Exercise-set (4):

Note: Only exercises marked in red are supposed to be handed in.

1. Assuming that the pre-exponential factor for surface diffusion is given by $\frac{k_B T}{h}$,

(a) How low must the diffusion activation energy be to give a diffusion length, λ, of roughly 100 nm between successive collisions with impinging vapor, for deposition of Si with the deposition flux of 1.4×10^{19} at/m^{2}s and T_s= 400 °C on Si(001)? Remember that at low temperature regime, desorption is negligible.

(b) How much of a decrease in T_s would correspond to a ×10 decrease in λ?

2. Exercise 5.4 from the course book.

3. Exercise 5.3 from the course book.

Ans: (a) E_d = 0.83 eV, E_a = 2.0 eV, (b) 1041 K and 759 K.

Note: At high temperature regime, the diffusion length is limited by the adsorption lifetime, thus the exponential behavior is affected by both the diffusion barrier and the adsorption energy. At low temperature regime, the exponential behavior is solely affected by the diffusion barrier.

4. (a) How many unsaturated bonds would be created on (100), (101) and (111) faces of an fcc lattice if the crystal is cleaved parallel to either of these faces?

(b) Calculate the surface atom density ($\rho = \frac{\text{number of atoms}}{\text{area of unit-cell}}$) for (100), (101) and (111) faces.

(c) The surface energy of each plane per unit area is defined as:

$$\gamma = \frac{\varepsilon}{2} \times \text{number of broken bonds/atom} \times \rho$$

where ε is the energy per bond, and ρ is the surface atom density. Factor 2 comes from the fact that on cleavage of a solid, two surfaces are generated, so half of the total bond energy is assured to each surface.

Calculate the surface energy of (100), (101) and (111) faces for Au. The lattice constant of gold is 4.08 Å and the Au-Au bond energy is 225 kJ/mole.

5. Describe in words and schematically, the 'reconstruction' and 'relaxation' of tetrahedrally coordinated bonds of a crystal surface.