HW 10.

Thursday, October 8, 2020 4:44 PM

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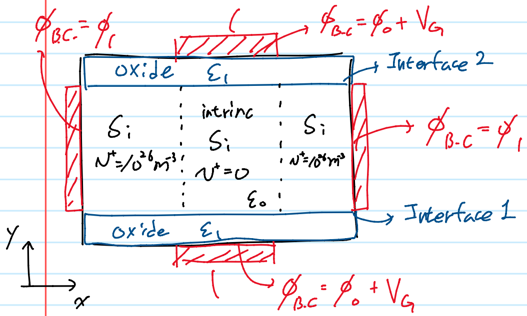
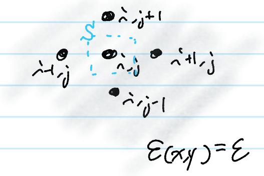


Edge 와 Bulk 와 Interface 부분으로 나누어 $\int_V d\tau\, \nabla\cdot(\varepsilon\nabla\phi(x,y)) = \int_V d\tau\, -\rho(x,y)$ 를 Discretization 했다.

ϕ_i은 $N^+ - n(\phi) + p(\phi) = 0$ 의 solution을 취했다.

가로 길이는 L_x, 세로 길이는 L_y.

i) Bulk



$$\int_V d\tau\, \varepsilon \nabla^2\phi(x,y) = \varepsilon\int_S d\vec{a}\cdot\nabla\phi(x,y) = \int_V d\tau\, -\rho(x,y)$$

$$= \int_V d\tau \left[q N_{acc} + q(n(\phi)-p(\phi))\right]$$

Discretization → grid spacing : Δ

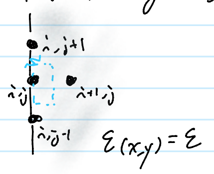
$$\varepsilon(-4\phi_{i,j}+\phi_{i+1,j}+\phi_{i-1,j}+\phi_{i,j+1}+\phi_{i,j-1}) = \Delta^2 q\left(N_{acc}+(n(\phi_{i,j})-p(\phi_{i,j}))\right)$$

Transform into $A\vec{\phi}=\vec{b}$

$$\begin{array}{r} \\ (jN_x+i)\text{th row} \leftarrow \\ \\ \end{array} \begin{pmatrix} \ddots & & & & \\ \varepsilon & \varepsilon & -4\varepsilon & \varepsilon & \varepsilon \\ & & & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \phi_{i,j-1} \\ \vdots \\ \phi_{i-1,j} \\ \phi_{i,j} \\ \phi_{i+1,j} \\ \vdots \\ \phi_{i,j+1} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \Delta^2 q\left(N_{acc}+2n_i \sinh\left(\frac{q\phi_{i,j}}{k_BT}\right)\right) \\ \vdots \end{pmatrix}$$

ii) Edge

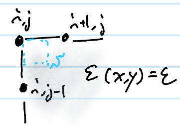
For homogeous Neumann B.C.,



By discretization,

$$\varepsilon\left(-2\phi_{i,j}+\phi_{i+1,j}+\frac{1}{2}\phi_{i,j+1}+\frac{1}{2}\phi_{i,j-1}\right)=0$$

$$\begin{array}{r} \\ (jN_x+i)\text{th row} \leftarrow \\ \\ \end{array} \begin{pmatrix} \ddots & & & \\ \frac{1}{2}\varepsilon & -2\varepsilon & \varepsilon & \frac{1}{2}\varepsilon \\ & & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \phi_{i,j-1} \\ \vdots \\ \phi_{i,j} \\ \phi_{i+1,j} \\ \vdots \\ \phi_{i,j+1} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ 0 \\ \vdots \end{pmatrix}$$



