Solution

A1. A given system of equations for scalar complex amplitudes must be performed at any point of the interface between media:

$$\forall y \quad E_y(x=-0) = E_y(x=+0); \begin{cases} E_y(x=-0) = f \cdot e^{-ik_{1y}y}, \ f \neq f(y), \\ E_y(x=+0) = g \cdot e^{-ik_{2y}y}, \ g \neq g(y). \end{cases}$$

This necessarily follows $k_{1y} = k_{2y}$. Similarly, considering the second boundary, we obtain $k_{2y} = k_{3y}$.

A2. Using the expression for k and the equality $k_y = k_{1y} = k_{2y} = k_{3y}$:

$$k = \sqrt{k_{1x}^2 + k_y^2} \Rightarrow k_{1x} = \sqrt{\frac{\varepsilon_1 \omega^2}{c^2} - k_y^2} = \frac{\sqrt{\varepsilon_1}\omega}{c}\cos\theta_1.$$

Similarly,

$$k_{2x} = \frac{\sqrt{\varepsilon_2}\omega}{c}\cos\theta_2 = \frac{\sqrt{\varepsilon_2}\omega}{c}\sqrt{1 - \frac{\varepsilon_1}{\varepsilon_2}\sin^2\theta_1},$$

$$k_{3x} = \frac{\sqrt{\varepsilon_3}\omega}{c}\cos\theta_3 = \frac{\sqrt{\varepsilon_3}\omega}{c}\sqrt{1 - \frac{\varepsilon_1}{\varepsilon_3}\sin^2\theta_1}.$$

$$\boxed{\begin{cases} k_{1x} = \dfrac{\sqrt{\varepsilon_1}\omega}{c}\cos\theta_1, \\ k_{2x} = \dfrac{\omega}{c}\sqrt{\varepsilon_2 - \varepsilon_1\sin^2\theta_1}, \\ k_{3x} = \dfrac{\omega}{c}\sqrt{\varepsilon_3 - \varepsilon_1\sin^2\theta_1} \end{cases}}$$

A3. Let's write down the boundary conditions for boundary 1-2 on the tangential components E and B, respectively, counting $x = 0$:

$$\mathcal{E} + r\mathcal{E} = a\mathcal{E} + b\mathcal{E},$$

$$k_{1x}\mathcal{E} - k_{1x}\mathcal{E}r = k_{2x}a\mathcal{E} - k_{2x}b\mathcal{E}.$$

And for the boundary 2-3:

$$a\mathcal{E}e^{ik_{2x}d} + b\mathcal{E}e^{-ik_{2x}d} = t\mathcal{E}\ ,$$

$$k_{3x}t\mathcal{E} = k_{2x}\mathcal{E}ae^{ik_{2x}d} - k_{2x}\mathcal{E}be^{-ik_{2x}d}.$$

Thus, we obtained a system of equations:

$$\begin{cases} 1 + r = a + b, \\ k_{1x}(1 - r) = k_{2x}(a - b), \\ ae^{i\phi} + be^{-i\phi} = t, \\ k_{3x}t = k_{2x}(ae^{i\phi} - be^{-i\phi}), \end{cases}$$

where the notation $\phi = k_{2x}d$ is introduced.

$$\boxed{\begin{cases} 1 + r = a + b, \\ k_{1x}(1 - r) = k_{2x}(a - b), \\ ae^{ik_{2x}d} + be^{-ik_{2x}d} = t, \\ k_{3x}t = k_{2x}(ae^{ik_{2x}d} - be^{-ik_{2x}d}). \end{cases}}$$

A4. From the **A3**, we get:

$$\begin{cases} t = (ae^{i\psi} - be^{-i\psi})\dfrac{k_{2x}}{k_{3x}}, \\ a = be^{-2i\psi} \cdot \dfrac{k_{2x}+k_{3x}}{k_{2x}-k_{3x}}, \\ a(k_{1x}+k_{2x}) + b(k_{1x}-k_{2x}) = 2k_{1x}, \\ r = \dfrac{a(k_{1x}-k_{2x}) + b(k_{1x}+k_{2x})}{2k_{1x}}. \end{cases}$$

Deciding, we come to the result:

$$r_s = \frac{(k_{1x}-k_{2x})(k_{2x}+k_{3x}) + (k_{1x}+k_{2x})(k_{2x}-k_{3x})e^{2i\phi}}{(k_{1x}-k_{2x})(k_{2x}-k_{3x})e^{2i\phi} + (k_{1x}+k_{2x})(k_{2x}+k_{3x})}.$$

Introducing the notation

$$\boxed{\begin{cases} A = \dfrac{k_{2x}+k_{3x}}{k_{2x}-k_{3x}}, \\ B = \dfrac{k_{1x}+k_{2x}}{k_{1x}-k_{2x}}. \end{cases}}$$

we get the expression reduced to the required form.

