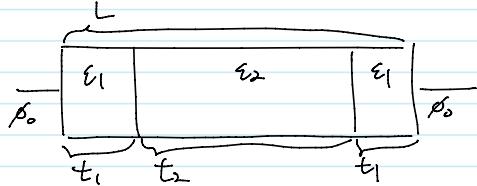


HW 6.

2020년 9월 22일 화요일 오후 6:42

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$$\frac{d}{dx} \left(\varepsilon(x) \frac{d\phi(x)}{dx} \right) = b(x) \quad \text{on } \mathcal{A},$$

$$\epsilon(x) = \begin{cases} \epsilon_1 & \text{for } 0 \leq x < t_1 \\ \epsilon_2 & \text{for } t_1 \leq x < t_1 + t_2 \\ \epsilon_1 & \text{for } t_1 + t_2 \leq x < L \end{cases}, \quad b(x) = \begin{cases} \phi_0 & \text{at } x=0 \\ 0 & \text{for } 0 < x < t_1 \\ \epsilon_{\text{Nacc}} & \text{for } t_1 < x < t_1 + t_2 \\ 0 & \text{for } t_1 + t_2 < x < L \\ \phi_0 & \text{at } x=L \end{cases}$$

when we take
the depletion approximation.

If we add an electron (hole) density to the $b(x)$ of the depletion approximation,

$$b(x) = \begin{cases} \phi_0 + V_G & \text{at } x=0 \\ 0 & \text{for } 0 < x < t_1 \\ g_{\text{Nuc}} + g_p(N(x) - P(x)) & \text{for } t_1 < x < t_1 + t_2 \\ 0 & \text{for } t_1 + t_2 < x < L \\ \phi_0 + V_G & \text{at } x=L \end{cases}$$

where V_g is a gate voltage, $N(x)$ ($p(x)$) is an electron (hole) density.

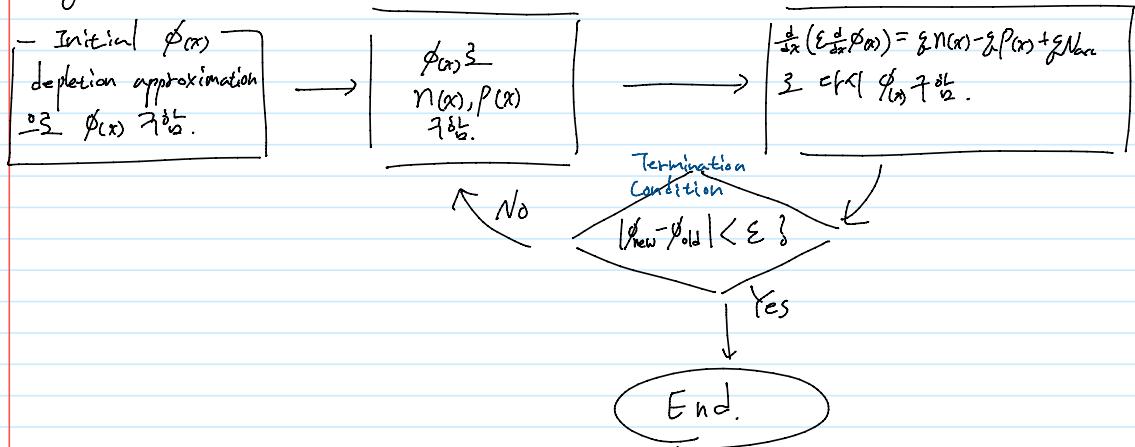
$$\begin{cases} N(x) = N_c \exp\left(-\frac{E_c - E_x}{k_B T}\right) \exp\left(\frac{g\phi}{k_B T}\right) \\ P(x) = N_c \exp\left(-\frac{E_c - E_x}{k_B T}\right) \exp\left(-\frac{g\phi}{k_B T}\right) \end{cases} \Rightarrow g(N(x) - P(x)) = 2gN_c e^{-\frac{E_c - E_x}{k_B T}} \sinh\left(\frac{g\phi}{k_B T}\right)$$

