Term project

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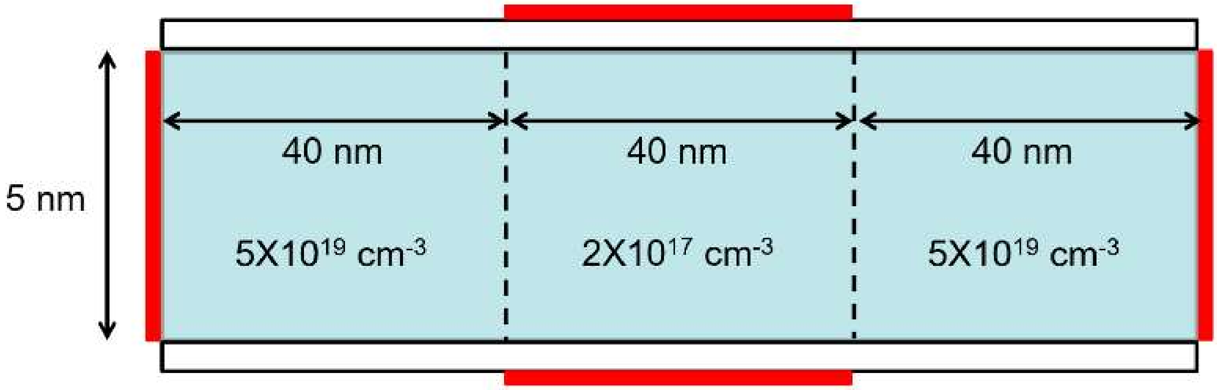
Entire structure (double gate, Work function = 4.3 eV)



Computational Microelectronics, 2018 Fall

1. Step 1.

For 2D simulation, by Stoke's Theorem,

$$\oint_{surface} \varepsilon \nabla \psi \cdot d\boldsymbol{a} = -\int_{Volume} q(N^{+} - n_i)$$

=> $$\oint_{surface} \varepsilon \nabla \psi \cdot d\boldsymbol{a} = -q(N^{+} - n_i)\Delta x\, \Delta y \Delta z$$

=>

$$\varepsilon_2\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j-1} + \varepsilon_3\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j+1} - \varepsilon_1\left(2\frac{\Delta z}{\Delta y} + 2\frac{\Delta y}{\Delta z}\right)\psi_{i,j} + \varepsilon_4\left(\frac{\Delta y}{\Delta z}\right)\psi_{i-1,j} + \varepsilon_5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i+1,j} = -q(N^{+} - n_i)\,\Delta y \Delta z$$

=>

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j-1} + \left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j+1} - \left(2\frac{\Delta z}{\Delta y} + 2\frac{\Delta y}{\Delta z}\right)\psi_{i,j} + \left(\frac{\Delta y}{\Delta z}\right)\psi_{i-1,j} + \left(\frac{\Delta y}{\Delta z}\right)\psi_{i+1,j}\right\} = -\frac{q(N^{+} - n_i)}{\varepsilon_0}\,\Delta y \Delta z$$

For each interface,

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j-1} + 0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j+1} - \left(\frac{\Delta z}{\Delta y} + \frac{\Delta y}{\Delta z}\right)\psi_{i,j} + \left(\frac{\Delta y}{\Delta z}\right)\psi_{i-1,j}\right\} = -0.5\frac{q(N^{+} - n_i)}{\varepsilon_0}\,\Delta y \Delta z (\text{위})$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j-1} + 0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j+1} - \left(\frac{\Delta z}{\Delta y} + \frac{\Delta y}{\Delta z}\right)\psi_{i,j} + \left(\frac{\Delta y}{\Delta z}\right)\psi_{i+1,j}\right\} = -0.5\frac{q(N^{+} - n_i)}{\varepsilon_0}\,\Delta y \Delta z (\text{아래})$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j+1} - \left(\frac{\Delta z}{\Delta y} + \frac{\Delta y}{\Delta z}\right)\psi_{i,j} + 0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i-1,j} + 0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i+1,j}\right\} = -0.5\frac{q(N^{+} - n_i)}{\varepsilon_0}\,\Delta y \Delta z (\text{왼쪽})$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j-1} - \left(\frac{\Delta z}{\Delta y} + \frac{\Delta y}{\Delta z}\right)\psi_{i,j} + 0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i-1,j} + 0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i+1,j}\right\} = -0.5\frac{q(N^{+} - n_i)}{\varepsilon_0}\,\Delta y \Delta z (\text{오른쪽})$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j+1}-0.5\left(\frac{\Delta z}{\Delta y}+\frac{\Delta y}{\Delta z}\right)\psi_{i,j}+0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i-1,j}\right\}=-0.25\frac{q(N^+-n_i)}{\varepsilon_0}\ \Delta y\Delta z\ \text{(왼쪽 위)}$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j+1}-0.5\left(\frac{\Delta z}{\Delta y}+\frac{\Delta y}{\Delta z}\right)\psi_{i,j}+0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i+1,j}\right\}=-0.25\frac{q(N^+-n_i)}{\varepsilon_0}\ \Delta y\Delta z\ \text{(왼쪽 아래)}$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j-1}-0.5\left(\frac{\Delta z}{\Delta y}+\frac{\Delta y}{\Delta z}\right)\psi_{i,j}+0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i-1,j}\right\}=-0.25\frac{q(N^+-n_i)}{\varepsilon_0}\ \Delta y\Delta z\ \text{(오른쪽 위)}$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j-1}-0.5\left(\frac{\Delta z}{\Delta y}+\frac{\Delta y}{\Delta z}\right)\psi_{i,j}+0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i+1,j}\right\}=-0.25\frac{q(N^+-n_i)}{\varepsilon_0}\ \Delta y\Delta z\ \text{(오른쪽 아래)}$$