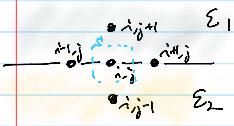
$$\varepsilon\left(-\phi_{i,j}+\frac{1}{2}\phi_{i+1,j}+\frac{1}{2}\phi_{i,j-1}\right)=0$$

$$\begin{array}{r} \\ (jN_x+i)\text{th row} \leftarrow \\ \\ \end{array} \begin{pmatrix} \ddots & & & \\ \frac{1}{2}\varepsilon & & -\varepsilon & \frac{1}{2}\varepsilon \\ & & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \phi_{i,j-1} \\ \vdots \\ \phi_{i,j} \\ \phi_{i+1,j} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ 0 \\ \vdots \end{pmatrix}$$

For Dirichlet B.C.,

$$\phi_{i,j} = \phi_{B.C.} \longrightarrow \begin{pmatrix} \ddots & & \\ & 1 & \\ & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \phi_{i,j} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \phi_{B.C.} \\ \vdots \end{pmatrix}$$

iii) Interface

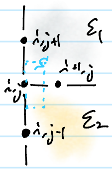


By discretization,

$$-2(\varepsilon_1+\varepsilon_2)\phi_{i,j} + \frac{(\varepsilon_1+\varepsilon_2)}{2}\phi_{i+1,j} + \frac{(\varepsilon_1+\varepsilon_2)}{2}\phi_{i-1,j} + \varepsilon_1\phi_{i,j+1} + \varepsilon_2\phi_{i,j-1}$$

$$= \Delta^2 q\left(N_{acc} + (n(\phi_{i,j}) - p(\phi_{i,j}))\right)$$

$$\begin{pmatrix} \ddots & & & & \\ \varepsilon_2 & \frac{\varepsilon_1+\varepsilon_2}{2} & -2(\varepsilon_1+\varepsilon_2) & \frac{\varepsilon_1+\varepsilon_2}{2} & \varepsilon_1 \\ & & & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \phi_{i,j-1} \\ \vdots \\ \phi_{i-1,j} \\ \phi_{i,j} \\ \phi_{i+1,j} \\ \vdots \\ \phi_{i,j+1} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \Delta^2 q\left(N_{acc} + 2n_i \sinh\left(\frac{q\phi_{i,j}}{k_B T}\right)\right) \\ \vdots \end{pmatrix}$$

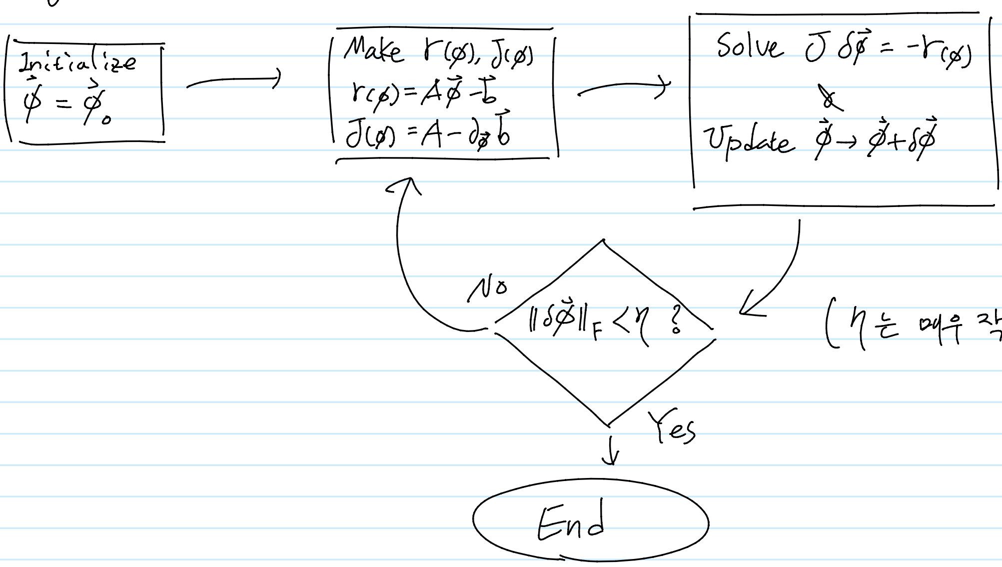


$$-(\varepsilon_1+\varepsilon_2)\phi_{i,j} + \frac{(\varepsilon_1+\varepsilon_2)}{2}\phi_{i+1,j} + \frac{\varepsilon_1}{2}\phi_{i,j+1} + \frac{\varepsilon_2}{2}\phi_{i,j-1} = 0$$