A5. Similarly, **A3** records the conditions at the two interfaces, taking into account the connection of electric and magnetic fields in the EM wave: $\sqrt{\varepsilon\varepsilon_0\mu_0}\mathcal{E} = \mathcal{B}$:

$$\begin{cases} 1 + r = a + b, \\ \dfrac{k_{1x}}{\varepsilon_1}(1-r) = \dfrac{k_{2x}}{\varepsilon_2}(a-b), \\ ae^{ik_{2x}d} + be^{-ik_{2x}d} = t, \\ \dfrac{k_{3x}}{\varepsilon_3}t = \dfrac{k_{2x}}{\varepsilon_2}(ae^{ik_{2x}d} - be^{-ik_{2x}d}). \end{cases}$$

Or, taking into account the reinterpretations proposed in the condition:

$$\boxed{\begin{cases} 1 + r = a + b, \\ \kappa_{1x}(1-r) = \kappa_{2x}(a-b), \\ ae^{i\phi} + be^{-i\phi} = t, \\ \kappa_{3x}t = \kappa_{2x}(ae^{i\phi} - be^{-i\phi}) \end{cases}}$$

A6. Note that the system in **A5** coincides with the system from **A3** up to the replacement of $\kappa_{ix} \leftrightarrow k_{ix}$. Accordingly, we immediately write down the answer:

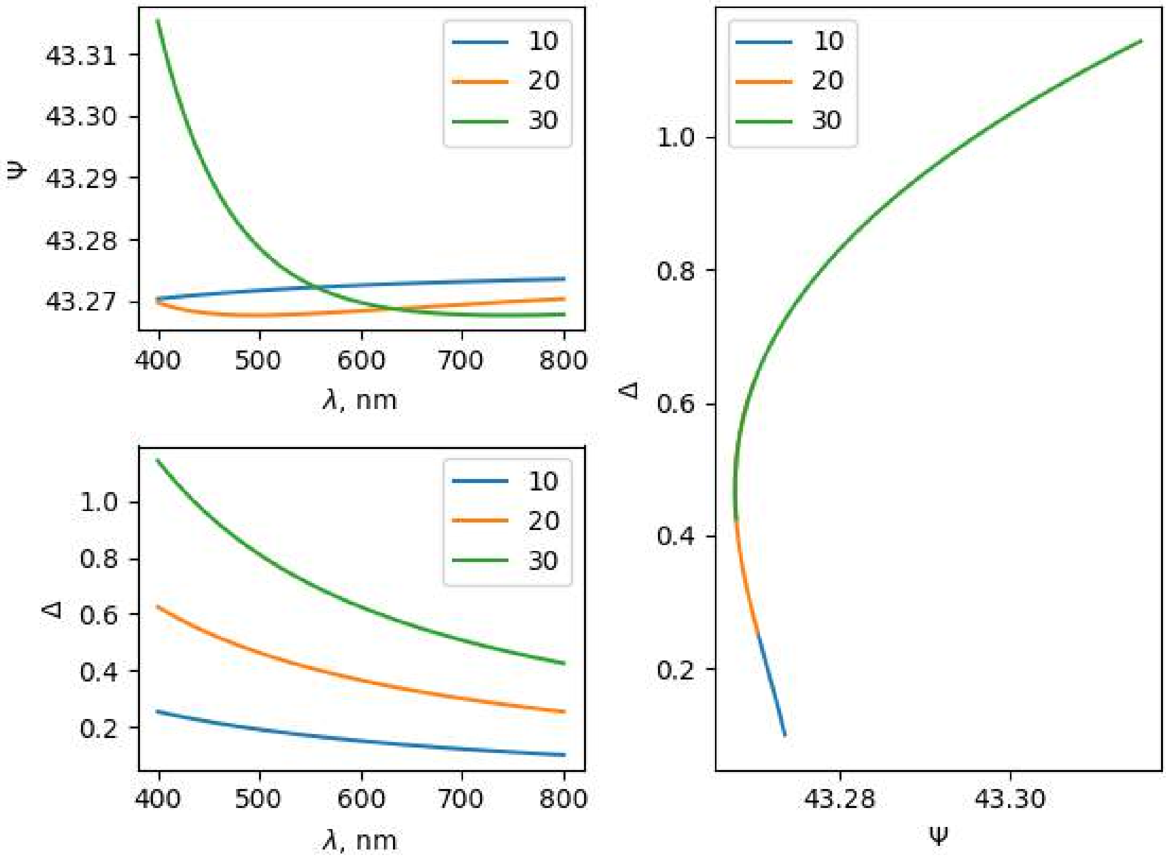
$$r_p = \frac{A + Be^{2i\phi}}{AB + e^{2\phi}},$$

