Drift-diffusion model

20202041 Park, Nuri

Gauss law :
$\nabla \cdot D = \rho = q(p - n + N^+), D = \epsilon E = -\epsilon \nabla \phi$
(it can be casted into poisson eqn in the vacuum.)

Electron/hole continuity :

$$\frac{\partial n}{\partial t} = -\nabla \cdot F_n = \frac{1}{q} \nabla \cdot J_n,$$
$$\frac{\partial p}{\partial t} = -\nabla \cdot F_p = -\frac{1}{q} \nabla \cdot J_p$$

Electron/hole current density :

$$J_n = q\mu_n nE + qD_n \nabla n,$$
$$J_p = q\mu_p pE - qD_p \nabla p$$

These 5 equations can be used to earn unknown 3 values: ϕ, n, p.

Electron current density + Electron continuity:

$$\frac{\partial n}{\partial t} = -\nabla \cdot F_n = \frac{1}{q} \nabla \cdot (q\mu_n nE + qD_n \nabla n)$$

$$(\text{steady state}) \rightarrow \nabla \cdot (+q\mu_n nE + qD_n \nabla n) = 0$$

We need to calculate ϕ as we did before. Now we can use ϕ as fixed values to insert in the above eqn.

1D, steady-state case :

$$\frac{d}{dx}\left(-q\mu_n n \frac{d\phi}{dx} + qD_n \frac{dn}{dx}\right) = 0$$

(Einstein relation: $D_n = \frac{k_B T}{q} \mu_n = V_T \mu_n$)

We need to integrate them to solve. Integrating above eqn from $x_{i-0.5}$ to $x_{i+0.5}$. Remember that $J_{n,i+0.5}$ is defined as :

$$J_{n,i+0.5} = -q\mu_n n_{i+0.5} \frac{d\phi}{dx}_{i+0.5} + qD_n \frac{dn}{dx}_{i+0.5}$$
$$= -q\mu_n \left(n_{i+0.5} \frac{d\phi}{dx}_{i+0.5} - V_T \frac{dn}{dx}_{i+0.5}\right), with\ Einstein\ relation.$$

Now we could have integrated form:

$$J_{n,i+0.5} - J_{n,i-0.5} = 0$$

$$n_{i+0.5} \frac{d\phi}{dx}_{i+0.5} - V_T \frac{dn}{dx}_{i+0.5} - n_{i-0.5} \frac{d\phi}{dx}_{i-0.5} + V_T \frac{dn}{dx}_{i-0.5} = 0$$

We have to discretize to define values on the point $i + 0.5$.

$$n_{i+0.5} = \frac{n_{i+1} + n_i}{2}, \frac{d\phi}{dx}_{i+0.5} = \frac{\phi_{i+1} - \phi_i}{\Delta x}, \frac{dn}{dx}_{i+0.5} = \frac{n_{i+1} - n_i}{\Delta x}$$

