HW8.

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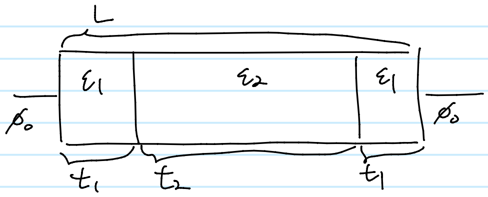


$\frac{d}{dx}\left(\varepsilon(x)\frac{d\phi(x)}{dx}\right) = b(x)$ 에서,

$$\varepsilon(x) = \begin{cases} \varepsilon_1 & \text{for } 0 \le x < t_1 \\ \varepsilon_2 & \text{for } t_1 \le x < t_1+t_2 \\ \varepsilon_1 & \text{for } t_1+t_2 \le x < L \end{cases}, \quad b(x) = \begin{cases} \phi_0 & \text{at } x=0 \\ 0 & \text{for } 0<x<t_1 \\ qN_{acc} & \text{for } t_1<x<t_1+t_2 \\ 0 & \text{for } t_1+t_2<x<L \\ \phi_0 & \text{at } x=L \end{cases}$$

when we take the depletion approximation.

$\phi(0) = \phi(L) = 0$.

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

$$b(x) = \begin{cases} \phi_0 + V_G & \text{at } x=0 \\ 0 & \text{for } 0<x<t_1 \\ qN_{acc} + q(n(x)-p(x)) & \text{for } t_1<x<t_1+t_2 \\ 0 & \text{for } t_1+t_2<x<L \\ \phi_0+V_G & \text{at } x=L \end{cases}$$

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

$$\begin{cases} n(x) = N_c \exp\left(-\frac{E_c-E_i}{k_BT}\right)\exp\left(\frac{q\phi}{k_BT}\right) \\ p(x) = N_c \exp\left(-\frac{E_c-E_i}{k_BT}\right)\exp\left(-\frac{q\phi}{k_BT}\right) \end{cases} \Rightarrow q(n(x)-p(x)) = 2qN_c e^{-\frac{E_c-E_i}{k_BT}} \sinh\left(\frac{q\phi}{k_BT}\right)$$

By finite difference,

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

$$
b(x) = (\Delta x)^2 \begin{pmatrix} \phi_0 + V_G \\ \vdots \\ 0 \\ \frac{\varepsilon_1 N_{acc}}{2} + \frac{\varepsilon_2}{2}(n(x) - p(x)) \\ \varepsilon_2 N_{acc} + \varepsilon_2 (n(x) - p(x)) \\ \vdots \\ \varepsilon_2 N_{acc} + \varepsilon_2 (n(x) - p(x)) \\ \frac{\varepsilon_2 N_{acc}}{2} + \frac{\varepsilon_2}{2}(n(x) - p(x)) \\ 0 \\ \vdots \\ \phi_0 + V_G \end{pmatrix} \begin{matrix} \\ \\ \\ \to x = t_1 \\ \\ \\ \\ \to x = t_1 + t_2 \\ \\ \\ \\ \end{matrix}, \quad \phi(x) = \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_N \end{pmatrix}
$$

* Algorithm with Newton method

Initial $\phi(x)$
$\phi(x) = \phi_0$

$\to$

Residue & Jacobian matrix
$r(\phi) = A\phi(x) - b(\phi)$
$J = A - \partial_\phi b(\phi)$

$\to$

Linear solver로
$J\,\delta\phi = -r(\phi)$ 에서 $\delta\phi$ 구함.
$\Rightarrow \phi \to \phi + \delta\phi$ 로 update

Termination Condition
$\| \delta\phi \|_F < \varepsilon$?