All of them are in oxide layer, therefore

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j-1}+0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j+1}-\left(\frac{\Delta z}{\Delta y}+\frac{\Delta y}{\Delta z}\right)\psi_{i,j}+\left(\frac{\Delta y}{\Delta z}\right)\psi_{i-1,j}\right\}=0\text{(위)}$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j-1}+0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j+1}-\left(\frac{\Delta z}{\Delta y}+\frac{\Delta y}{\Delta z}\right)\psi_{i,j}+\left(\frac{\Delta y}{\Delta z}\right)\psi_{i+1,j}\right\}=0\text{(아래)}$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j+1}-\left(\frac{\Delta z}{\Delta y}+\frac{\Delta y}{\Delta z}\right)\psi_{i,j}+0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i-1,j}+0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i+1,j}\right\}=0\text{(왼쪽)}$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j-1}-\left(\frac{\Delta z}{\Delta y}+\frac{\Delta y}{\Delta z}\right)\psi_{i,j}+0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i-1,j}+0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i+1,j}\right\}=0\text{(오른쪽)}$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j+1}-0.5\left(\frac{\Delta z}{\Delta y}+\frac{\Delta y}{\Delta z}\right)\psi_{i,j}+0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i-1,j}\right\}=0\ \text{(왼쪽 위)}$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j+1}-0.5\left(\frac{\Delta z}{\Delta y}+\frac{\Delta y}{\Delta z}\right)\psi_{i,j}+0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i+1,j}\right\}=0\ \text{(왼쪽 아래)}$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j-1}-0.5\left(\frac{\Delta z}{\Delta y}+\frac{\Delta y}{\Delta z}\right)\psi_{i,j}+0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i-1,j}\right\}=0\ \text{(오른쪽 위)}$$

$$\frac{\varepsilon_{sil}}{\varepsilon_0}\left\{0.5\left(\frac{\Delta z}{\Delta y}\right)\psi_{i,j-1}-0.5\left(\frac{\Delta z}{\Delta y}+\frac{\Delta y}{\Delta z}\right)\psi_{i,j}+0.5\left(\frac{\Delta y}{\Delta z}\right)\psi_{i+1,j}\right\}=0\ \text{(오른쪽 아래)}$$

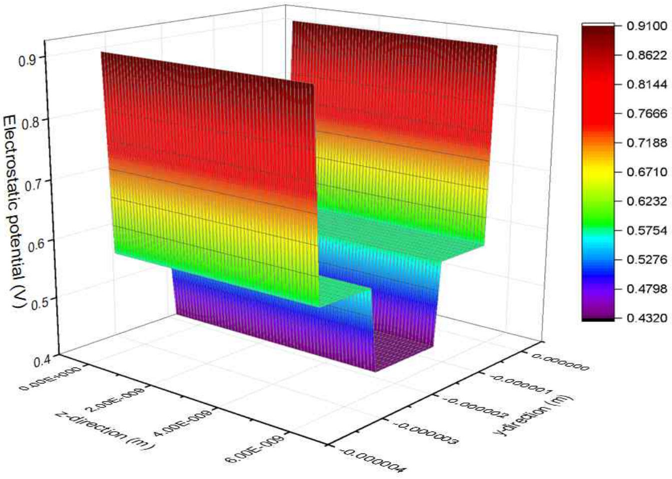
Also, for boundary condition between oxide layer and silicon layer,

$$\varepsilon_1\frac{\psi_{i,j}-\psi_{i-1,j}}{\Delta z}=\varepsilon_2\frac{\psi_{i+1,j}-\psi_{i,j}}{\Delta z}$$