$$\boxed{\begin{cases} A = \dfrac{\kappa_{2x}+\kappa_{3x}}{\kappa_{2x}-\kappa_{3x}}, \\ B = \dfrac{\kappa_{1x}+\kappa_{2x}}{\kappa_{1x}-\kappa_{2x}}. \end{cases}}$$

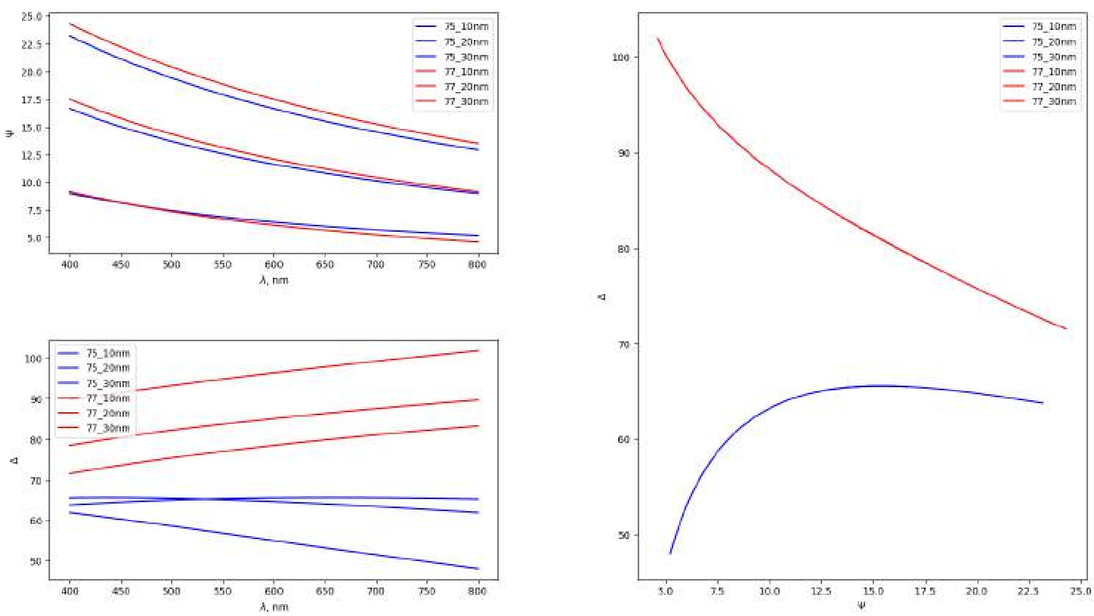
A7. We will receive graphs for three thicknesses: 10, 20 and 30 nm. At low angles of incidence, it can be seen that the maximum range of Ψ is hundredths degrees, while $\theta \sim 70°$, the maximum range of Φ is tens of degrees . The maximum sufficiency is reached when