By finite difference,

$$\frac{d}{dx} \left(\varepsilon(x) \frac{du}{dx} \right) \Rightarrow A = \begin{pmatrix} 0 & - & - & - & \cdot & \cdot & \cdot \\ \varepsilon_1 - 2\varepsilon_1 & \varepsilon_1 & & & & & \\ \vdots & & & & & & \\ \varepsilon_1 & \rightarrow \varepsilon_1 & \varepsilon_1 & & & & \\ \varepsilon_1 - \varepsilon_1 \varepsilon_2 & \varepsilon_2 & & & & & \\ \varepsilon_2 - 2\varepsilon_2 & \varepsilon_2 & & & & & \\ \vdots & & & & & & \\ \varepsilon_2 & \rightarrow \varepsilon_2 & \varepsilon_2 & & & & \\ \varepsilon_2 - \varepsilon_1 \varepsilon_2 & \varepsilon_1 & & & & & \\ \varepsilon_1 - 2\varepsilon_1 & \varepsilon_1 & & & & & \\ \vdots & & & & & & \\ 0 & 1 & & & & & \end{pmatrix}$$

$$b(x) = (\Delta x)^2 \begin{pmatrix} \phi_0 + V_G \\ \vdots \\ 0 \\ \frac{\epsilon_{\text{Nacc}}}{2} \\ \epsilon_{\text{Nacc}} + g(N(x) - P(x)) \\ \vdots \\ \frac{\epsilon_{\text{Nacc}}}{2} \\ 0 \\ \vdots \\ \phi_0 + V_G \end{pmatrix} \rightarrow \begin{cases} x = t_1 \\ x = t_1 + t_2 \end{cases}, \quad \phi(x) = \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_N \end{pmatrix}$$

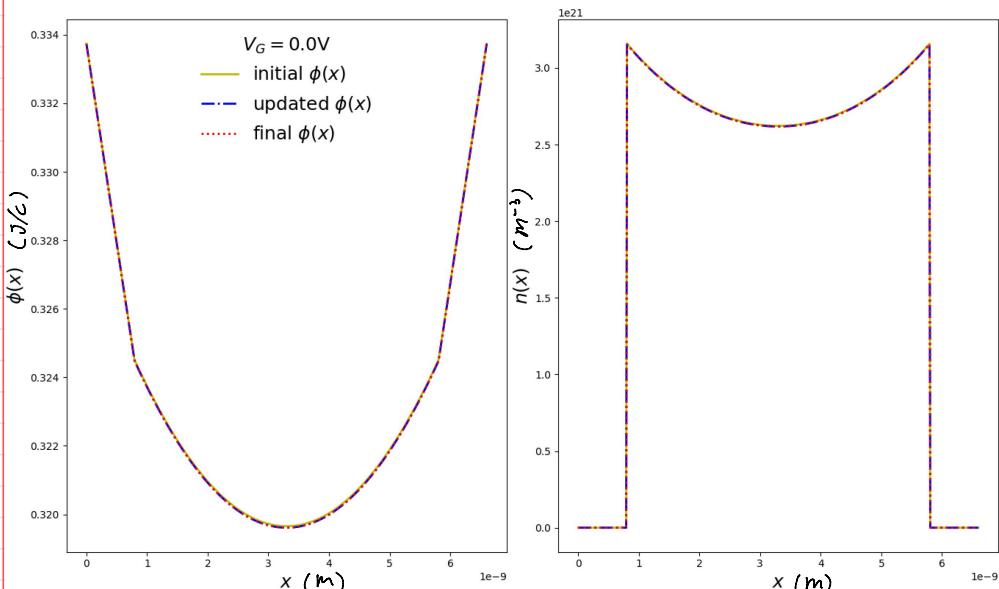
* Algorithm.



Results.

