Lecture4

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Source-free case

- Once again, the "source-free" Poisson equation is the Laplace equation.
  - Since we are (incorrectly) calling the $\nabla \cdot \mathbf{D} = \rho(\mathbf{r})$ as the Poisson equation, the source-free case (no net charge, $\rho(\mathbf{r}) = 0$) is not reduced to the Laplace equation.
  - Instead, (under the electrostatic approximation)
$$\nabla \cdot [\epsilon(\mathbf{r}) \nabla \phi(\mathbf{r})] = 0$$
  - In the 1D strcture,
$$\frac{d}{dx}\left[\epsilon(x)\frac{d}{dx}\phi(x)\right] = 0$$

Comparison

- Laplace equation

$$\frac{d}{dx}\left[\frac{d}{dx}\phi(x)\right] = 0$$

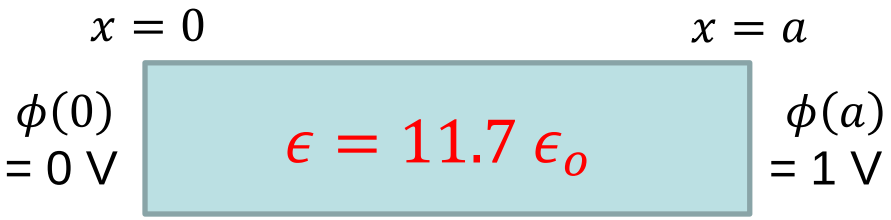
- (Generalized) Poisson equation with the source-free condition

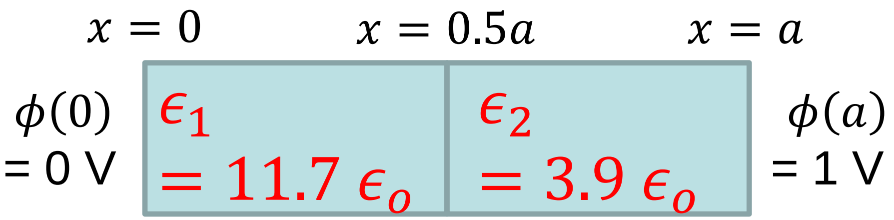
$$\frac{d}{dx}\left[\epsilon(x)\frac{d}{dx}\phi(x)\right] = 0$$

  – They look quite similar. However, they are not.

Two capacitors

- Capacitor made of a single dielectric layer
  - Its thickness is 5 nm. Its relative permittivity is 11.7.
- Capacitor made of two dielectric layers
  - Each of them is 2.5 nm thick. Their relative permittivity is 11.7 and 3.9, respectively.





$$\phi(x) = \frac{x}{a}$$

$$\phi(x) = \frac{x}{2a} \qquad \phi(x) = \frac{3x}{2a} - \frac{1}{2}$$

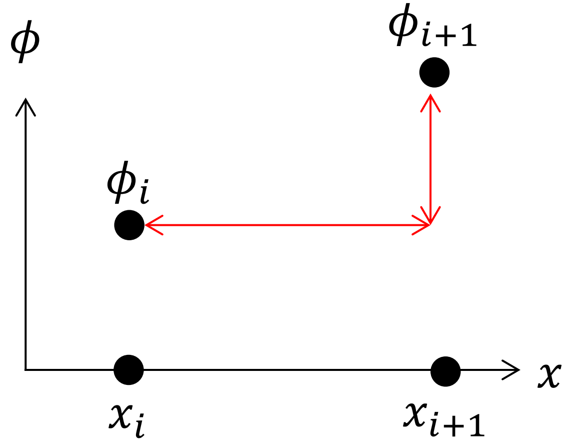
Discretization

- How to treat the position-dependent permittivity
  - For $2 \leq i \leq N-1$, the integration from $x_{i-0.5}$ to $x_{i+0.5}$ yields

$$\epsilon(x_{i+0.5}) \left.\frac{d\phi}{dx}\right|_{x_{i+0.5}} - \epsilon(x_{i-0.5}) \left.\frac{d\phi}{dx}\right|_{x_{i-0.5}} = 0$$

  - The first derivative is approximated by

$$\left.\frac{d\phi}{dx}\right|_{x_{i+0.5}} \approx \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i}$$



$N = 5$ example

- At x_3, two layers ($\epsilon_1 = 11.7\ \epsilon_0$ and $\epsilon_2 = 3.9\ \epsilon_0$) meet.
  - It is simply given by

$$Ax = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ \epsilon_1 & -2\epsilon_1 & \epsilon_1 & 0 & 0 \\ 0 & \epsilon_1 & -\epsilon_2 - \epsilon_1 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_2 & -2\epsilon_2 & \epsilon_2 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \phi(x_1) \\ \phi(x_2) \\ \phi(x_3) \\ \phi(x_4) \\ \phi(x_5) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = b$$

  - Note that the third row has different coefficients.
  - When $\epsilon_1 = \epsilon_2$, it is reduced to the Laplace equation.