HW14

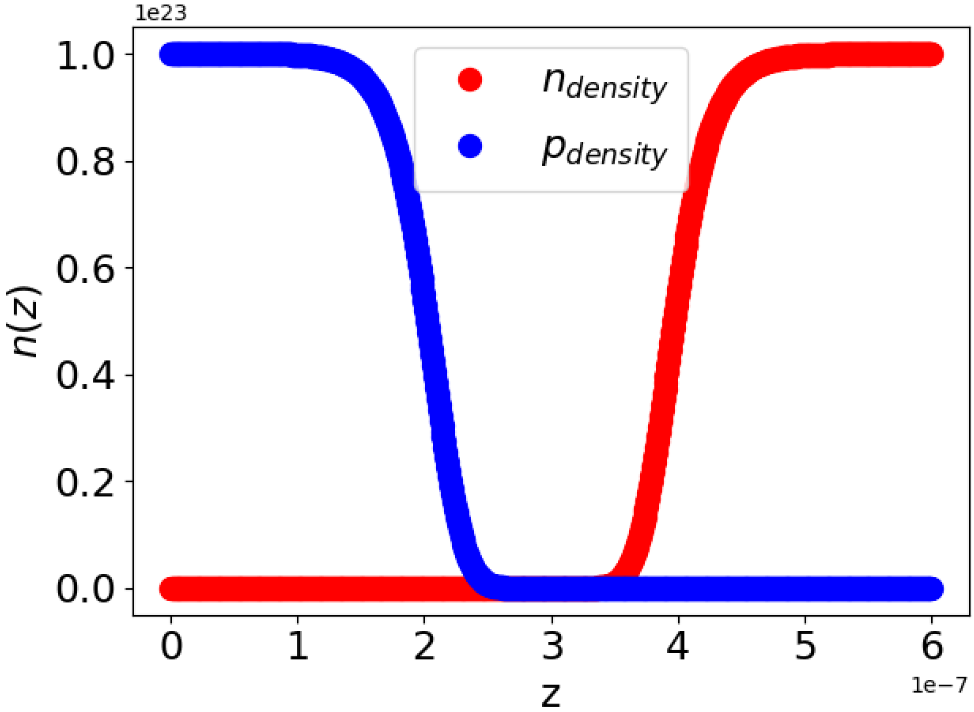
PN junction

$$\frac{\epsilon_{si}(\phi_{i+1}+\phi_{i-1})-2\epsilon\phi_i}{\Delta x^2} = qN_{acc}+2qsinh\left(\frac{\phi}{V_T}\right), \quad \left(x<\frac{N}{2}\right)$$
$$= 2qsinh\left(\frac{\phi}{V_T}\right), \quad \left(x=\frac{N}{2}\right)$$
$$= -qN_{acc}+2qsinh\left(\frac{\phi}{V_T}\right), \quad \left(x>\frac{N}{2}\right)$$

Boundary conditions:

$$\phi_{N-1}=\frac{k_BT}{q}\log\left(\frac{N_{acc}}{n_i}\right), \phi_0=-\frac{k_BT}{q}\log\left(\frac{N_{acc}}{n_i}\right), n_{N-1}=N^+, n_0=\frac{n_i^2}{N^+}$$

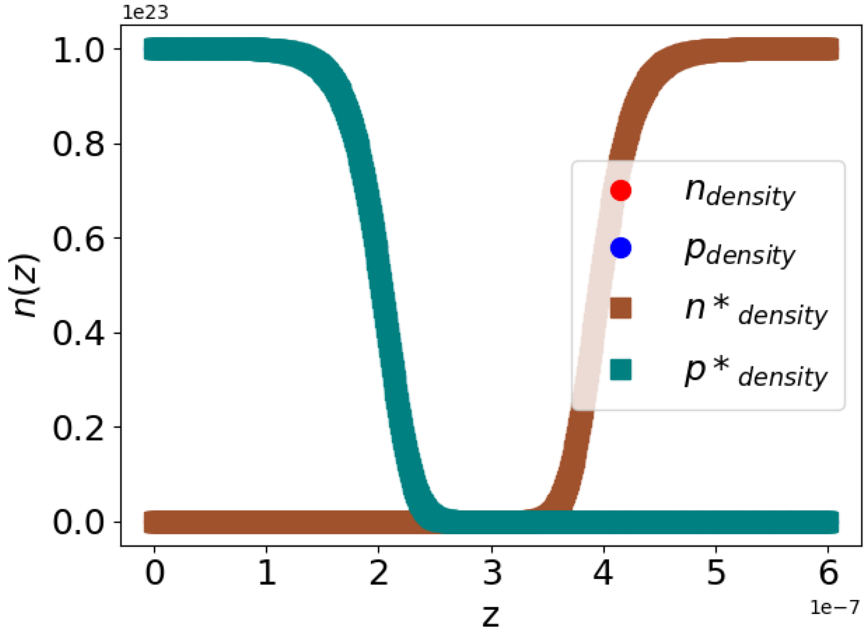
This is the semi-classical result of density:



