Exercise 11 (online: Mo 10.07.2023. Return by: **Mo 17.07.2023 10:00**) **12P**

1. **Statistical growth** 3P

   Consider a statistical growth of a film, for which the coverage $\Theta_n(t)$ of the nth layer is given by

   $$\Theta_n(t) = 1 - \exp(-t/\tau) \sum_{k=0}^{n-1} \frac{1}{k!} \left(\frac{t}{\tau}\right)^k. \tag{1}$$

   (a) Show that equation (1) can be written as (1P)

   $$\Theta_n(t) = \exp(-t/\tau) \sum_{k=n}^{\infty} \frac{1}{k!} \left(\frac{t}{\tau}\right)^k. \tag{2}$$

   (b) Starting from equation 2, show that the total coverage $\Theta(t)$ equals to (2P)

   $$\Theta(t) = \sum_{n=1}^{\infty} \Theta_n(t) = \frac{t}{\tau}. \tag{3}$$

   Hint: write out $\Theta(t)$ and rearrange the order of the sums with the proper limits.

2. **Step flow** 9P

   Consider deposition of a material with flux F on a flat surface with straight steps separated by a distance L. The concentration $n(x,t)$ of adatoms at the surface satisfies the following differential equation (modification of the second Fick's law):

   $$\frac{\partial n(x,t)}{\partial t} = F - \frac{n(x,t)}{\tau_s} + D_s \cdot \frac{\partial^2 n(x,t)}{\partial x^2}, \tag{4}$$

   where the flux F describes deposition, $\frac{n(x,t)}{\tau_s}$ - desorption of adatoms (with a characteristic time scale τ_s), and $D_s \cdot \frac{\partial^2 n(x,t)}{\partial x^2}$ - surface diffusion of adatoms (with a surface diffusion coefficient D_s). Let us make the assumption that the movement of the step can be neglected in the diffusion problem, so that the adatoms have a steady distribution on either side of the step which is practically the same as though the step were adsorbing adatoms without movement. In this case, $\frac{\partial n(x,t)}{\partial t} = 0$, meaning that the equilibrium concentration of adatoms $n(x)$ does not depend on time and satisfies the equation

   $$D_s \cdot \frac{d^2 n(x)}{dx^2} - \frac{n(x)}{\tau_s} = -F. \tag{5}$$

   (a) Check that $n(x) = F\tau_s$ is a partial solution for $n(x)$ of the inhomogeneous equation 5. (1P)

   (b) Check that $n(x) = A \cdot \sinh(x \,/\, x_s) + B \cdot \cosh(x \,/\, x_s)$ is a general solution of the homogeneous differential equation $D_s \cdot \frac{d^2 n(x)}{dx^2} - \frac{n(x)}{\tau_s} = 0$. Here A and B are constants, and the characteristic surface diffusion length x_s depends on the coefficients D_s and τ_s. Give an explicit expression for x_s. (1P)

   (c) The general solution for the inhomogeneous differential equation 5 can be given as a sum of the solutions from two previous steps, i.e. $n(x) = F\tau_s + A \cdot \sinh(x \,/\, x_s) + B \cdot \cosh(x \,/\, x_s)$. The constants A and B are to be determined from the boundary conditions. Assuming that Ehrlich-Schwöbel barrier is low, the concentration of the adatoms on both sides of the steps in equilibrium is n_{eq}. This allows us to sketch the concentration of the adatoms on the surface $n(x)$ between two steps on the surface as it is shown in Fig. 1.

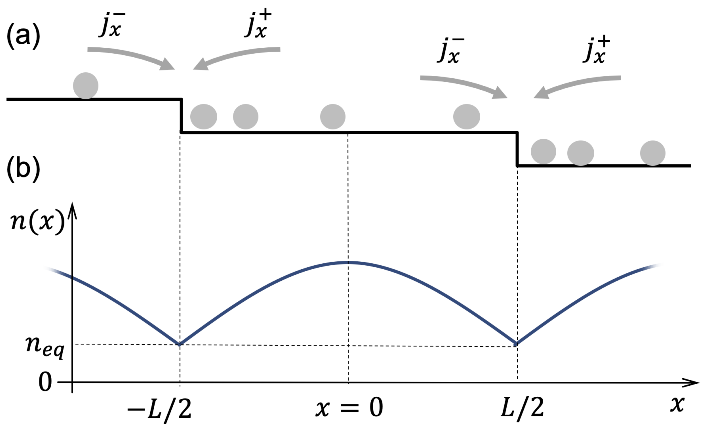

Figure 1: (a) Surface with steps and adatoms (b) Concentration profile $n(x)$ of adatoms between two steps. The arrows above the sketch represent flux of the adatoms j_x from both sides towards a step.

Determine the constants A and B from the boundary conditions $n(x = \pm\frac{L}{2}) = n_{eq}$. Find the analytical expression for $n(x)$ for $-L/2 \leq x \leq L/2$. (2P)

(d) The first Fick's law,

$$j_x = -D_s \cdot \frac{dn(x)}{dx}, \tag{6}$$

can be used to calculate the projection of the flux of the adatoms onto the x-axis. Using the result for $n(x)$ from the previous step, calculate the flux j_x^+ and j_x^- of the adatoms towards the step from both sides. (2P)

(e) Assuming that adatoms that are flowing towards the step will all stick to it, calculate the speed of the step propagation as $v_{step} = (j_x^+ + j_x^-)/n_0$. Here j_x^+ and j_x^- are fluxes of adatoms calculated in the previous step, and n_0 is the 2D density of the material in crystalline form. For a square lattice with the lattice parameter a, we can assume $n_0 = 1/a^2$. (1P)

(f) How the speed of the step propagation depends on the terrace length L? Plot the dependence of the step propagation speed as a function of L (1P) .

(g) If all the terraces have the same length L, all steps will propagate with the same speed, calculated in section 2f. How the step propagation will change, if one of the terraces have a smaller length $L' < L$ (Fig. 2)? Is the system of equidistant steps stable? (1P) .

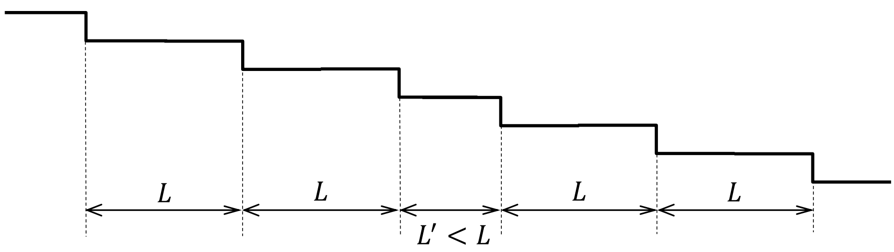

Figure 2: Stability of the step flow.