MATLAB example

- Step-by-step procedure
  - First, set the matrix, A.

```
A = zeros(5,5);
A(1,1) = 1.0;
A(2,1) = 11.7; A(2,2) = -23.4; A(2,3) = 11.7;
A(3,2) = 11.7; A(3,3) = -15.6; A(3,4) = 3.9;
A(4,3) = 3.9; A(4,4) = -7.8; A(4,5) = 3.9;
A(5,5) = 1.0;
```

  - Next , set the vector, b.

```
b = zeros(5,1); b(5,1) = 1.0;
```

  - Finally, get the solution vector, x.

```
x = A \ b
```

Homework#3

- Due: AM08:00, September 17
- Problem#1
  - In your own research work, you may consider a heterostructure.
  - Specify your own heterostructure. Specifiy the thickness and the relative permittivity of each layer. (Ignore mobile carriers.)
  - Then, calculate the capacitance per area. (F/cm^2)
  - Compare your result with the analytic expression.

  - (When you have no idea about the heterostructure, please select any one available to you.)

Poisson equation

- Fixed-source case

$$\frac{d}{dx}\left[\epsilon(x)\frac{d}{dx}\phi(x)\right] = -\rho(x)$$

  - The net charge density, $\rho(x)$, is given by

$$\rho(x) = qp(x) - qn(x) + qN_{dop}^{+}(x)$$

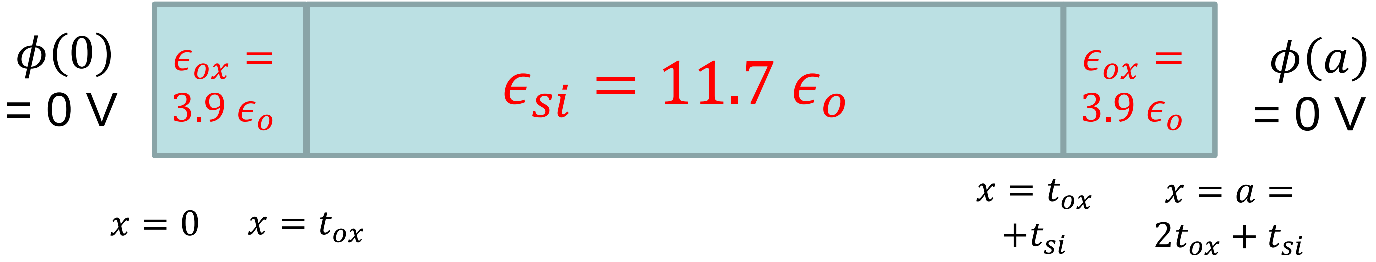
$p(x)$: Hole density, $n(x)$: Electron density, $N_{dop}^{+}(x)$: Net doping density

  - Calculating $p(x)$ and $n(x)$ is not a trivial task.
  - Let us assume that all mobile carriers are depleted.

$$\frac{d}{dx}\left[\epsilon(x)\frac{d}{dx}\phi(x)\right] = -qN_{dop}^{+}(x)$$

Double-gate MOS

- Real engineering problem
  - A silicon layer (whose thickness is t_{si}) surrounded by two oxide layers (whose thickness is t_{ox})

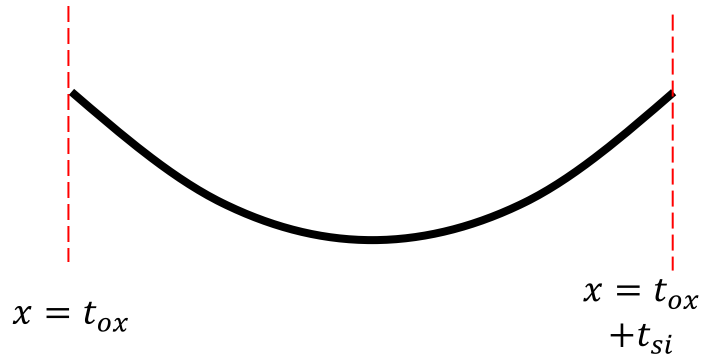


  - The silicon layer is doped with p-type dopants. The doping density is N_{acc}. Since the p-type dopant provides a hole, the dopant itself is negatively charged. $N_{dop}^{+} = -N_{acc}$.