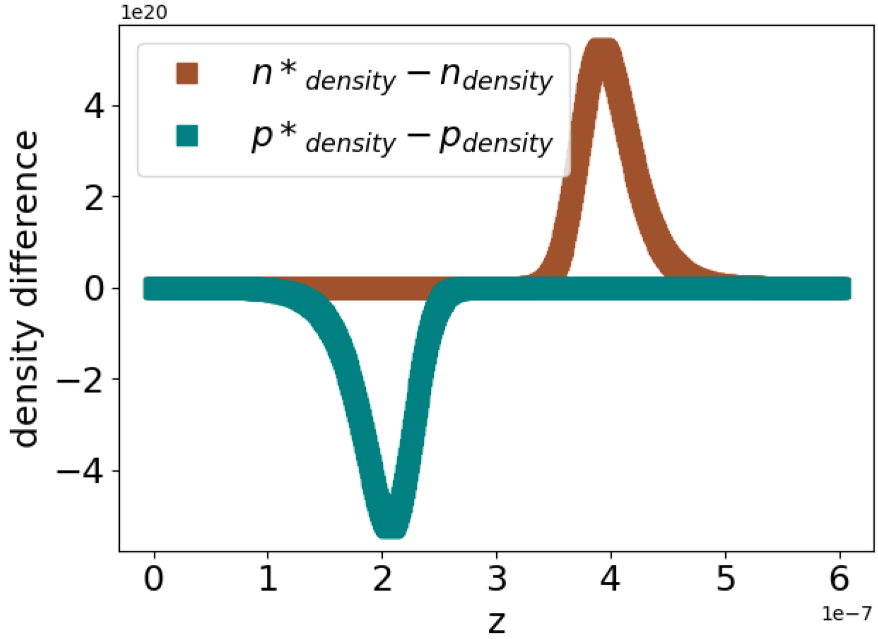
Now let's consider Drift-Diffusion model.

$$J_{n,i+0.5}=-q\mu_n\left(n_{i+0.5}\frac{d\phi}{dx}_{i+0.5}-V_T\frac{dn}{dx}_{i+0.5}\right)$$

$$residue=J_{n,i+0.5}-J_{n,i-0.5}=\frac{n_{i+1}+n_i}{2}\left(\frac{\phi_{i+1}-\phi_i}{\Delta x}\right)-V_T\frac{n_{i+1}-n_i}{\Delta x}-\frac{n_i+n_{i-1}}{2}\frac{\phi_i-\phi_{i-1}}{\Delta x}+V_T\frac{n_i-n_{i-1}}{\Delta x}$$
$$Jaco_{i-1}=-\frac{1}{2}\frac{\phi_i-\phi_{i-1}}{\Delta x}-V_T\frac{1}{\Delta x}$$
$$Jaco_i=\frac{1}{2}\left(\frac{\phi_{i+1}-\phi_i}{\Delta x}\right)+V_T\frac{1}{\Delta x}-\frac{1}{2}\frac{\phi_i-\phi_{i-1}}{\Delta x}+V_T\frac{1}{\Delta x}$$
$$Jaco_{i+1}=\frac{1}{2}\left(\frac{\phi_{i+1}-\phi_i}{\Delta x}\right)-V_T\frac{1}{\Delta x}$$



Star means the density is updated with drift-diffusion model. It looks similar adapting drift-diffusion model with not adapted model. The difference with them is shown below.



The difference is largest at the midpoint of densities(~0.5).

Now we couple the Poisson equation and the continuity equation.

Poisson equation :

$$R_\phi = \frac{\epsilon_{i+0.5}\phi_{i+1} - (\epsilon_{i+0.5} + \epsilon_{i-0.5})\phi_i + \epsilon_{i-0.5}\phi_{i-1}}{\epsilon_0} + \frac{\Delta x^2 q}{\epsilon_0}(N^+ - n_i) = 0$$

$$\frac{\partial R_\phi}{\partial \phi_{i+1}} = \frac{\epsilon_{i+0.5}}{\epsilon_0}, \qquad \frac{\partial R_\phi}{\partial \phi_i} = -\frac{\epsilon_{i+0.5} + \epsilon_{i-0.5}}{\epsilon_0}, \qquad \frac{\partial R_\phi}{\partial \phi_{i-1}} = \frac{\epsilon_{i+0.5}}{\epsilon_0},$$

$$\frac{\partial R_\phi}{\partial n_i} = -\frac{\Delta x^2 q}{\epsilon_0}$$

Continuity equation:

$$R_n = \left(\frac{n_{i+1} + n_i}{2}\right)\left(\frac{\phi_{i+1} - \phi_i}{\Delta x}\right) - V_T\frac{n_{i+1} - n_i}{\Delta x} - \left(\frac{n_i + n_{i-1}}{2}\right)\left(\frac{\phi_i - \phi_{i-1}}{\Delta x}\right) + V_T\frac{n_i - n_{i-1}}{\Delta x} = 0$$

$$\frac{\partial R_n}{\partial n_{i+1}} = \frac{1}{2}\frac{\phi_{i+1} - \phi_i}{\Delta x} - V_T\frac{1}{\Delta x},$$

