomistic surface growth. Results obtained for Si/Si(001) deposition for both flat and stepped substrates will be presented.