($\because$ Neumann B.C.)

$$\begin{pmatrix} \ddots & & & \\ \frac{\varepsilon_2}{2} & -(\varepsilon_1+\varepsilon_2) & \frac{\varepsilon_1+\varepsilon_2}{2} & \frac{\varepsilon_1}{2} \\ & & \ddots & \end{pmatrix} \begin{pmatrix} \vdots \\ \phi_{i,j-1} \\ \vdots \\ \phi_{i,j} \\ \phi_{i+1,j} \\ \vdots \\ \phi_{i,j+1} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ 0 \\ \vdots \end{pmatrix}$$

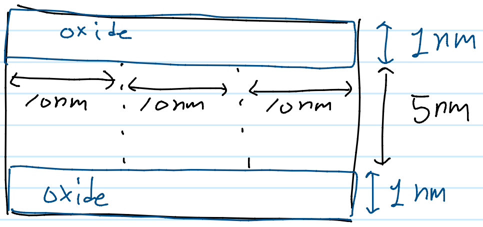
* Algorithm



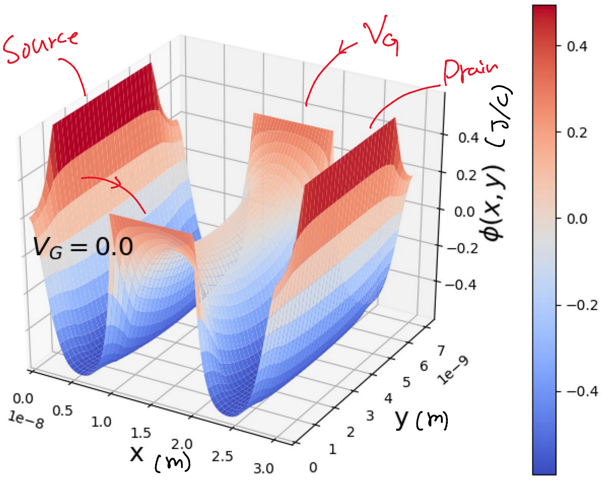
(η는 매우 작은 수)