$$\frac{\partial R_n}{\partial n_i} = \frac{1}{2}\frac{\phi_{i+1} - \phi_i}{\Delta x} + \frac{V_T}{\Delta x} - \frac{1}{2}\left(\frac{\phi_i - \phi_{i-1}}{\Delta x}\right) + \frac{V_T}{\Delta x},$$

$$\frac{\partial R_n}{\partial n_{i-1}} = -\frac{1}{2}\frac{\phi_i - \phi_{i-1}}{\Delta x} - \frac{V_T}{\Delta x}$$

$$\frac{\partial R_n}{\partial \phi_{i+1}} = \frac{n_{i+1} + n_i}{2}\frac{1}{\Delta x}, \qquad \frac{\partial R_n}{\partial \phi_i} = -\frac{n_{i+1} + n_i}{2}\frac{1}{\Delta x} - \left(\frac{n_i + n_{i-1}}{2}\right)\frac{1}{\Delta x}, \qquad \frac{\partial R_n}{\partial \phi_{i-1}} = \frac{n_i + n_{i-1}}{2}\frac{1}{\Delta x}$$

HW 15

N^+NN^+ structure.

Boundary condition : $\phi_0 = \phi_{N-1} = V_T \log(5 \times 10^{23} m^{-3}/n_{int})$

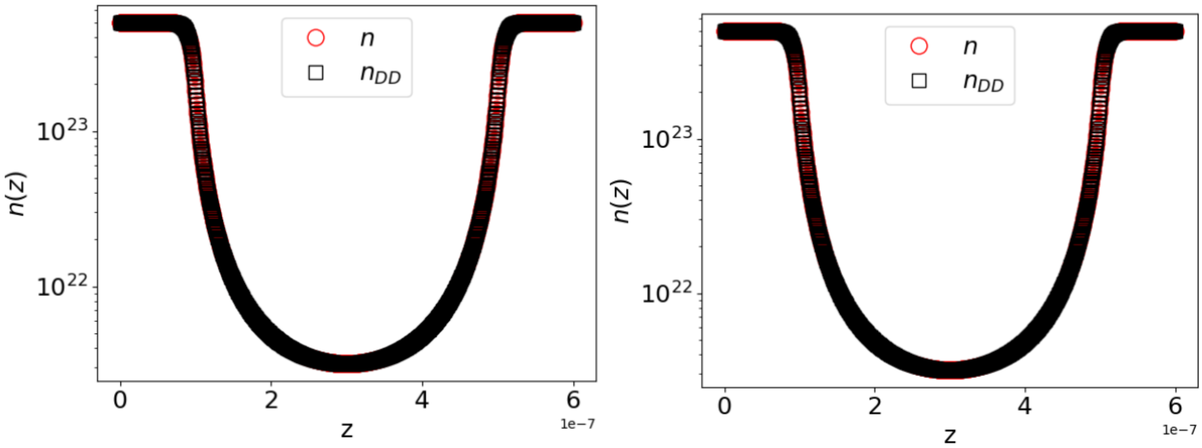
600nm long structure : 0.5nm, 1nm, and 10nm spacing

