

## Drift-diffusion model

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### 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 :

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

### Electron/hole current density :

$$\begin{aligned}J_n &= q\mu_n nE + qD_n \nabla n, \\ J_p &= q\mu_p pE - qD_p \nabla p\end{aligned}$$

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

### 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  $\phi$  as we did before. Now we can use  $\phi$  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 :

$$\begin{aligned}J_{n,i+0.5} &= -q\mu_n n_{i+0.5} \frac{d\phi}{dx_{i+0.5}} + qD_n \frac{dn}{dx_{i+0.5}} \\ &= -q\mu_n \left( n_{i+0.5} \frac{d\phi}{dx_{i+0.5}} - V_T \frac{dn}{dx_{i+0.5}} \right), \text{ with Einstein relation.}\end{aligned}$$

Now we could have integrated form:

$$\begin{aligned}J_{n,i+0.5} - J_{n,i-0.5} &= 0 \\ n_{i+0.5} \frac{d\phi}{dx_{i+0.5}} - V_T \frac{dn}{dx_{i+0.5}} - n_{i-0.5} \frac{d\phi}{dx_{i-0.5}} + V_T \frac{dn}{dx_{i-0.5}} &= 0\end{aligned}$$

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

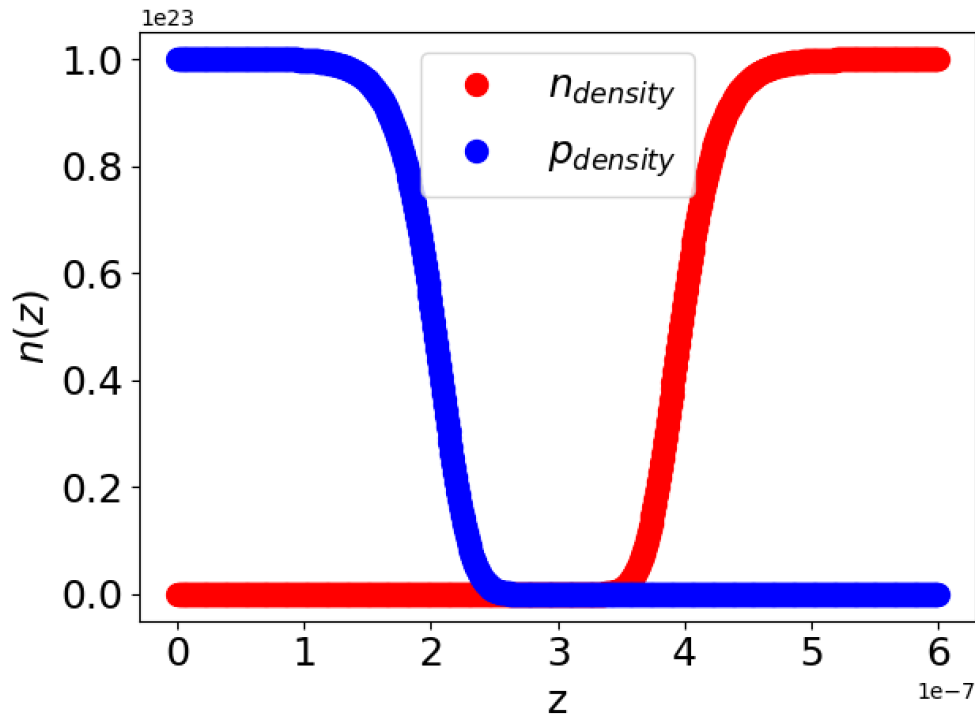
### PN junction

$$\begin{aligned}\frac{\epsilon_{si}(\phi_{i+1} + \phi_{i-1}) - 2\epsilon\phi_i}{\Delta x^2} &= qN_{acc} + 2q\sinh\left(\frac{\phi}{V_T}\right), & (x < \frac{N}{2}) \\ &= 2q\sinh\left(\frac{\phi}{V_T}\right), & (x = \frac{N}{2}) \\ &= -qN_{acc} + 2q\sinh\left(\frac{\phi}{V_T}\right), & (x > \frac{N}{2})\end{aligned}$$

Boundary conditions:

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

This is the semi-classical result of density:



Now let's consider Drift-Diffusion model.