$$\theta_{\text{opt}} = 77°.$$

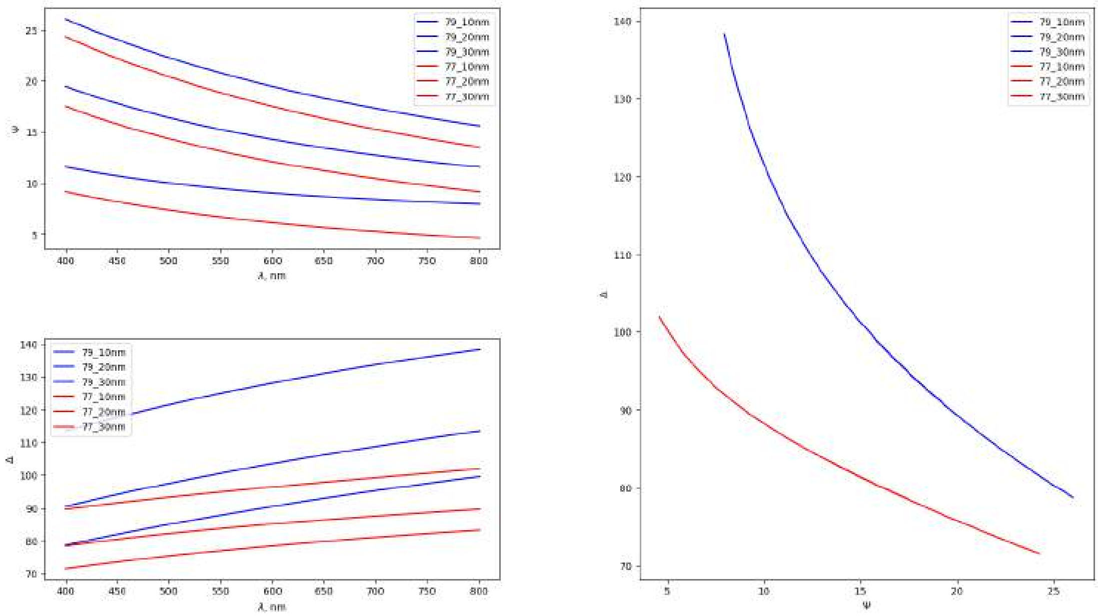
The corresponding graphs for comparison are given below.



Dependencies for the angle of incidence of 20° and film thicknesses of 10 nm, 20 nm and 30 nm.



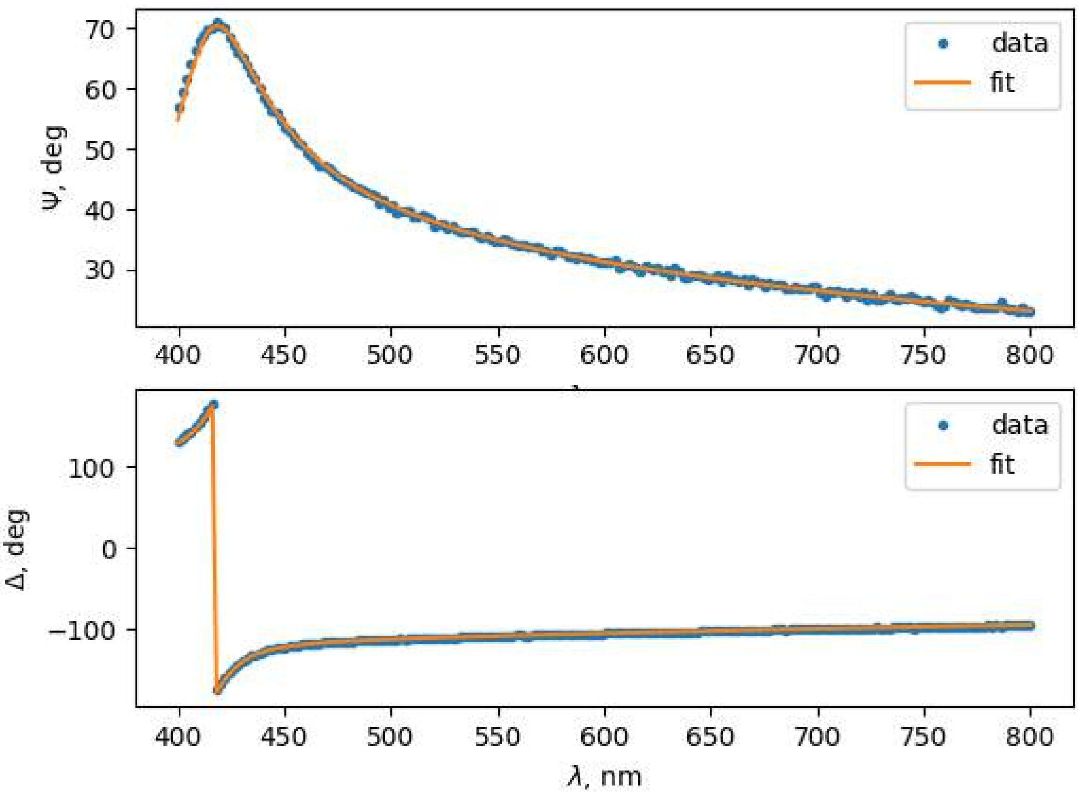
A comparison of the dependencies for the angles of incidence of 75° and 77° and the film thickness of 10 nm, 20 nm and 30 nm.