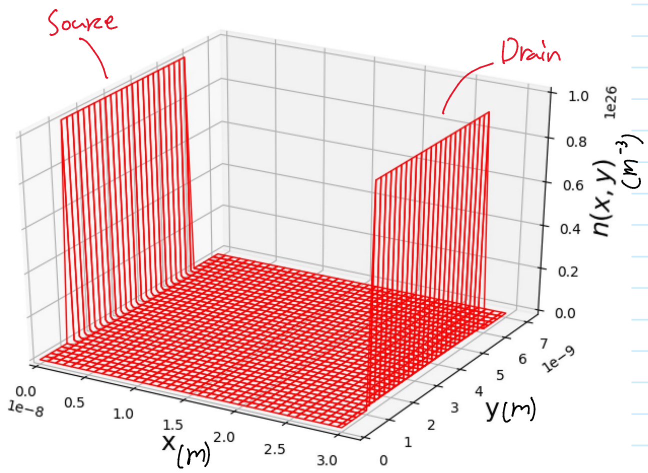
Results

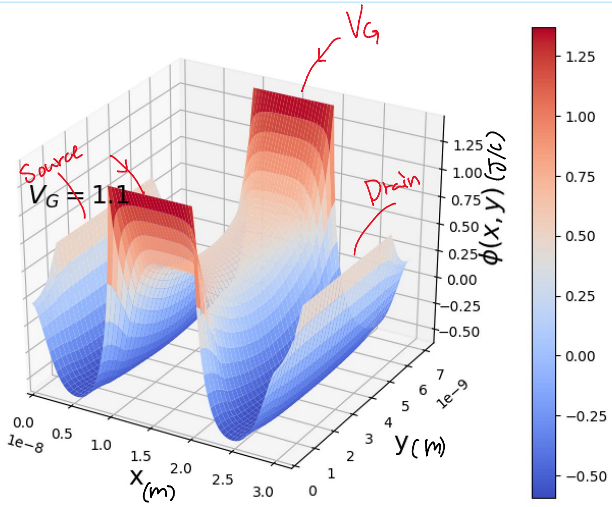
$\Delta = 0.2nm$, $L_x = 30nm$, $L_y = 7nm$

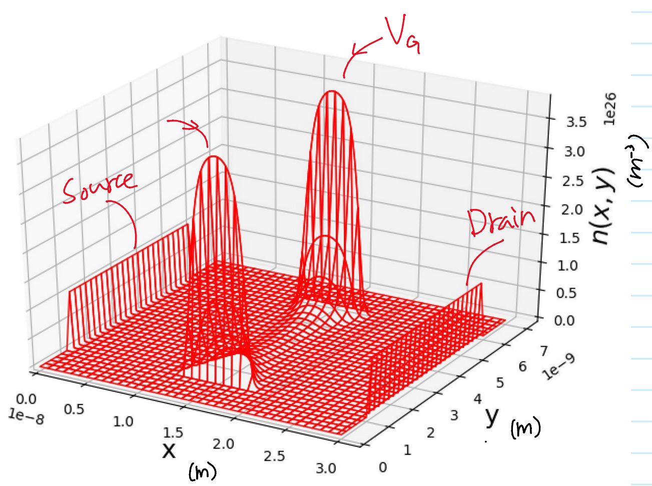


1) $\phi(x,y)$ & $n(x,y)$ for V_G









Homogeneous Neumann B.C. 부분에선 $\nabla\phi\cdot\vec{n}=0$ 인 것이 잘 나타난다.

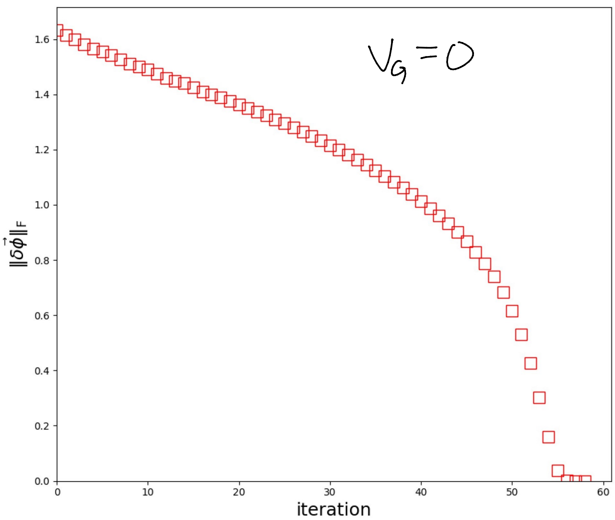
Gate voltage 가 커지면서 gate 쪽 electron density 가 증가한다.