No

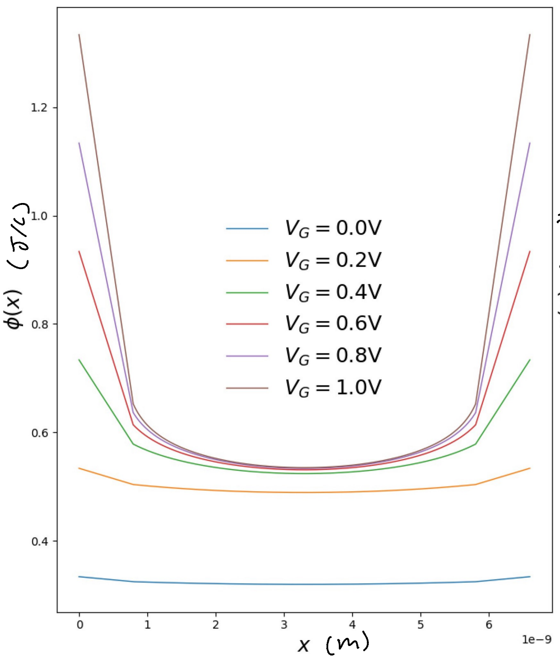
Yes

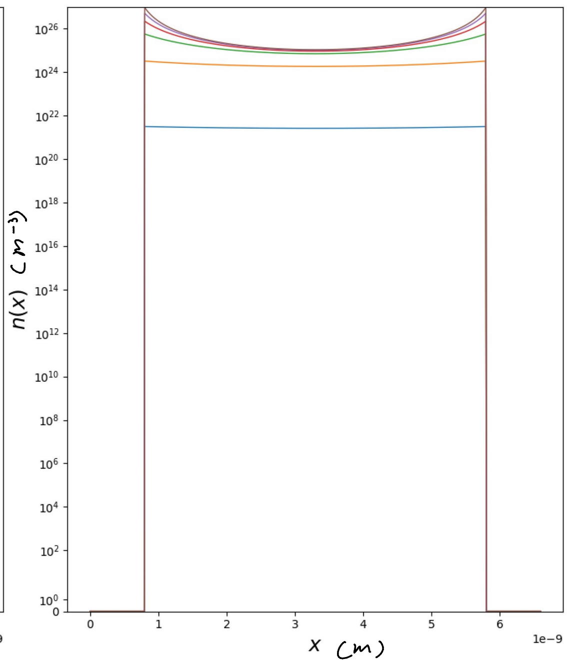
End.

* $\| \cdot \|_F$는 Frobenius norm.

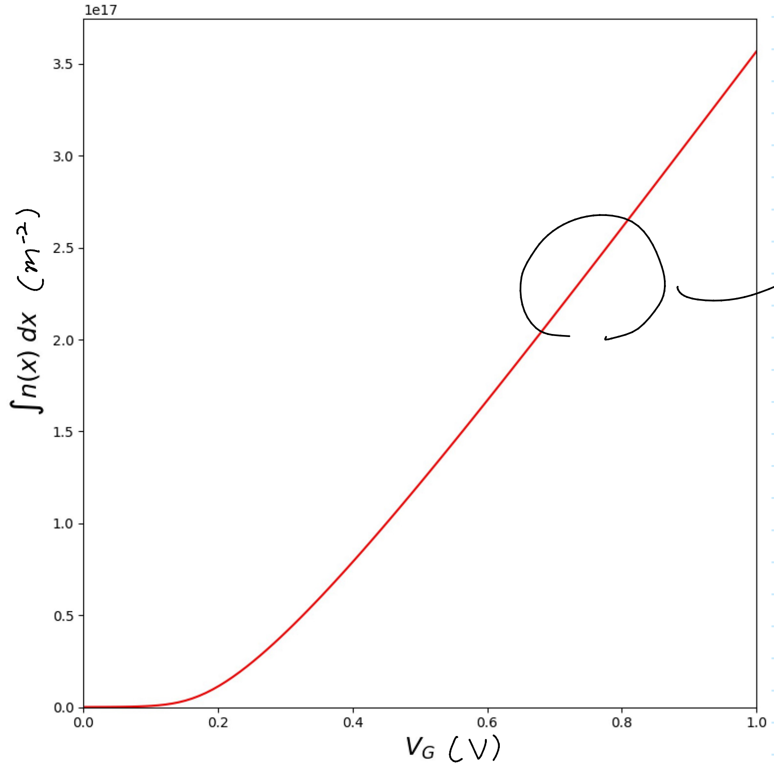
Results.

$\phi_0 = 0.33374\,V$, $N = 800$, $N_{acc} = 10^{24}\,m^{-3}$,
$t_1 = 0.8\,nm$, $t_2 = 5\,nm$, $\varepsilon_1 = 3.9\varepsilon_0$, $\varepsilon_2 = 11.7\varepsilon_0$, $T = 300K$.





$n(\frac{L}{2})$은 V_G가 커져도 $\sim 10^{25}\ m^{-3}$ 에서 수렴한다. 하지만 interface에서 electron density가 급격하게 커짐을 알 수 있다.
Newton method를 이용하면 HW 6. 와 다르게 발산하는 문제가 사라진다.



: integrated electron density를 V_G에 따라 보았다.

→ Linear growth