A comparison of the dependencies for the angles of incidence of 77° and 79° and the film thickness of 10 nm, 20 nm and 30 nm.

$$\boxed{\theta_{\text{opt}} = 77^\circ}$$

B1.



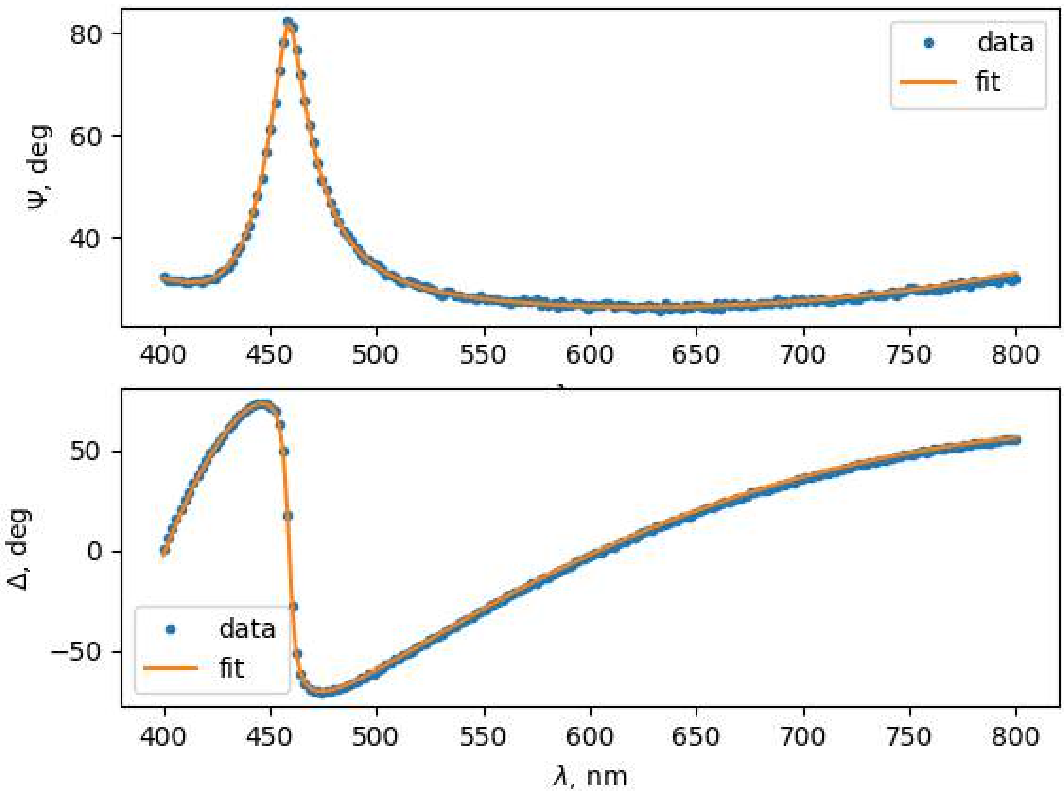
The graph for $\Phi = 71^\circ, d = 67$ nm.

Let us describe the search algorithm for optimal Φ and d. First enter arbitrary Φ and d in B1.py. Next, on each step we try to change Φ or d a bit, and look at the "error" given out by the program B1.py. If the error decreases, we continue to change Φ or d in the same direction (e.g. if we have lowered Φ by 1°, and the error have decreased, then on the next step we also lower Φ by 1°). Finally, we will reach such Φ and d that any small changes of them lead to the increasing of the error, i.e. we reach the minimal possible error. It means that we have found optimal Φ and d.

One can see on the graph how fitting data correspond to the colleague's ones, but the numerical parameter of the approximation quality is the error giving by the program B1.py.