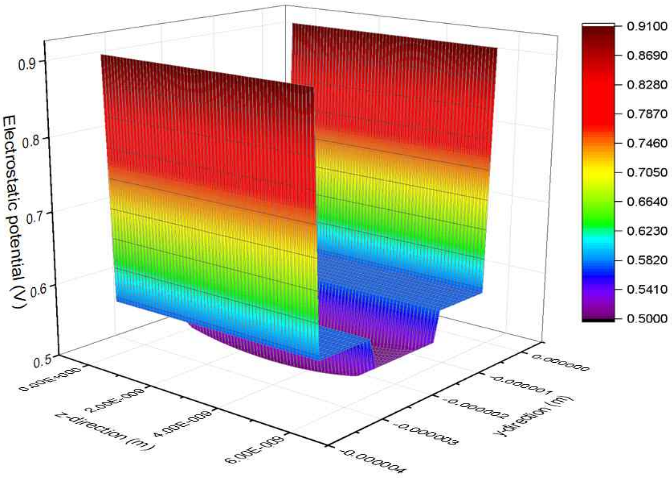
=> $\varepsilon_1\psi_{i-1,j}+\varepsilon_2\psi_{i+1,j}-(\varepsilon_1+\varepsilon_2)\psi_{i,j}=0$

Solution Vg = 0.1V to 1.0V with Newton-Rapson method is below.

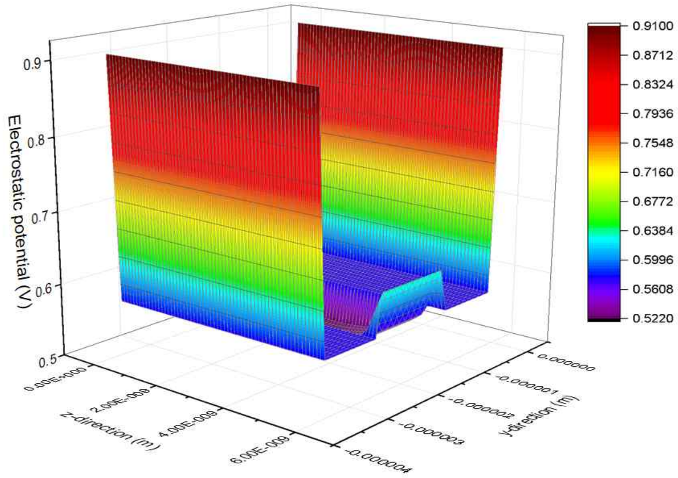
Vg = 0.1V


Electrostatic potential (V)
0.9
0.8
0.7
0.6
0.5
0.4
0.00E+000
2.00E-009
4.00E-009
6.00E-009
z-direction (m)
0.000000
-0.000001
-0.000002
-0.000003
-0.000004
y-direction (m)
0.9100
0.8622
0.8144
0.7666
0.7188
0.6710
0.6232
0.5754
0.5276
0.4798
0.4320

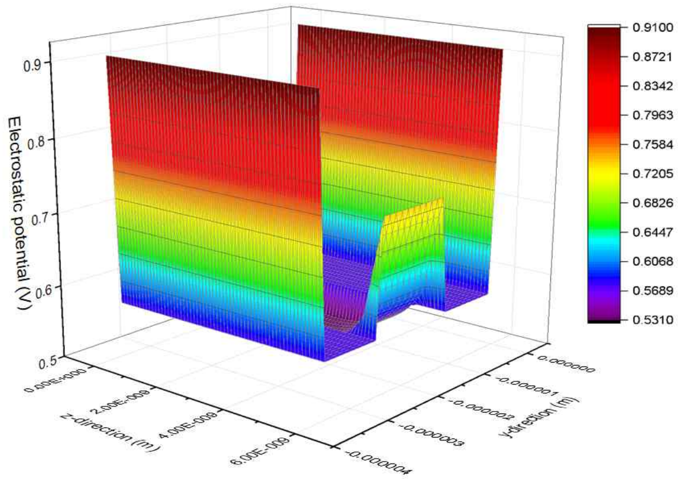
Vg = 0.2V


Electrostatic potential (V)
0.9
0.8
0.7
0.6
0.5
0.00E+000
2.00E-009
4.00E-009
6.00E-009
z-direction (m)
0.000000
-0.000001
-0.000002
-0.000003
-0.000004
y-direction (m)
0.9100
0.8690
0.8280
0.7870
0.7460
0.7050
0.6640
0.6230
0.5820
0.5410
0.5000