60nm short structure : 0.2nm, 1nm and 5nm spacing

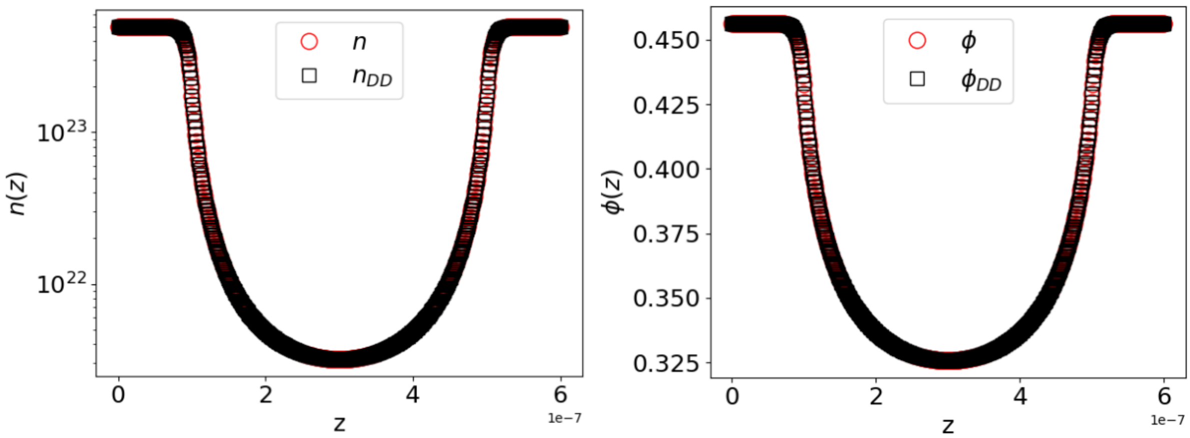
$$\begin{pmatrix} \frac{\partial R_{\phi_1}}{\partial \phi_1} & \frac{\partial R_{\phi_1}}{\partial n_1} & \frac{\partial R_{\phi_1}}{\partial \phi_2} & \frac{\partial R_{\phi_1}}{\partial n_2} & \cdots \\ \frac{\partial R_{n_1}}{\partial \phi_1} & \frac{\partial R_{n_1}}{\partial n_1} & \frac{\partial R_{n_1}}{\partial \phi_2} & \frac{\partial R_{n_1}}{\partial n_2} & \\ \frac{\partial R_{\phi_2}}{\partial \phi_1} & \frac{\partial R_{\phi_2}}{\partial n_1} & \frac{\partial R_{\phi_2}}{\partial \phi_2} & \frac{\partial R_{\phi_2}}{\partial n_2} & \\ & \vdots & & & \ddots \end{pmatrix} \begin{pmatrix} \delta\phi_1 \\ \delta n_1 \\ \delta\phi_2 \\ \delta n_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} R_{\phi_1} \\ R_{n_1} \\ R_{\phi_2} \\ R_{n_2} \\ \vdots \end{pmatrix}$$