Analytic solution (1)

- Qualitative analysis
  - Due to the mirror symmetry, the electrostatic potential is also mirror symmetric.
  - Inside the oxide layer, the electrostatic potential must be linear.
  - Inside the silicon layer, the Poisson equation reads ($N_{acc} > 0$)

$$\frac{d}{dx}\left[\frac{d}{dx}\phi(x)\right] = \frac{qN_{acc}}{\epsilon_{si}}$$



Analytic solution (2)

- Solution
  - Integrating the Poisson equation inside the silicon layer,

$$\left.\frac{d\phi}{dx}\right|_{x=t_{ox}+t_{si}} - \left.\frac{d\phi}{dx}\right|_{x=t_{ox}} = \frac{qN_{acc}}{\epsilon_{si}} t_{si}$$

  - We know that

$$\left.\frac{d\phi}{dx}\right|_{x=t_{ox}} = \frac{\phi(t_{ox})}{3t_{ox}}$$

  - The electrostatic potential at $x = t_{ox}$ is given by

$$\phi(t_{ox}) = -\frac{3t_{ox}qN_{acc}t_{si}}{2\epsilon_{si}}$$

Scaling

- A suitable form
  - The original form

$$\frac{d}{dx}\left[\epsilon(x)\frac{d}{dx}\phi(x)\right] = qN_{acc}(x)$$

  - However, the values of $\epsilon(x)$ and dx in the SI unit is very small.
  - Equivalently, we will use the following form:

$$(\Delta x)\frac{d}{dx}\left[\frac{\epsilon(x)}{\epsilon_0}\frac{d}{dx}\phi(x)\right] = (\Delta x)\frac{qN_{acc}(x)}{\epsilon_0}$$

  - The discretized version at $x = x_i$ is

$$\frac{\epsilon(x_{i+0.5})}{\epsilon_0}\phi_{i+1} - \frac{\epsilon(x_{i+0.5}) + \epsilon(x_{i-0.5})}{\epsilon_0}\phi_i + \frac{\epsilon(x_{i-0.5})}{\epsilon_0}\phi_{i-1} = (\Delta x)^2\frac{qN_{acc}(x_i)}{\epsilon_0}$$

MATLAB example (1)

- Step-by-step procedure
  - First, set up the structure.

```
q = 1.602192e-19; % Elementary charge, C
eps0 = 8.854187817e-12; % Vacuum permittivity, F/m
Deltax = 0.1e-9; % 0.1 nm spacing
N = 61; % 6 nm thick
interface1 = 6; % At x=0.5 nm
interface2 = 56; % At x=5.5 nm
eps_si = 11.7; eps_ox = 3.9; % Relative permittivity
Nacc = 1e24; % 1e18 /cm^3
```

MATLAB example (2)

- Step-by-step procedure (continued)
  - Next, set the matrix, A. (Five cases)

```
A = zeros(N,N);
A(1,1) = 1.0;
for ii=2:N-1
   if     (ii< interface1) A(ii,ii-1) = eps_ox; A(ii,ii) = -2*eps_ox;      A(ii,ii+1) = eps_ox;
   elseif (ii==interface1) A(ii,ii-1) = eps_ox; A(ii,ii) = -eps_ox-eps_si; A(ii,ii+1) = eps_si;
   elseif (ii< interface2) A(ii,ii-1) = eps_si; A(ii,ii) = -2*eps_si;      A(ii,ii+1) = eps_si;
   elseif (ii==interface2) A(ii,ii-1) = eps_si; A(ii,ii) = -eps_si-eps_ox; A(ii,ii+1) = eps_ox;
   elseif (ii> interface2) A(ii,ii-1) = eps_ox; A(ii,ii) = -2*eps_ox;      A(ii,ii+1) = eps_ox;
   end
end
A(N,N) = 1.0;
```

MATLAB example (3)

- The vector, b, contains the doping effect.

```
b = zeros(N,1);
for ii=interface1:interface2
   if     (ii==interface1) b(ii,1) = Deltax*Deltax*q*Nacc/eps0*0.5;
   elseif (ii==interface2) b(ii,1) = Deltax*Deltax*q*Nacc/eps0*0.5;
   else                    b(ii,1) = Deltax*Deltax*q*Nacc/eps0;
   end
end
```