$$\boxed{\Phi = 71.1^\circ \quad d = 66.7\text{ nm}}$$

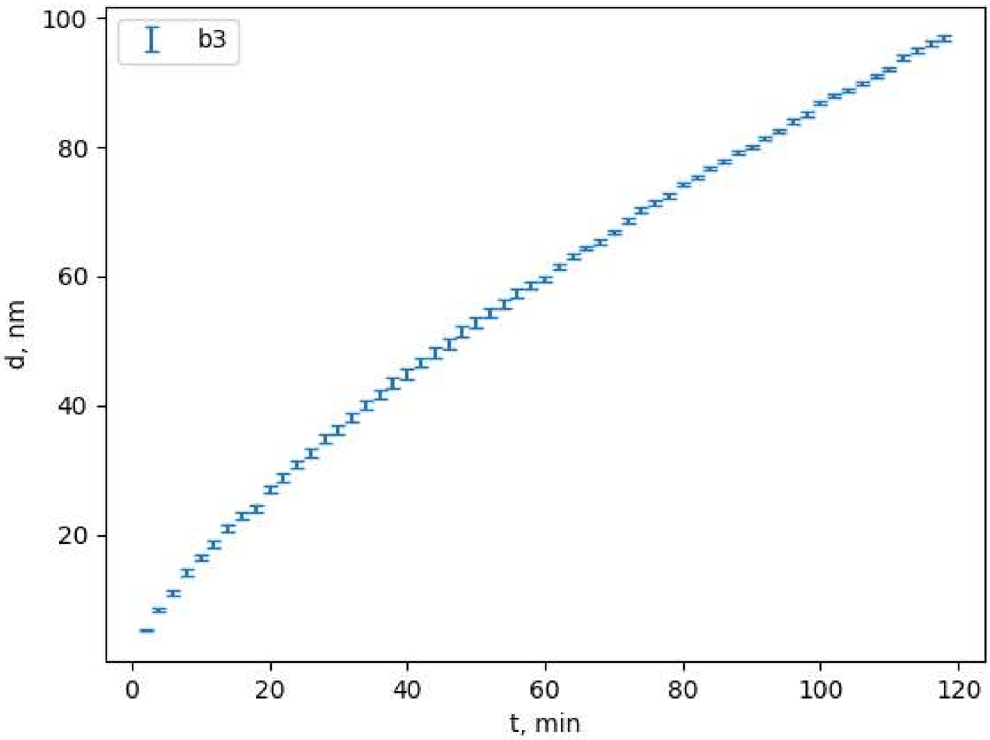
B2. The search algorithm for optimal Φ and d coincides with the such one in part **B1**.



The graph for $\Phi = 57°, d = 232$ nm.

$$\boxed{\Phi = 57^\circ \quad d = 232\text{ nm}}$$

B3. Set name = b3, Phi = 77, T = 1000, $t_{\max}$ = 120 in B_in.txt, then run gen_data.exe and B.py consistently. In "res" folder we get the file with desired graph. Note that we substitute $\Phi = \theta_{\text{opt}}$ from **A7** in order to increase the quality of the experiment.



B4. Consider a small time period Δt and a part of SiO_2-Si border having the area S. Then the mass of the Si oxided during Δt equals $\Delta m = F_3\,\Delta t\,S\,\mu_{SiO_2}$. On the other hand, the SiO_2-Si border will move by $v\,\Delta t$, so the mass of SiO_2 appeared equals $\Delta m = \rho_{SiO_2}\,S\,v\,\Delta t$. Thus $\rho_{SiO_2}\,v\,S\,\Delta t = F_3\,\Delta t\,S\,\mu_{SiO_2}$, so $\rho_{SiO_2}\,v = F_3\,\mu_{SiO_2}$.

$$\boxed{v = F_3\frac{\mu_{SiO_2}}{\rho_{SiO_2}}}$$

B5. Stationarity conditions gives $F_1 = F_2 = F_3$, i.e. $h(C^* - C_0) = \frac{D}{d}(C_0 - C_i) = kC_i$. From the second equality we get $C_0 = (1 + \frac{kd}{D})C_i$. Substitute it in $h(C^* - C_0) = kC_i$ and get $h(C^* - (1 + \frac{kd}{D})C_i) = kC_i$, what implies $C^* = (\frac{k}{h} + \frac{kd}{D} + 1)C_i$, so

$$C_i = \frac{C^*}{1 + \frac{k}{h} + \frac{kd}{D}}, \quad C_0 = \left(1 + \frac{kd}{D}\right)C_i = C^*\frac{1 + \frac{kd}{D}}{1 + \frac{k}{h} + \frac{kd}{D}}$$

$$\boxed{C_0 = C^*\frac{1 + \dfrac{kd}{D}}{1 + \dfrac{k}{h} + \dfrac{kd}{D}}, \qquad C_i = C^*\frac{1}{1 + \dfrac{k}{h} + \dfrac{kd}{D}}}$$