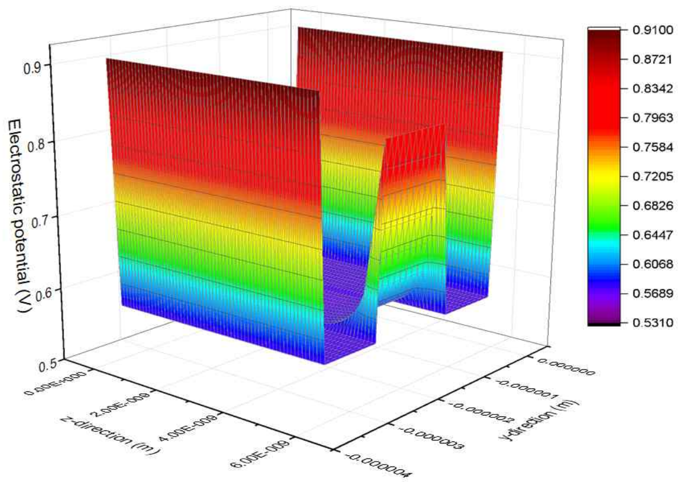
Vg = 0.3V



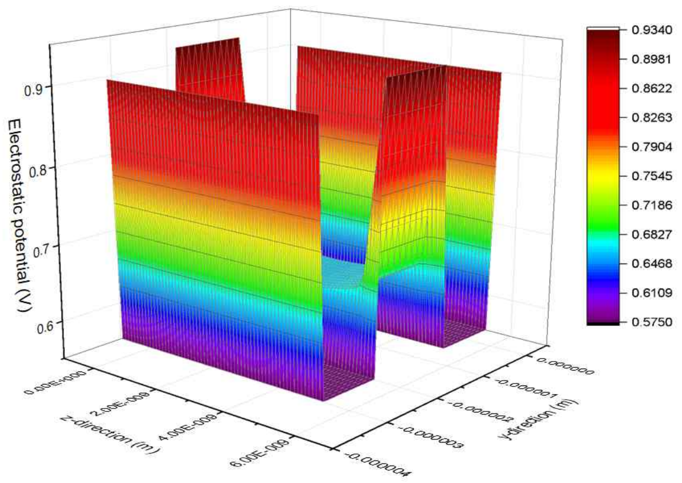
Vg = 0.4V



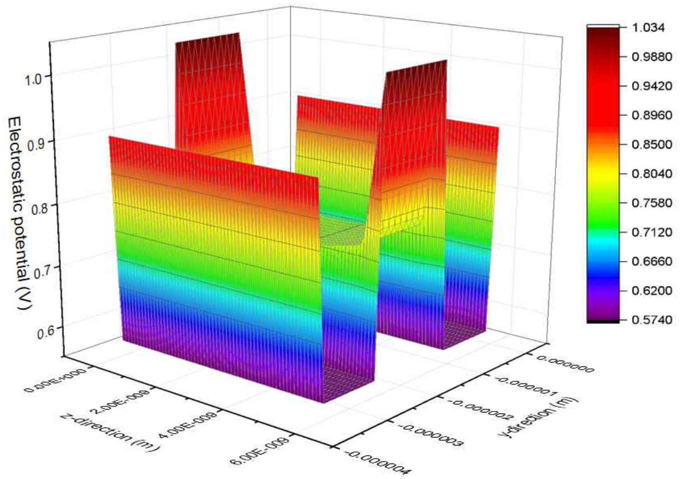
Vg = 0.5V



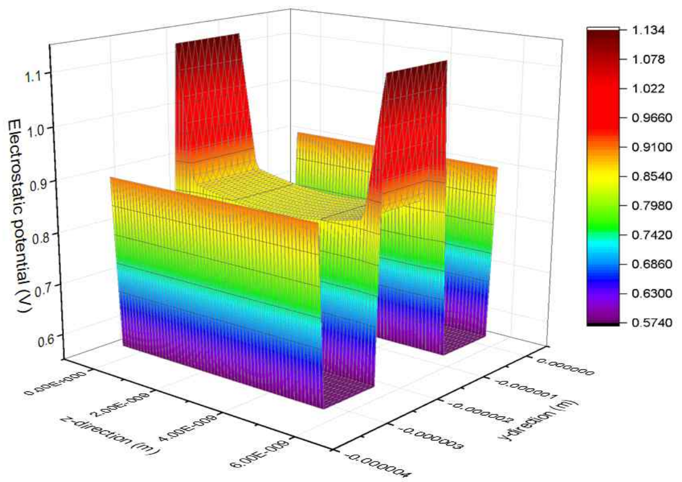
Vg = 0.6V



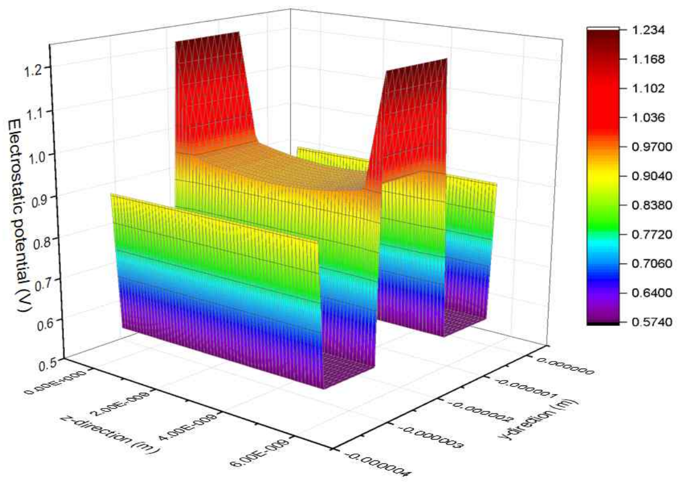
Vg = 0.7V



Vg = 0.8V

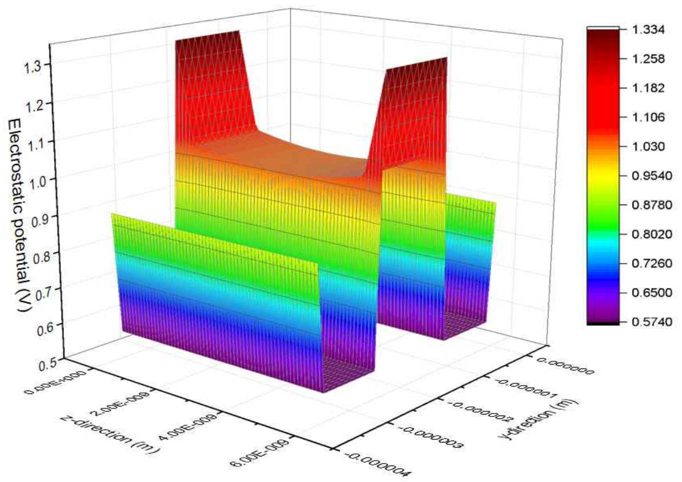


Vg = 0.9V



Electrostatic potential (V)
z-direction (m)
y-direction (m)
