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.

$x = 0$ $x = a$

$\phi(0)$ = 0 V $\epsilon = 11.7\,\epsilon_o$ $\phi(a)$ = 1 V

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

$x = 0$ $x = 0.5a$ $x = a$

$\phi(0)$ = 0 V $\epsilon_1 = 11.7\,\epsilon_o$ $\epsilon_2 = 3.9\,\epsilon_o$ $\phi(a)$ = 1 V

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

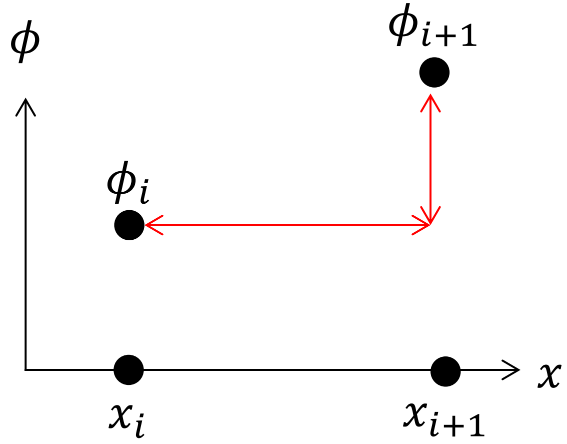
Discretization

- How to treat the position-dependent permittivity
  - For $2 \le i \le N-1$, 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.)