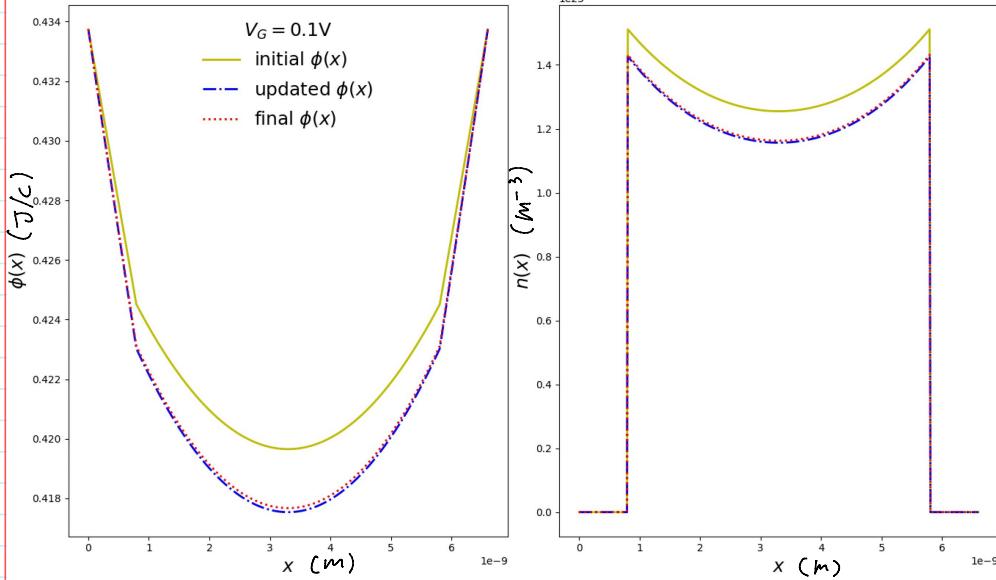
$$\phi_0 = 0.33374 \text{ V}, N = 500, N_{\text{acc}} = 10^{24} \text{ m}^{-3},$$

$$t_1 = 0.8 \text{ nm}, t_2 = 5 \text{ nm}, \epsilon_1 = 3.9\epsilon_0, \epsilon_2 = 11.7\epsilon_0, T = 300 \text{ K}.$$

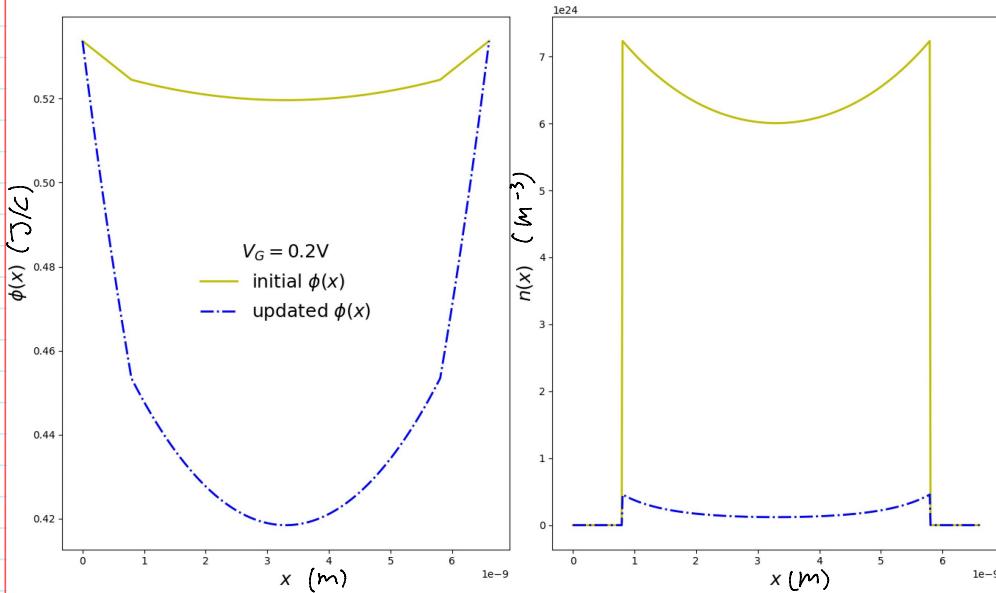


Updated는 loop를 1번만 거쳤을 때, final은 termination 때, $\phi(x)$ 이다.

