Surface roughening in homoepitaxy on flat and stepped Si(001) substrates: A numerical simulation

A. Saxena.[1,*], R. A. Budiman[2], A. Gerisch[3], A. T. Lawniczak[4], H. E. Ruda[5], and H. Fukś[6]

[1,*,2] *Dept. of Mechanical and Manufacturing Engineering, University of Calgary, Canada,*
[3] *Dept. of Mathematics and Computer Science, University of Halle, Germany,*
[4] *Dept. of Mathematics and Statistics, University of Guelph, Canada,*
[5] *Dept. of Materials Science and Engineering, University of Toronto, Canada,*
[6] *Dept. of Mathematics, Brock University, Canada*

Abstract

We[1] outline a 1+1-dimensional lattice gas cellular automaton (LGCA) approach to simulate atomistic processes in thin film deposition. The main objective of our simulations is to comprehend the atomistic processes leading to the formation of mesoscopic (10-1000 nm) structures. The computer simulation approach is based on a discrete description of atoms so that the unit length scale coincides with the atom diameter. The computational goal of our simulation is to boost the computation speed without compromising with the atomistic details in order to predict the structural evolution of thin films on the order of seconds and even minutes. This is done by putting the unit time scale in the nearest neighbor atomic jump time, which is around several microseconds for typical deposition conditions. Long deposition times, up to several minutes, can be simulated with this method.

Our approach is based on the lattice gas cellular automata (LGCA) models of chemical reactions and waves, where individual particles interact with surroundings through assumed local driving forces. We present local rules, that define the LGCA approach, for the homoepitaxial deposition, which are derived from the propensity of an atom to establish as many chemical bonds as possible to the underlying substrate atoms when it executes surface diffusion. Our simulation differs from the kinetic Monte Carlo in that : (i) the unit time step in our simulation is explicitly determined by the nearest neighbor atomic jump, thus without assuming that atomistic processes have probabilities following the Poisson process ; (ii) more than one adatom is allowed to diffuse on the surface at any given time, and (iii) surface atoms, be they adatoms or already incorporated into the film, always have finite probabilities to jump from their current sites.

We use a one-dimensional lattice of length L with periodic boundary conditions. The lattice sites are denoted by $r = 0, 1, 2, ..., L-1$; and, in arithmetic expressions always understood to be modulo L. We consider discrete time points $k = 0, 1, 2, ...$The LGCA's state at an individual site r at time k is described by an integer-valued variable $h(r, k)$,which repre-

[1,*]A. Saxena, Address: Department of Mechanical and Manufacturing Engineering, 2500 University Drive NW, University of Calgary, Calgary, Alberta T2N 1N4 CANADA
Phone +1-403-220-7185, Fax +1-403-282-8406, E-mail asaxena@ucalgary.ca

sents the site's film height (thickness). We initialize the LGCA with the values $h(r,0)$ for all r at time $k = 0$. The state $h(r,k) \geq 0$ at time k represents the height, *i.e.*number of one atomic-height layers, of the grown structure on the lattice at site r and time k.

All deposited atoms at site r below the adatom are called *bulk* atoms. Once an adatom becomes a bulk atom by virtue of the presence of a freshly landing atom above the adatom, then this bulk atom is not allowed to move anymore. We thus assume that all adatoms, and only these, are mobile and can move to neighboring lattice sites. The rules that describe their motion are outlined below.

The time evolution of the LGCA from time k to time $k+1$, *i.e.* one simulation step proceeds in three sub-steps: (*i*) Particle Landing, (*ii*) Adatom velocity Computation, and (*iii*) Adatom motion. Each sub-step is performed at each lattice site r independently from the other lattice sites and the next sub-step is started only after the previous sub-step has been completed on all sites of the lattice.

We assume that each simulation step from simulation time k to simulation time $k+1$ corresponds to an *effective time step* denoted by $\triangle t_{eff}$(in seconds [s]) leading to $t = k\triangle t_{eff}$. The effective time step $\triangle t_{eff}$ corresponds to the average time taken by adatoms to jump to the nearest atomic site(includng the waiting time before the actual hop). To achieve computational efficiency, we fix $\triangle t_{eff}$ to a constant value.

The expected value (in space) of the random variable $h(r,k)$ at time k is approximated by:

$$\overline{h}(k) := \frac{1}{L}\sum_{r=0}^{L-1} h(r,k) \qquad (1)$$

The surface roughening evolution is analysed by evaluating the interface width:

$$w(L,k) = \sqrt{\frac{1}{L}\sum_{r=0}^{L-1}[h(r,k)^2 - \overline{h}(k)^2]} \qquad (2)$$

$w(L,k)$ measures the roughness of the evolving thin film surface.

We also compute the "step-density" as defined by

$$\rho_{step}(k) = \frac{1}{2L}\sum_{r=0r'\in\{r-1,r+1\}}^{L-1} [1 - \delta_{h(r,k),h(r',k)}] \qquad (3)$$

where $\delta_{j,k}$ is the Kronecker δ-function, which is equal to unity if $j = k$ and is equal to zero otherwise. The step-density ρ_{step} above measures the number of surface height discontinuities, *i.e.*, steps. The step-density of a flat surface is zero, whereas the step-density of a surface that has no two neighbouring sites of the same height is equal to unity. The quantities herein the analysis are plotted as a function of real time t, instead of as a function of simulation time k.

In this paper we focus on the deposition of Si atoms on initially flat Si(001) and initially structured Si(001) substrate. Since both the thin film being deposited and the substrate are of identical chemical nature, there is no lattice constant mismatch between them. The number of parameters required to run the simulations is minimal; thus this method can prove quite useful in predicting the structural evolution of various semiconductor thin film systems.

KEYWORDS : *Computational material science, surface growth, thin film deposition, Coarse-grained description of surface forces, lattice gas cellular automata*