1.234
1.168
1.102
1.036
0.9700
0.9040
0.8380
0.7720
0.7060
0.6400
0.5740

Vg = 1.0V



Electrostatic potential (V)
z-direction (m)
y-direction (m)
1.334
1.258
1.182
1.106
1.030
0.9540
0.8780
0.8020
0.7260
0.6500
0.5740

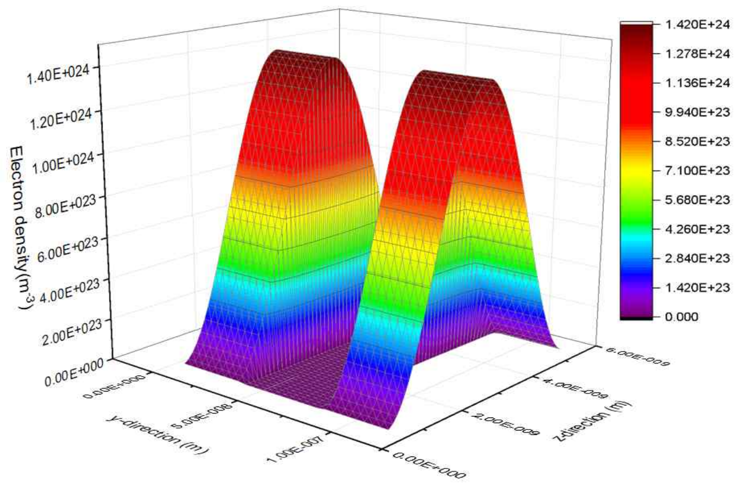
2. Step 2 (죄송합니다. 이 부분은 생략하겠습니다. Step3에 필요한 electrostatic potential은 Non-linear Poisson Solver with N-R method : Step1으로 대체하겠습니다.)