B6. From **B4** we have $v = \dot{d} = \frac{F_3\mu_{SiO_2}}{\rho_{SiO_2}} = \frac{kC_i\mu_{SiO_2}}{\rho_{SiO_2}}$. Taking into account the expression for C_i obtained in **B5** we get

$$\dot{d} = C^*\frac{\mu_{SiO_2}}{\rho_{SiO_2}}\frac{1}{\frac{1}{k} + \frac{1}{h} + \frac{d}{D}}$$

or, equivalently,

$$\frac{\dot{d}\cdot d}{D} + \dot{d}\cdot\left(\frac{1}{k} + \frac{1}{h}\right) - C^*\frac{\mu_{SiO_2}}{\rho_{SiO_2}} = 0$$

Note that the left hand side equals

$$\frac{d}{dt}\left(\frac{d^2}{2D}+d\cdot\left(\frac{1}{k}+\frac{1}{h}\right)-t\cdot C^*\frac{\mu_{\mathrm{SiO_2}}}{\rho_{\mathrm{SiO_2}}}\right)=0$$

So

$$\frac{d^2}{2D}+d\cdot\left(\frac{1}{k}+\frac{1}{h}\right)-t\cdot C^*\frac{\mu_{\mathrm{SiO_2}}}{\rho_{\mathrm{SiO_2}}}=\mathrm{const}$$

where const can be found from the initial consition $d(t_0)=d_0$. Namely,

$$\mathrm{const}=\frac{d_0^2}{2D}+d_0\cdot\left(\frac{1}{k}+\frac{1}{h}\right)-t_0\cdot C^*\frac{\mu_{\mathrm{SiO_2}}}{\rho_{\mathrm{SiO_2}}}$$

So we get

$$d^2+2D\cdot\left(\frac{1}{k}+\frac{1}{h}\right)\cdot d=2DC^*\frac{\mu_{\mathrm{SiO_2}}}{\rho_{\mathrm{SiO_2}}}(t+\tau)$$

where $\tau=\frac{\mathrm{const}\cdot\rho_{\mathrm{SiO_2}}}{2DC^*\mu_{\mathrm{SiO_2}}}$.

$$\boxed{A=2D\left(\frac{1}{k}+\frac{1}{h}\right),\quad B=2DC^*\frac{\mu_{\mathrm{SiO_2}}}{\rho_{\mathrm{SiO_2}}}}$$

B7. First create data necessary for B7.py. Set T, $\Phi=\theta_{\mathrm{opt}}=77°$, $t_{\mathrm{max}}=120$ in B_in.txt, then run gen_data.exe and B.py, and finally, run B7.py five times, on each time entering name, T and Φ from B_in.txt. We write every output of B7.py in the file B8_in.txt and get the table below.

Note that even for $T=850°C$ we get an error "Final layer is too thin to approximate", and for $T=900°C$ we get too high error rate, so it is reasonable to start with $T=950°C$ with a step $50°C$.

T, $°C$	B, nm^2/min	ΔB, nm^2/min	B/A, nm/min	$\Delta(B/A)$, nm/min
950	85	6	0.780	0.044
1000	160	6	1.017	0.027
1050	251	4	2.310	0.044
1100	389	2	4.636	0.070
1150	551	4	7.751	0.188

B8.

First plot the graphs $\ln B\left(\frac{1}{T}\right)$ and $\ln\frac{B}{A}\left(\frac{1}{T}\right)$ using the program B8.py. In the console one can see the slopes of proposed linear approximations. Namely, the slope coefficient of $\ln B\left(\frac{1}{T}\right)$ equals $-(14671\pm 625)\,°C$, and the slope coefficient of $\ln\frac{B}{A}\left(\frac{1}{T}\right)$ equals $-(23418\pm 1730)\,°C$ (where K means one kelvin).