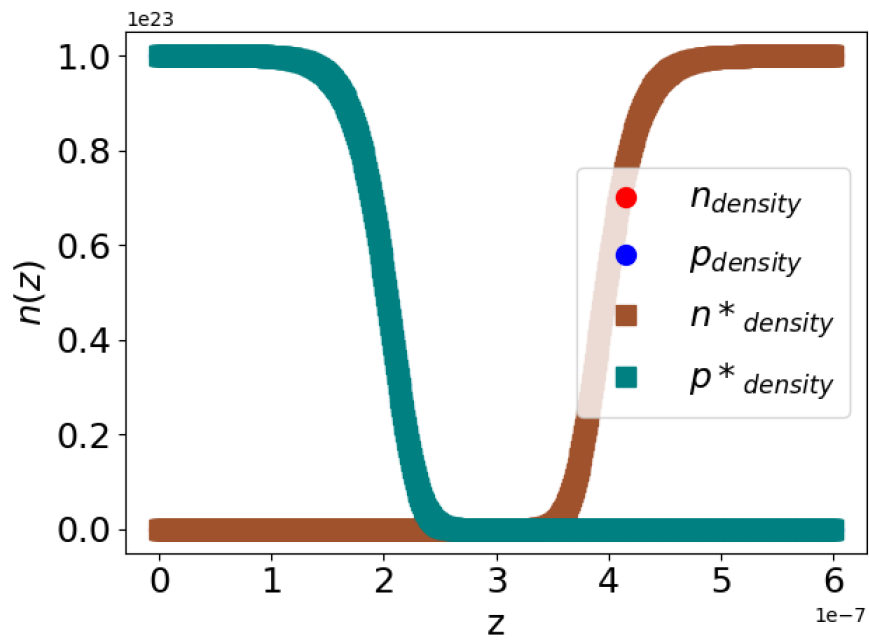
$$J_{n,i+0.5} = -q\mu_n \left( n_{i+0.5} \frac{d\phi}{dx_{i+0.5}} - V_T \frac{dn}{dx_{i+0.5}} \right)$$

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

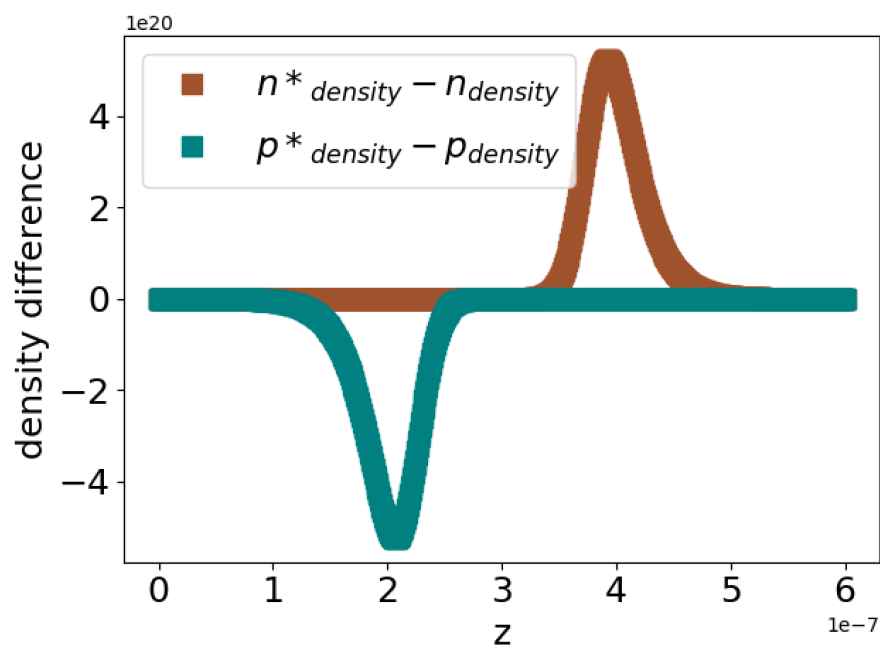
$$Jaco_{i-1} = -\frac{1}{2} \frac{\phi_i - \phi_{i-1}}{\Delta x} - V_T \frac{1}{\Delta x}$$

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

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



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( $\sim 0.5$ ).

Now we couple the Poisson equation and the continuity equation.

**Poisson equation :**

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

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

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

**Continuity equation:**

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

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

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

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

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

**HW 15**

$N^+NN^+$  structure.

