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 ϵ_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 μ 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 ϵ_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.