Problem #1

Oxide	Gate(Workfunction = 4.3eV)	
Source(1e20/cm³)	Interface2 Channel(intrinsic) Interface1	Drain(1e20/cm³)
Oxide	Gate(Workfunction - 4.3eV)	

10번 과제에서의 Poisson equation 부분

Red circle: dirichlet boundary condition.

Gate : $res = \phi_{i,j} - 0.33374 - V_g$

Drain: $\operatorname{res} = \phi_{i,j} - \phi_0 - V_d$ Source: $\operatorname{res} = \phi_{i,j} - \phi_0$, $\phi_0 = V_T \sinh^{-1}\left(\frac{N_d}{2n_i}\right)$

Blue line: neaumann boundary condition.

 $\text{Bottom} \ : \ \operatorname{res} = \epsilon_{\operatorname{ox}} \left(\phi_{i,j+1} \tfrac{\Delta x}{\Delta y} + 0.5 \phi_{i+1,j} \tfrac{\Delta y}{\Delta x} + 0.5 \phi_{i-1,j} \tfrac{\Delta y}{\Delta x} - \phi_{i,j} (\tfrac{\Delta x}{\Delta y} + \tfrac{\Delta y}{\Delta x}) \right)$

 $\text{Top: res} = \epsilon_{\text{ox}} \Big(\phi_{i,j-1} \tfrac{\Delta x}{\Delta y} + 0.5 \phi_{i+1,j} \tfrac{\Delta y}{\Delta x} + 0.5 \phi_{i-1,j} \tfrac{\Delta y}{\Delta x} - \phi_{i,j} (\tfrac{\Delta x}{\Delta y} + \tfrac{\Delta y}{\Delta x}) \Big)$

 $\mbox{Right : res} = \epsilon_{\mbox{\scriptsize ox}} \Big(0.5 \phi_{i,j+1} \frac{\Delta x}{\Delta y} + 0.5 \phi_{i,j-1} \frac{\Delta x}{\Delta y} + \phi_{i-1,j} \frac{\Delta y}{\Delta x} - \phi_{i,j} (\frac{\Delta x}{\Delta y} + \frac{\Delta y}{\Delta x}) \Big)$

 $\mathsf{Left} \ : \ \mathsf{res} = \epsilon_{\mathsf{ox}} \Big(0.5 \phi_{i,j+1} \tfrac{\Delta x}{\Delta y} + 0.5 \phi_{i,j-1} \tfrac{\Delta x}{\Delta y} + \phi_{i+1,j} \tfrac{\Delta y}{\Delta x} - \phi_{i,j} (\tfrac{\Delta x}{\Delta y} + \tfrac{\Delta y}{\Delta x}) \Big)$

Orange line: Si-Oxide interface.

 $Interface 1 : res = \epsilon_{si} \left(\phi_{i,j+1} - \phi_{i,j}\right) \frac{\Delta x}{\Delta y} + \epsilon_{ox} \left(\phi_{i,j-1} - \phi_{i,j}\right) \frac{\Delta x}{\Delta y} + 0.5 (\epsilon_{si} + \epsilon_{ox}) \left(\phi_{i+1,j} + \phi_{i-1,j} - 2\phi_{i,j}\right) \frac{\Delta y}{\Delta x} + 0.5 \Delta x \Delta y q \rho(i,j)$

 $\label{eq:interface2} \text{Interface2} \ : \ \text{res} = \epsilon_{\text{si}} \big(\phi_{i,j-1} - \phi_{i,j} \ \big) \frac{\Delta x}{\Delta y} + \epsilon_{\text{ox}} \big(\phi_{i,j+1} - \phi_{i,j} \ \big) \frac{\Delta x}{\Delta y} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i-1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 \Delta x \Delta y q \rho(i,j) \big) \\ = \frac{\Delta x}{\Delta y} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i-1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 \Delta x \Delta y q \rho(i,j) \big) \\ = \frac{\Delta x}{\Delta y} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i-1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 \Delta x \Delta y q \rho(i,j) \big) \\ = \frac{\Delta x}{\Delta y} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i-1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 \Delta x \Delta y q \rho(i,j) \big) \\ = \frac{\Delta x}{\Delta y} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i-1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 \Delta x \Delta y q \rho(i,j) \big) \\ = \frac{\Delta x}{\Delta y} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 \Delta x \Delta y q \rho(i,j) \big) \\ = \frac{\Delta x}{\Delta y} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i,j}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{si}} + \epsilon_{\text{ox}}) \big(\phi_{i+1,j} + \phi_{i+1,j} - 2\phi_{i+1,j}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{ox}} + 2\phi_{\text{ox}}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{ox}} + 2\phi_{\text{ox}}\big) \frac{\Delta y}{\Delta x} + 0.5 (\epsilon_{\text{ox}} + 2\phi_{\text{ox}}\big) \frac{\Delta y}{\Delta x} + 0.5$