3. Step 3

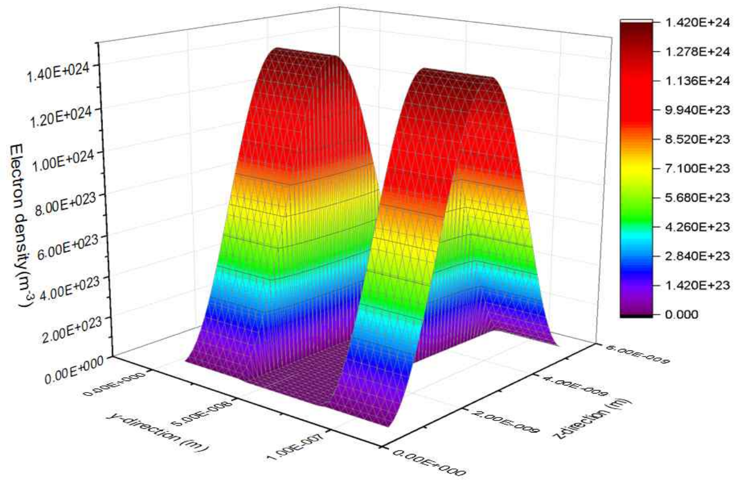
We assume that Lx = 100nm, Ly = 120nm, then we calculate the electron density except both end of y-direction with Schrodinger Solver.

1) Vg = 0.1V, Vd = 0.1V

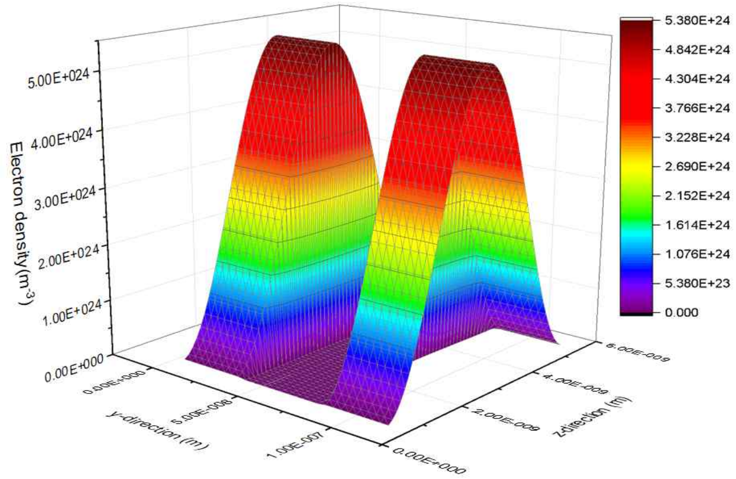
- x-valley (mx = 0.19m0)



- y-valley (my = 0.19m0)

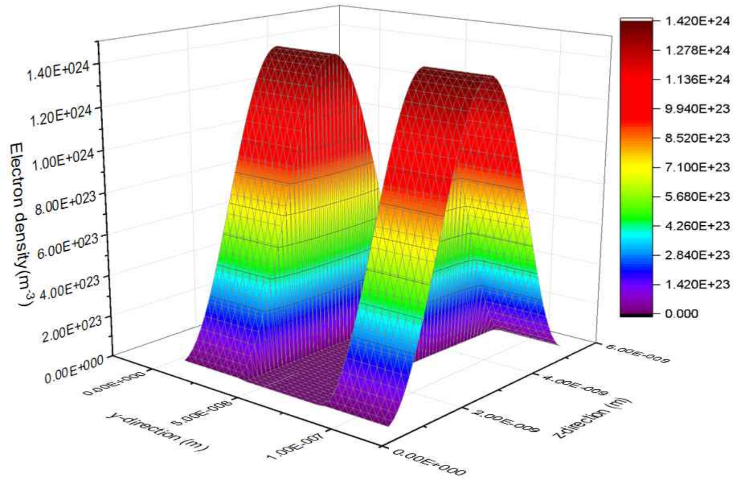


- z-valley (mz = 0.19m0)

