Exercise 12 (online: Mo 17.07.2023. Return by: **Mo 24.07.2023 10:00**) **14P**

1. **Layer-by-layer growth** 5P

   Assume a layer-by-layer growth of organic molecules during a thin film deposition. One molecular layer has a thickness d. Assume the constant flux of organic molecules on the substrate, so that the total amount of the deposited material $\Theta = t/\tau$ linearly increases with the time t.

   (a) How does the coverage Θ_n of n-th layer change with the total deposition Θ? Plot $\Theta_n(\Theta)$ for $n = 1, 2, 3, 4, ...$ and write the formula, which describes this behavior mathematically. (2P)

   (b) Plot the exposed layer coverage $\phi_n = \Theta_n - \Theta_{n+1}$ as a function of total deposition Θ for $n = 1, 2, 3, 4, ...$ and write the corresponding mathematical expression for ϕ_n. (1P)

   (c) Calculate the roughness $\sigma = d \cdot \sqrt{\langle n^2 \rangle - \langle n \rangle^2}$ as a function of total deposition Θ and plot it. What is the maximum roughness and when is it achieved? *Hint: it is enough to consider the growth from n fully covered layers till $n+1$ fully covered layer.* (2P)

2. **X-ray scattering during the layer-by-layer film growth** 9P

   Assume again a layer-by-layer growth of organic molecules during a thin film deposition. Consider now an X-ray scattering experiment from such a film, assuming that the incidence and exit angles are equal to θ, as shown in Fig. 1 (do not confuse the total coverage Θ, the coverage of the n-th layer Θ_n and the scattering angle θ). The scattering from the substrate can be neglected and the scattering intensity of one monolayer is normalized to 1 (in an actual experiment, one should take the scattering from the substrate into account).

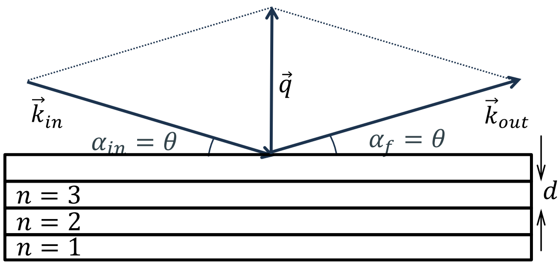

Figure 1: X-ray scattering from a multilayer film.

   (a) For the thickness of a single molecular layer $d = 1.5$ nm, calculate the value of the scattering vector q_B, at which the first Bragg peak appears. Calculate the corresponding scattering angle θ if one uses X-rays with photon energy $\hbar\omega = 8.04$ keV. (2P)

   (b) Calculate the scattered intensity $I_B(\Theta)$ at Bragg condition (at the scattering vector q_B) and plot it as a function of total deposition Θ. (1P)

   (c) Calculate the scattered intensity $I_{AB}(\Theta)$ at anti-Bragg condition (at the scattering vector $\frac{1}{2}q_B$) and plot it as a function of total deposition Θ. (2P)

   (d) Calculate the scattered intensity $I(\Theta)$ at the scattering vector $\frac{1}{3}q_B$ and plot it as a function of total deposition Θ. *Hint: note that the X-rays scattered from three successive completely filled layer interfere with each other in such a way that they cancel out (because the scattering phase is given by $e^{-i\boldsymbol{qr}}$ and $e^{-i(2\pi/3)} + e^{-2i(2\pi/3)} + e^{-3i(2\pi/3)} = 0$). This means that one needs to consider only the growth of the three layers. For the sake of simplicity, one can take layers with $n = 1, 2, 3$, because for the higher layers the scattered intensity will change with Θ in exactly the same way as for the first three layers.* (4P)