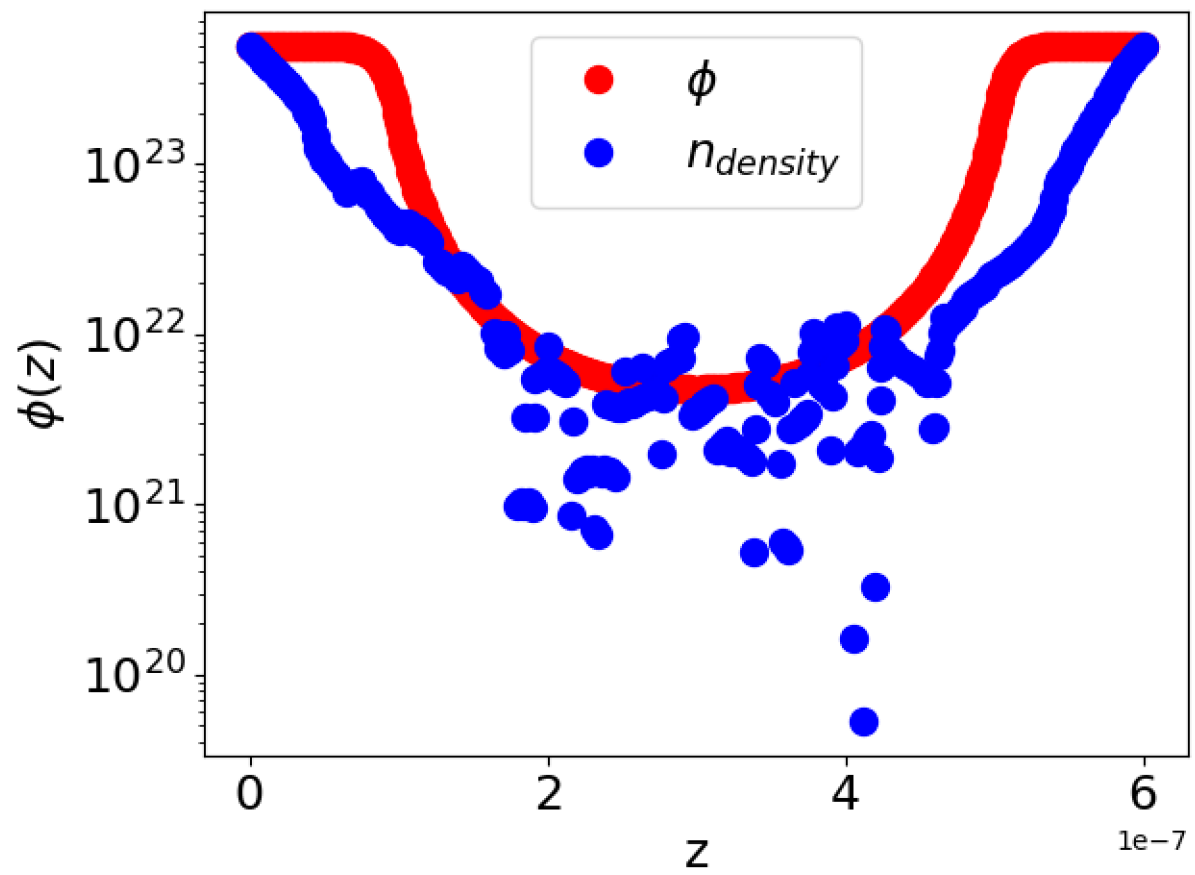
Boundary condition :  $\phi_0 = \phi_{N-1} = V_T \log(5 \times 10^{23} m^{-3} / n_{int})$

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

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

$$\begin{pmatrix} \frac{\partial R_\phi}{\partial \phi_1} & \frac{\partial R_\phi}{\partial n_1} & \frac{\partial R_\phi}{\partial \phi_2} & \frac{\partial R_\phi}{\partial n_2} & \dots \\ \frac{\partial R_n}{\partial \phi_1} & \frac{\partial R_n}{\partial n_1} & \frac{\partial R_n}{\partial \phi_2} & \frac{\partial R_n}{\partial n_2} \\ \frac{\partial R_\phi}{\partial \phi_1} & \frac{\partial R_\phi}{\partial n_1} & \frac{\partial R_\phi}{\partial \phi_2} & \frac{\partial R_\phi}{\partial n_2} \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} \phi_1 \\ n_1 \\ \phi_2 \\ n_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} R_\phi \\ R_n \\ R_\phi \\ R_n \\ \vdots \end{pmatrix}$$

Result



I need to update figures to make it right... it is a disappointing result.