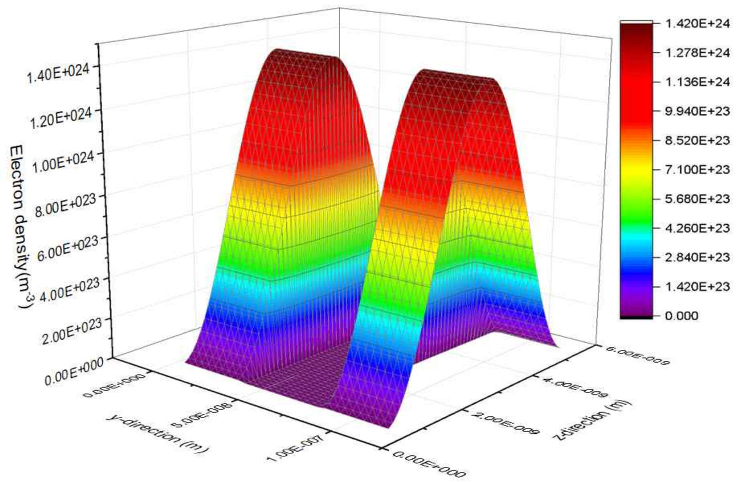


2) Vg = 0.1V, Vd = 0.5V

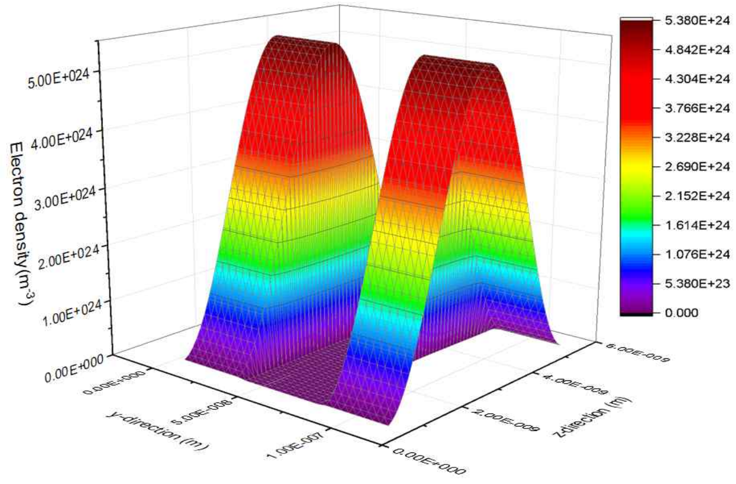
- x-valley



- y-valley

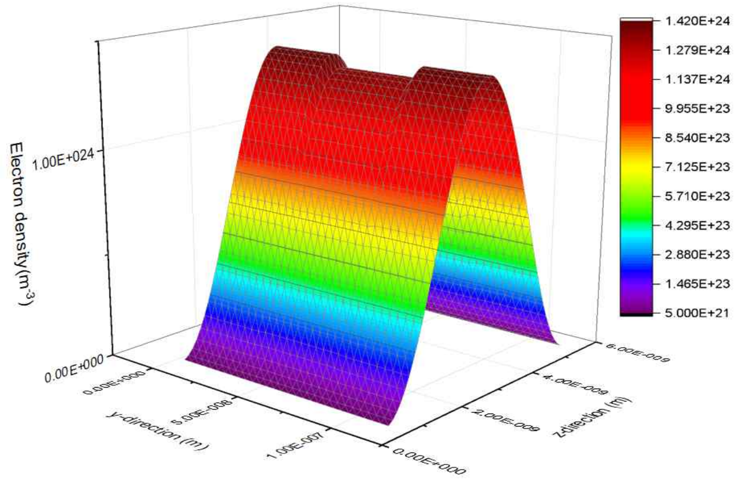


- z-valley

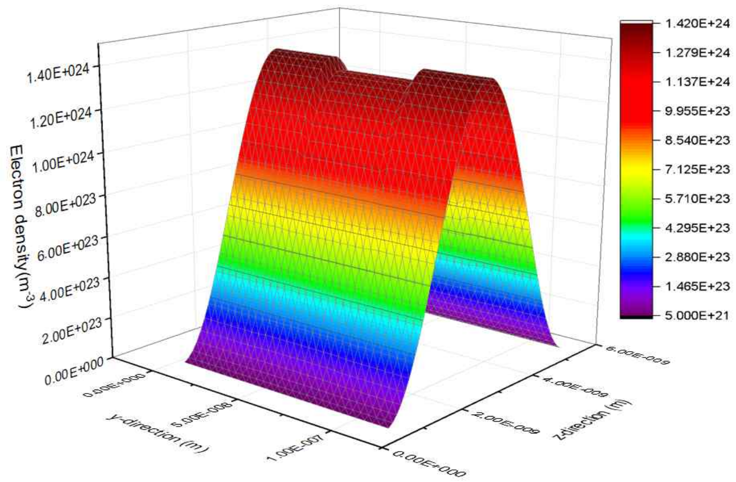


3) Vg = 0.5V, Vd = 0.1V

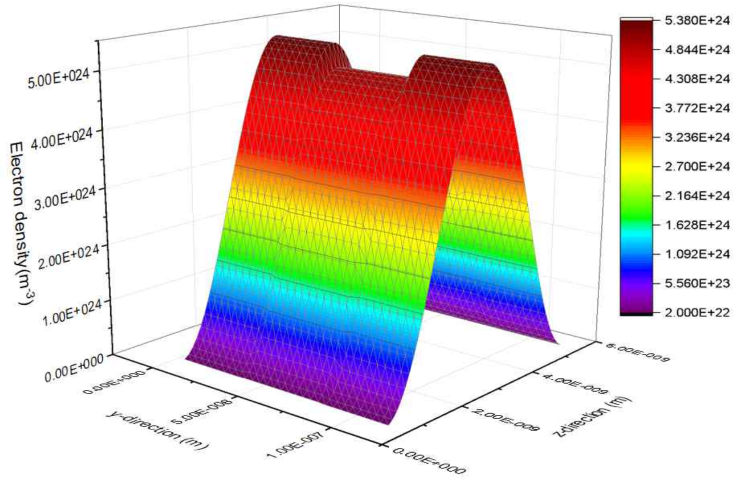
- x-valley



