Master en Sciences Physiques

**Nanophysique PHYS-F-475**

## CHAPITRE 4. Crystal Growth

### Exercices

1. **kMC algorithm** Write out the kMC algorithm for crystal growth in detail: what must be calculated, how are the parameters chosen? (Use pseudocode if you know how.)

2. **kMC dynamics** Based on the dynamics of the kinetic Monte Carlo algorithm, develop an equation for the number of adatoms on the surface of a crystal. Assume that there are no steps (the surface is flat) and that interaction between the adatoms can be neglected. What is the general solution? What is the equilibrium number of adatoms as a function of supersaturation?

3. **Line tension** Using simple arguments based on bond counting, what is the line tension of an island of impurities surrounded by crystal molecules if the bond strength between an impurity atom and crystal atoms is $\epsilon_I$?

4. **Thermodynamics.**

   - A crystal surface is comprised of N sites. What is the difference in (free) energy between a crystal with $n$ layers in a solution with chemical potential $\mu$ and a crystal with $n+1$ layers. (i.e. what is the energy of N atoms in solution? What is their energy if they form a new layer of crystal?) Assume the crystal bond energy is $\epsilon < 0$.
   - Repeat the calculation but assume that there is an impurity on surface which is square with sides of $L$ lattice sites in length and crystal-impurity bond energy of $\epsilon_I$.
   - Generalize to the case of $N_I$ such impurities.
   - Generalize to rectangular impurities with sides of length $L_x, L_y$.
   - Generalize to impurities that each occupy $M$ sites and have perimeter $S$.

5. **Diffsion and the crystal growth rate.** Consider the model for crystal growth that couples the SOS model for the surface with the diffusional model for transport in the fluid above the surface. In the following, assume that all quantities depend only on the coordinate in the direction perpindicular to the crystal surface (the z-direction). Let the height of the crystal surface at time $t$ be $z = H_t$ and the concentration in the fluid at position $z$ at time $t$ be $c_t(z)$. The total height of the computational cell is $L_z$ and the dimensions in the other directions are $L_x$ and $L_y$. Assume that the concentration in the fluid obeys the diffusion equation.

   - If the rate at which a given molecule in the fluid executes a jump in some direction is $\nu_{\text{jump}}$ and the rate at which a molecule enters a given cell at the top of the fluid is $\nu_{\text{add}}$ then what is the equilibrium concentration in the fluid (i.e. one in which the concentration is independent of position)?
   - In the non-equilibrium case (i.e. in which concentration depends on position), what is the equation for the rate of change of the concentration in the top layer of the fluid? (Assume the concentration in each "layer" of the fluid is constant. Consider the rate at which molecules enter and leave the top of the layer and that at which they enter and leave the bottom of the layer.) Show that this reproduces your previous result when the concentration is uniform.
   - What is the relation between $dH_t/dt$ and the step velocity at time $t$?
   - What is the net flux of molecules at the crystal surface according to the diffusion equation?
   - Relate the next flux of the previous question to the step velocity (the flux of molecules arriving at the surface must equal the rate of consumption of material by step growth).
   - Put all of this together into a closed set of equations for the concentration. Assume the relation between step velocity and concentration at the crystal surface, $v(c_t(z))$ is known.
   - There is a natural small (dimensionless) parameter in the problem: can you identify it?
   - Use this to develop an approximate solution to the problem. (Hint: consider

eliminating time derivatives, $d/dt$ in favor of $d/dH_t$).