$V_G = 0 \text{ V}$ 인 경우, $N_{\text{acc}} \gg n_{\text{init}}(x)$ 인 경우 $\phi_{\text{init}}(x) \approx \phi_{\text{final}}(x)$ 이다.



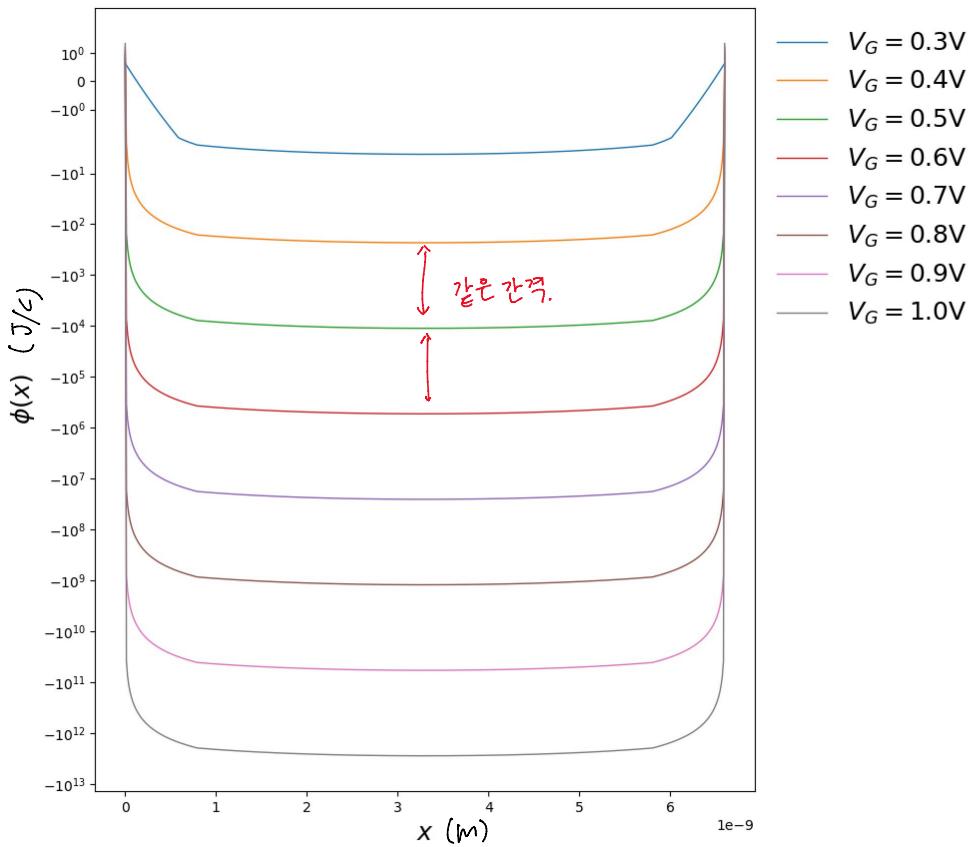
$V_G = 0.1\text{V}$ 경우 $\phi(x)$ 가 잘 수렴한다. 아직 $N_{acc} \gg n_{init}(x)$ 이기 때문에 보여진다.



$V_G = 0.2\text{V}$ 에서 $N_{acc} \lesssim n_{init}(x)$ 가 된다. 이 때문에 loop를 진행하면, $\phi(x)$ 가 초기에 진동하면서 수렴하지 않는다.

$V_G > 0.2\text{V}$ 부터는 $N_{acc} \ll n_{init}(x)$ 가 되면서 loop를 진행하게 되면, $b(x)$ 가 발산하여 $\phi(x)$ 가 수렴하지 않는다.

이는 $V_G > 0.2\text{V}$ 에서 depletion approximation이 적절하지 않다는 걸 의미한다.



log scale $\phi_{\text{updated}}(x)$ 을 그려보면 $V_G \geq 0.3 \text{ V}$ 이상에서 $\phi(\frac{L}{2})$ 이 log scale로 증가함을 알 수 있다.