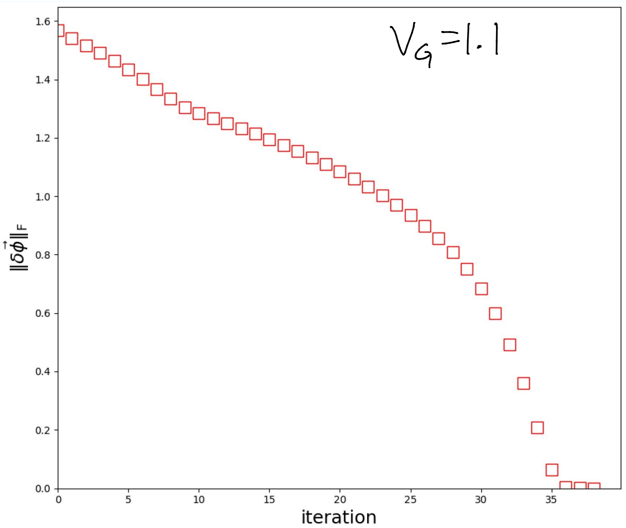
2) Converge trend for initial $\vec{\phi}$.

initial ϕ에 따라 Newton-Raphson method 의 Converge 가 어떻게 달라지는지 관찰해보았다. $\eta = 10^{-7}$으로 하였다.

i) $\vec{\phi}_{init.} = [\vec{\phi}]_{w\backslash o\ n(\phi),p(\phi)}$

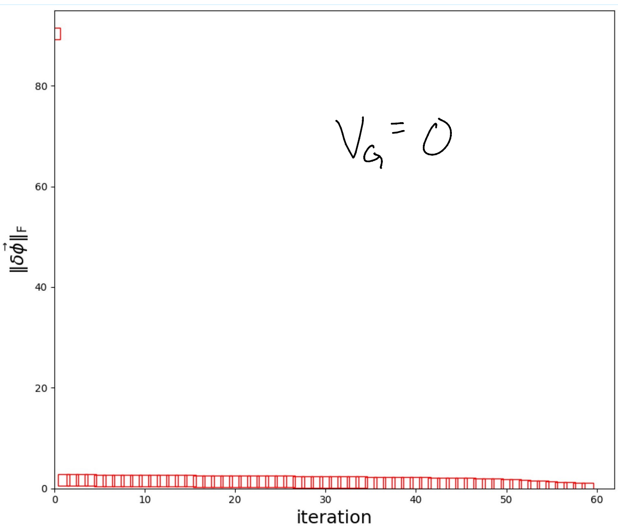
Initial $\vec{\phi}$를 선택할 때, $\nabla\cdot(\varepsilon\nabla\phi) = -\rho$ 에서 $\rho = qN^+$ 라 생각하고
$A\vec{\phi} = \vec{b}$ 를 풀어 구한 $\vec{\phi}$를 이용했다.

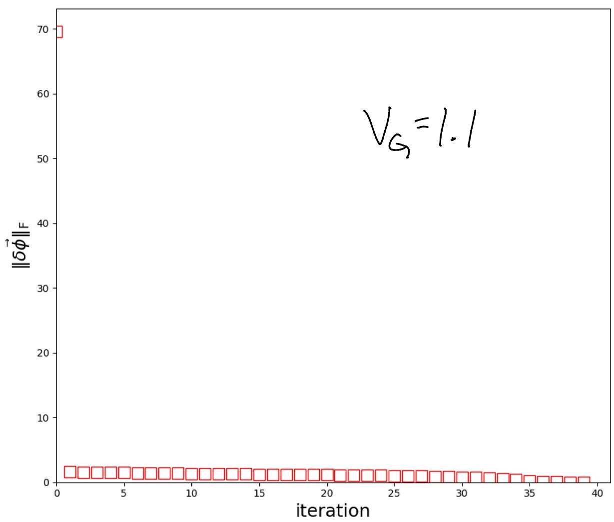




대략 40 ~ 60 iteration 에서 Converge 함을 알 수 있다.

ii) $\vec{\phi}_{init.} = \vec{0}$





대략 40~60 iteration에서 Converge 함을 알 수 있다.
그러나, $\|\delta\phi\|_F$의 trend가 다름을 알 수 있다.

i)와 ii)를 보면 initial ϕ에 따라 수렴 조건이
꽤 차이남을 알 수 있다.