We get from **B6** that

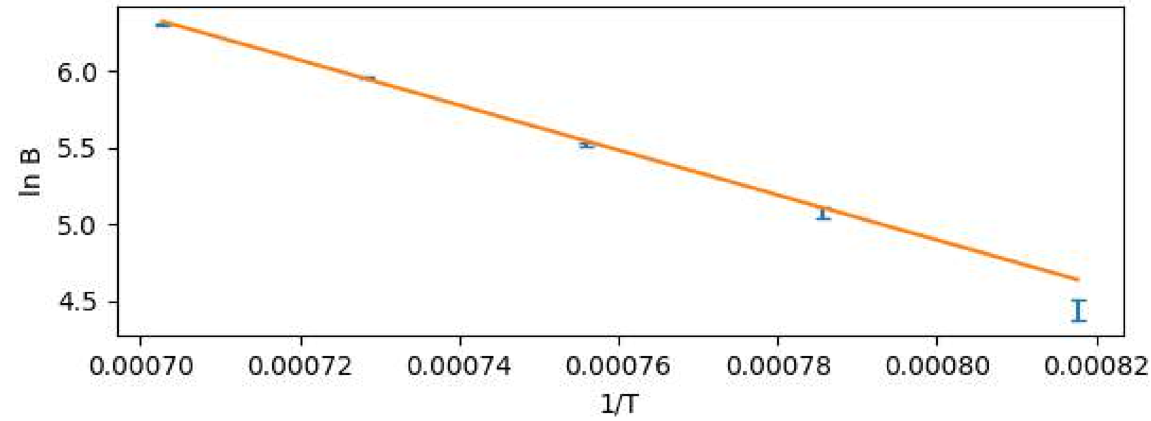
$$B=2DC^*\frac{\mu_{\mathrm{SiO_2}}}{\rho_{\mathrm{SiO_2}}}\propto e^{-\frac{\Delta E_a}{k_BT}}$$

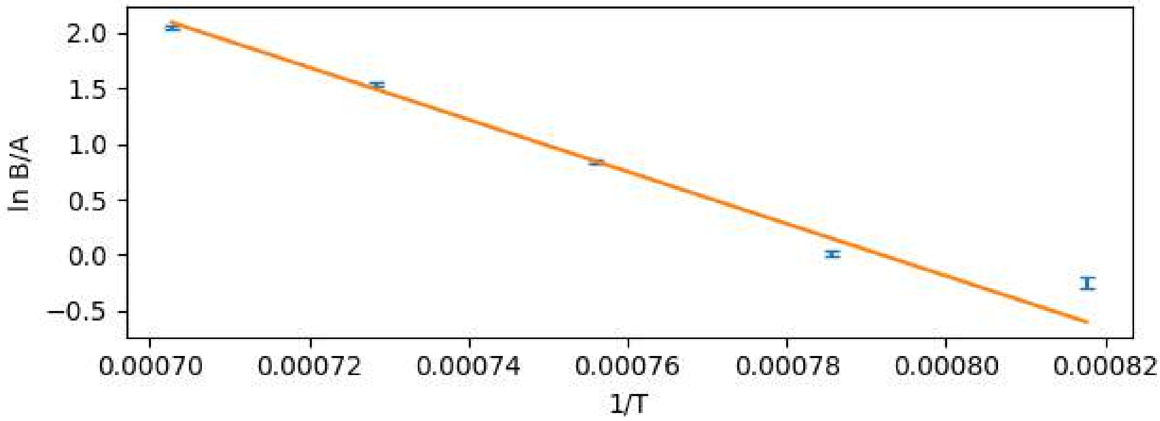
Thus the slope coefficient of the graph $\ln B\left(\frac{1}{T}\right)$ equals $-\frac{\Delta E_a}{k_B}$. So $\Delta E_a=(2.208\pm 0.086)\cdot 10^{-19}$ J, or, equivalently,

$$\Delta E_a=\frac{(2.208\pm 0.086)\cdot 10^{-19}}{1.60\cdot 10^{-19}}\,eV=(1.38\pm 0.05)\,eV$$

Next, $h\gg k$ implies $A\approx\frac{2D}{k}$, so

$$\frac{B}{A}\approx kC^*\frac{\mu_{\mathrm{SiO_2}}}{\rho_{\mathrm{SiO_2}}}\propto e^{-\frac{\Delta E_b}{k_BT}}$$





the slope coefficient of the graph $\ln \frac{B}{A}\left(\frac{1}{T}\right)$ equals $-\frac{\Delta E_b}{k_B}$. So $\Delta E_b = (3.23 \pm 0.23) \cdot 10^{-19}$ J, or, equivalently,

$$\Delta E_b = \frac{(3.23 \pm 0.23) \cdot 10^{-19}}{1.60 \cdot 10^{-19}}\, eV = (2.02 \pm 0.14)\, eV$$

$$\boxed{\Delta E_a = (1.38 \pm 0.05)\, eV, \quad \Delta E_b = (2.02 \pm 0.14)\, eV}$$