Result

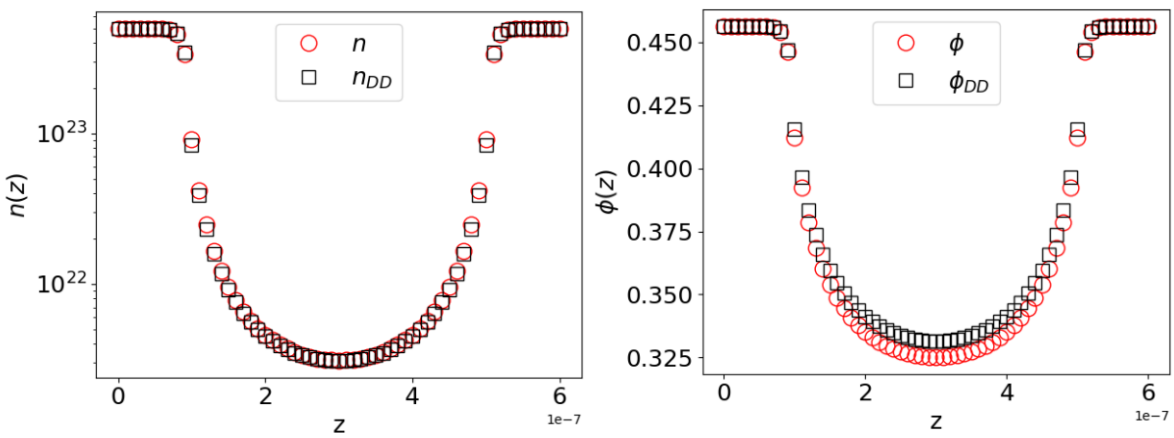
1-1. L = 600nm, 0.5nm spacing



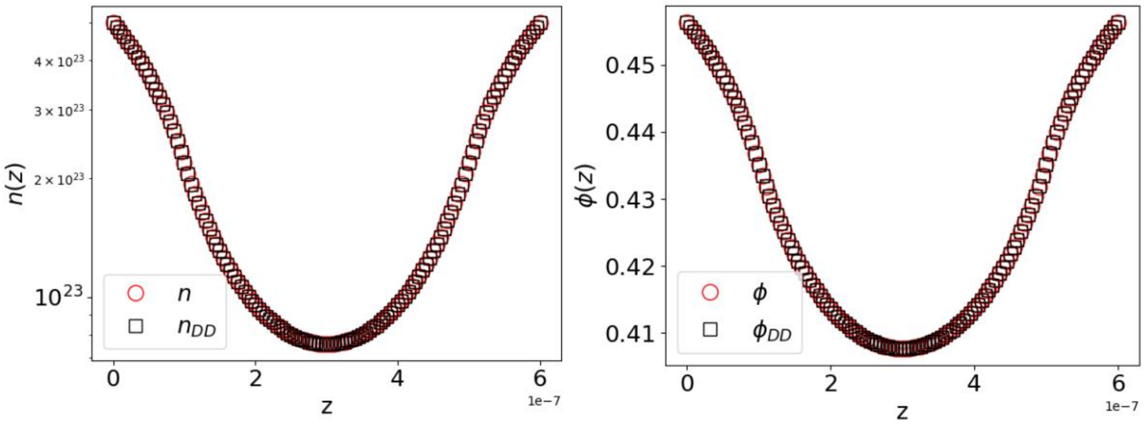
1-2. L = 600nm, 1nm spacing



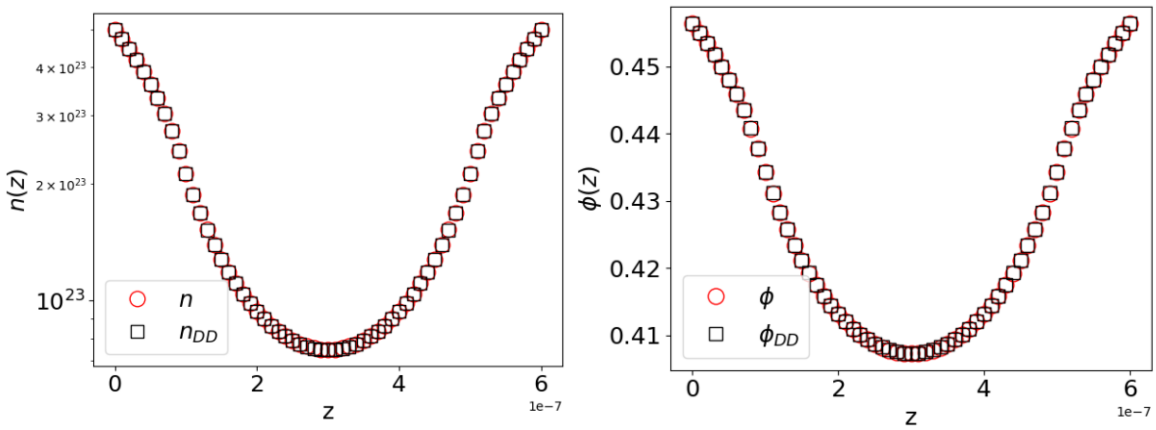
1-3. L = 600nm, 10nm spacing



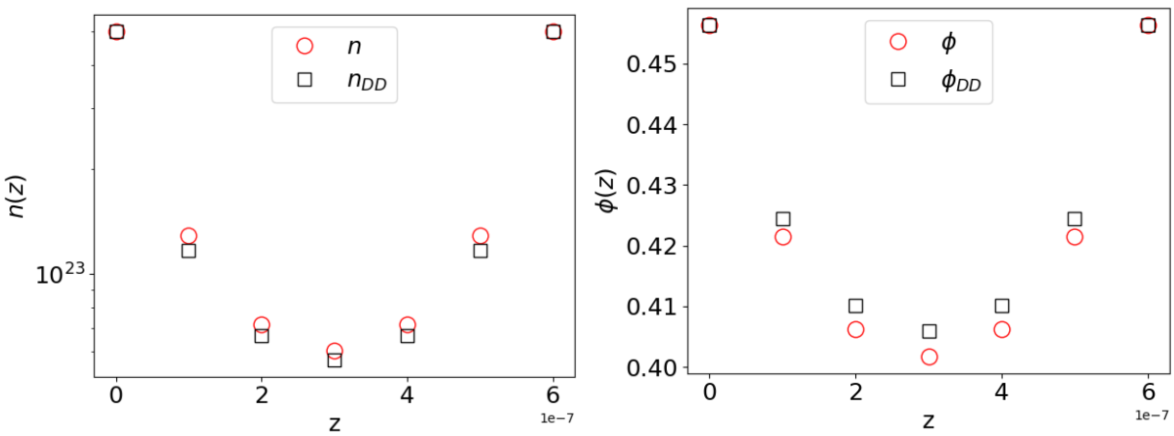
2-1. L=60nm, 0.5nm spacing



2-1. L=60nm, 1nm spacing



2-1. L=60nm, 10nm spacing



We found that more dense slicing makes more similar result.