Oxide

$$\text{res} = \epsilon_{\text{ox}} \left(\phi_{i,j+1} \frac{\Delta x}{\Delta y} + \phi_{i,j-1} \frac{\Delta x}{\Delta y} + \phi_{i+1,j} \frac{\Delta y}{\Delta x} + \phi_{i-1,j} \frac{\Delta y}{\Delta x} - 2\phi_{i,j} (\frac{\Delta x}{\Delta y} + \frac{\Delta y}{\Delta x}) \right)$$

Silicon

$$\operatorname{res} = \epsilon_{\operatorname{si}} \left(\phi_{i,j+1} \frac{\Delta x}{\Delta y} + \phi_{i,j-1} \frac{\Delta x}{\Delta y} + \phi_{i+1,j} \frac{\Delta y}{\Delta x} + \phi_{i-1,j} \frac{\Delta y}{\Delta x} - 2\phi_{i,j} \left(\frac{\Delta x}{\Delta y} + \frac{\Delta y}{\Delta x} \right) \right) + \Delta x \Delta y q \rho(i,j), \qquad \rho = N_d - n + p$$

이번 과제는 지난 10번 과제에서 했던 equilibrium에서 풀었던 2D Poisson equation을 확장시키는 과제로, drain에 bias를 가해서 전류를 계산하는 과제이다. Electrostatic potential, electron, hole 3개의 변수에 대해서 계산이 필요하므로, 3N*3N의 Jacobian과 3N*1의 residue가 필요하다. Residue는 poisson equation, electron의 scharffeter gummel, hole의 scharffeter gummel을 가진다. Poisson equation의 경우는 이전 과제와 같으며, 다만 source와 drain contact에서 source는 $\phi_0 = V_T \sinh^{-1}\left(\frac{N_d}{2n_t}\right)$ 를 가지고, drain은 $\sinh^{-1}\left(\frac{N_d}{2n_t}\right) + V_d$ 의 값을 가지게 된다.

Scharffeter gummel은 electron의 경우,

$$\begin{split} \operatorname{res} &= n_{i+1} B \left(\frac{\phi_{i+1} - \phi_i}{V_T} \right) - n_i B \left(\frac{\phi_i - \phi_{i+1}}{V_T} \right) - n_i B \left(\frac{\phi_i - \phi_{i-1}}{V_T} \right) + n_{i-1} B \left(\frac{\phi_{i-1} - \phi_i}{V_T} \right) \\ & \frac{\partial \operatorname{res}}{\partial n_{i+1}} = B \left(\frac{\phi_{i+1} - \phi_i}{V_T} \right), \qquad \frac{\partial \operatorname{res}}{\partial n_i} = B \left(\frac{\phi_i - \phi_{i+1}}{V_T} \right) - n_i B \left(\frac{\phi_i - \phi_{i-1}}{V_T} \right), \qquad \frac{\partial \operatorname{res}}{\partial n_{i-1}} = B \left(\frac{\phi_{i-1} - \phi_i}{V_T} \right) \\ & \frac{\partial \operatorname{res}}{\partial \phi_{i+1}} = n_{i+1} \frac{\partial B}{\partial \phi_{i+1}} - n_i \frac{\partial B}{\partial \phi_{i+1}}, \qquad \frac{\partial \operatorname{res}}{\partial \phi_i} = n_{i+1} \frac{\partial B}{\partial \phi_i} - n_i \frac{\partial B}{\partial \phi_i} - n_i \frac{\partial B}{\partial \phi_i} + n_{i-1} \frac{\partial B}{\partial \phi_i}, \qquad \frac{\partial \operatorname{res}}{\partial \phi_{i-1}} = -n_i \frac{\partial B}{\partial \phi_{i-1}} + n_{i-1} \frac{\partial B}{\partial \phi_{i-1}} - n_i \frac{\partial B}{\partial$$