- y-valley

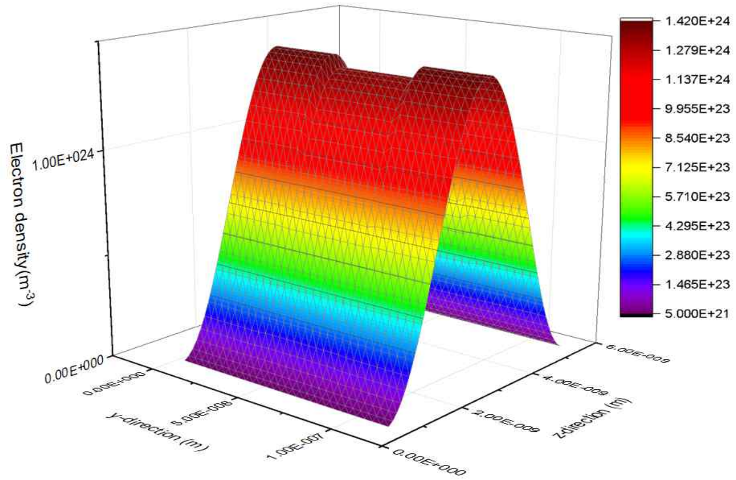


- z-valley

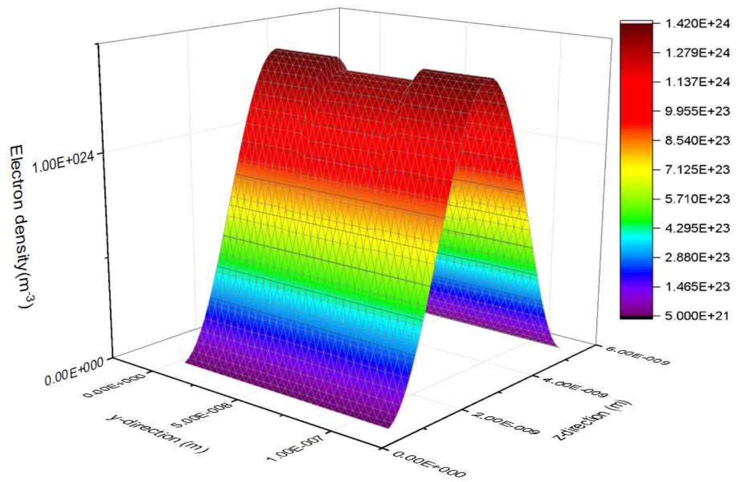


4) Vg = 0.5V, Vd = 0.5V

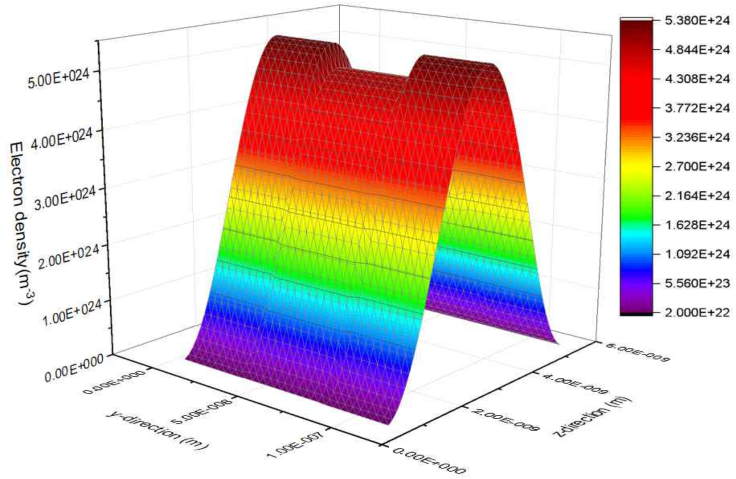
- x-valley



- y-valley



- z-valley



4. Step 4.

We assume that H = 2.0eV,

(f0에 대한 code와 raw data는 만들었으나, 이에 대한 plot과 I값을 구하지 못했습니다.)