위의 식으로 residue와 jacobian을 정리할 수 있다. Bernoulli function B(x)는 x가 0 근처일 때, 근사를 시켜주어야 한다. Hole 또한,

$$\begin{split} \operatorname{res} &= p_{i+1} B\left(\frac{\phi_i - \phi_{i+1}}{V_T}\right) - p_i B\left(\frac{\phi_{i+1} - \phi_i}{V_T}\right) - p_i B\left(\frac{\phi_{i-1} - \phi_i}{V_T}\right) + p_{i-1} B\left(\frac{\phi_i - \phi_{i-1}}{V_T}\right) \\ &\frac{\partial \operatorname{res}}{\partial p_{i+1}} = B\left(\frac{\phi_i - \phi_{i+1}}{V_T}\right), \quad \frac{\partial \operatorname{res}}{\partial \mathbf{p}_{\mathbf{i}}} = B\left(\frac{\phi_{i+1} - \phi_i}{V_T}\right) - n_i B\left(\frac{\phi_{i-1} - \phi_i}{V_T}\right), \quad \frac{\partial \operatorname{res}}{\partial p_{i-1}} = B\left(\frac{\phi_i - \phi_{i-1}}{V_T}\right) \\ &\frac{\partial \operatorname{res}}{\partial \phi_{\mathbf{i}+1}} = p_{i+1} \frac{\partial \mathbf{B}}{\partial \phi_{\mathbf{i}+1}} - p_i \frac{\partial \mathbf{B}}{\partial \phi_{\mathbf{i}+1}}, \quad \frac{\partial \operatorname{res}}{\partial \phi_{\mathbf{i}}} = p_{i+1} \frac{\partial \mathbf{B}}{\partial \phi_{\mathbf{i}}} - p_i \frac{\partial \mathbf{B}}{\partial \phi_{\mathbf{i}}} + p_{i-1} \frac{\partial \mathbf{B}}{\partial \phi_{\mathbf{i}}}, \quad \frac{\partial \operatorname{res}}{\partial \phi_{\mathbf{i}+1}} = -p_i \frac{\partial \mathbf{B}}{\partial \phi_{\mathbf{i}+1}} + p_{i-1} \frac{\partial \mathbf{B}}{\partial \phi_{\mathbf{i}+1}} - p_i \frac{\partial \mathbf{B}}{\partial \phi_{\mathbf{i}+1}} + p_{i-1} \frac{\partial \mathbf{B}}{\partial \phi_{\mathbf{i}+1}} - p_i \frac{\partial \mathbf{B}}{\partial \phi_{\mathbf{i}+1}} -$$

위와 같이 정리된다. 여기서, $\frac{\partial B}{\partial \phi_{1+1}}$ 와 같은 potential로 bernoulli function을 미분하는 항들에서 B는 같은 값은 아니고, residue 식에 있는 각각의 bernoulli function들로 다른 값들이다. 추가로 oxide 영역에서는 electron과 hole이 없다고 풀게 되므로 jacobian과 residue가 모두 0이 된다. 그러면 update의 값에 NaN이 발생하게 된다. 이를 막기 위해, 자기 자신으로 미분하는 jacobian 부분을 1로 설정하였다.

위의 residue와 jacobian을 가지고 계산이 아래와 같이 진행된다.

먼저, 2D Poisson equation만을 target gate voltage 까지 증가시켜서 풀어주어 초기의 electrostic potential을 얻는다. 그리고 얻어진 electrostatic potential을 이용하여서 초기의 electron과 hole density를 얻어낸다. 얻어진 potential과 density를 가지고 poisson equation과 scharffeter gummel을 coupling 하여서 풀게 된다. 이 때, drain voltage를 증가시키면서 계산을 하고, 얻어진 전자 농도와 electrostatic potential을 이용하여서 terminal current를 계산하면 된다. Hole의 농도는 매우낮으므로, current 계산에는 이용하지 않았다. 계산된 결과는 아래와 같다.

