Computational Microelectronics L6 (Pre-recorded)

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1D source-free Poisson equation

A rare case

- MOS capacitor with a uniform doping concentration
  - An analytic expression is available.

$$\left(\left.\frac{d\phi}{dx}\right|_0\right)^2 = \frac{2k_BT}{\epsilon_{si}} n_{int}$$
$$\times\left[\exp\left(-\frac{q\phi_\infty}{k_BT}\right)\left\{\exp\left(-\frac{q\phi_s}{k_BT}\right) - 1 + \frac{q\phi_s}{k_BT}\right\} + \exp\left(\frac{q\phi_\infty}{k_BT}\right)\left\{\exp\left(\frac{q\phi_s}{k_BT}\right) - 1 - \frac{q\phi_s}{k_BT}\right\}\right]$$

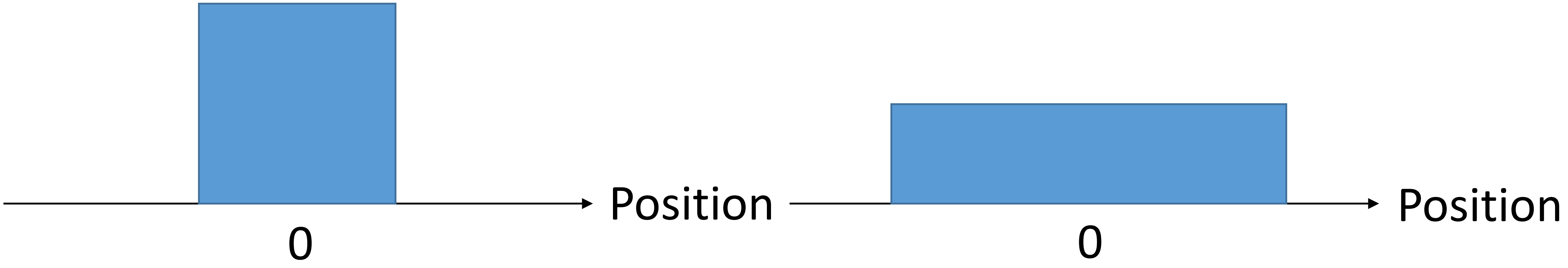
  - However, it is a rare case. We can make it much more difficult by introducing additional conditions.
  - We need a general way.

Integration

- The major step for simplification is integration.
  - For example, we perform

$$\int_{\phi_s}^{0}[\dots]d\bar{\phi}$$

  - Internal distribution of a quantity is expressed as a single scalar.



Simulation domain

- Assume the simulation domain of $[L_1, L_2]$.
  - We introduce a finite number of points,
  $$x_0(\equiv L_1), x_1, \ldots, x_{N-1}(\equiv L_2)$$
  - For a uniform grid,
  $$x_i = i \times \frac{L_2 - L_1}{N - 1} + L_1 = i \times \Delta x + L_1$$
  - Also, we introduce the electrostatic potential at those points,
  $$\phi(x_0), \phi(x_1), \ldots, \phi(x_{N-1})$$
  - Instead of finding out $\phi(x)$ everywhere, we try to find a solution vector, $[\phi(x_0)\ \phi(x_1)\ \ldots\ \phi(x_{N-1})]^T$, which satisfies an appropriate equation (or the boundary conditions) at those discretized points only.

Poisson equation

- Poisson equation
  - It is Gauss' law, $\nabla \cdot \mathbf{D}(\mathbf{r}) = \rho(\mathbf{r})$, written with the electrostatic assumption, $\mathbf{E}(\mathbf{r}) = -\nabla\phi$:
$$\nabla \cdot [\epsilon(\mathbf{r})\nabla\phi] = -\rho(\mathbf{r})$$
  - When the permittivity is a constant,
$$\nabla \cdot (\nabla\phi) = -\frac{\rho(\mathbf{r})}{\epsilon}$$
  - When there is no net charge,
$$\nabla \cdot (\nabla\phi) = 0$$
- We keep the position-dependent permittivity:
$$\nabla \cdot [\epsilon(\mathbf{r})\nabla\phi] = 0$$

Discretization of $\nabla \cdot [\epsilon(\mathbf{r})\nabla\phi]$

- 1D

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

  – Integration from $x_{i-0.5}$ to $x_{i+0.5}$

$$\int_{x_{i-0.5}}^{x_{i+0.5}} \frac{d}{dx}\left[\epsilon(x)\frac{d\phi}{dx}\right]dx = \epsilon(x_{i+0.5})\frac{d\phi}{dx}\bigg|_{x_{i+0.5}} - \epsilon(x_{i-0.5})\frac{d\phi}{dx}\bigg|_{x_{i-0.5}}$$

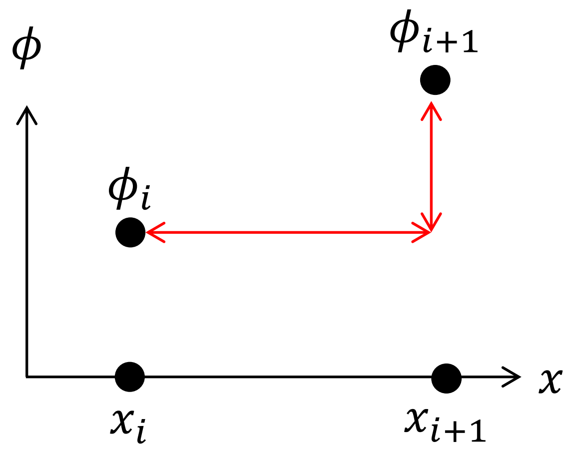
Discretization of ${d\phi}/{dx}$

- The first derivative is approximated by

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

  - Then, (integrated) $\frac{d}{dx}\left[\epsilon(x)\frac{d\phi}{dx}\right]$ becomes

$$\epsilon(x_{i+0.5})\frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} - \epsilon(x_{i-0.5})\frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}}$$



1D example

- Source-free Poisson equation
  - Consider a capacitor with two layers.
  - Each layer is 2.5-nm-thick.
  - The first layer (from 0 to 2.5 nm) has a relative permittivity of 11.7.
  - The second layer (from 2.5 nm to 5 nm) has a relative permittivity of 3.9.
  - $\phi(0)$ = 0 V and $\phi(5\ \mathrm{nm})$ = 1 V. Calculate the potential, ϕ.

Consider five points.

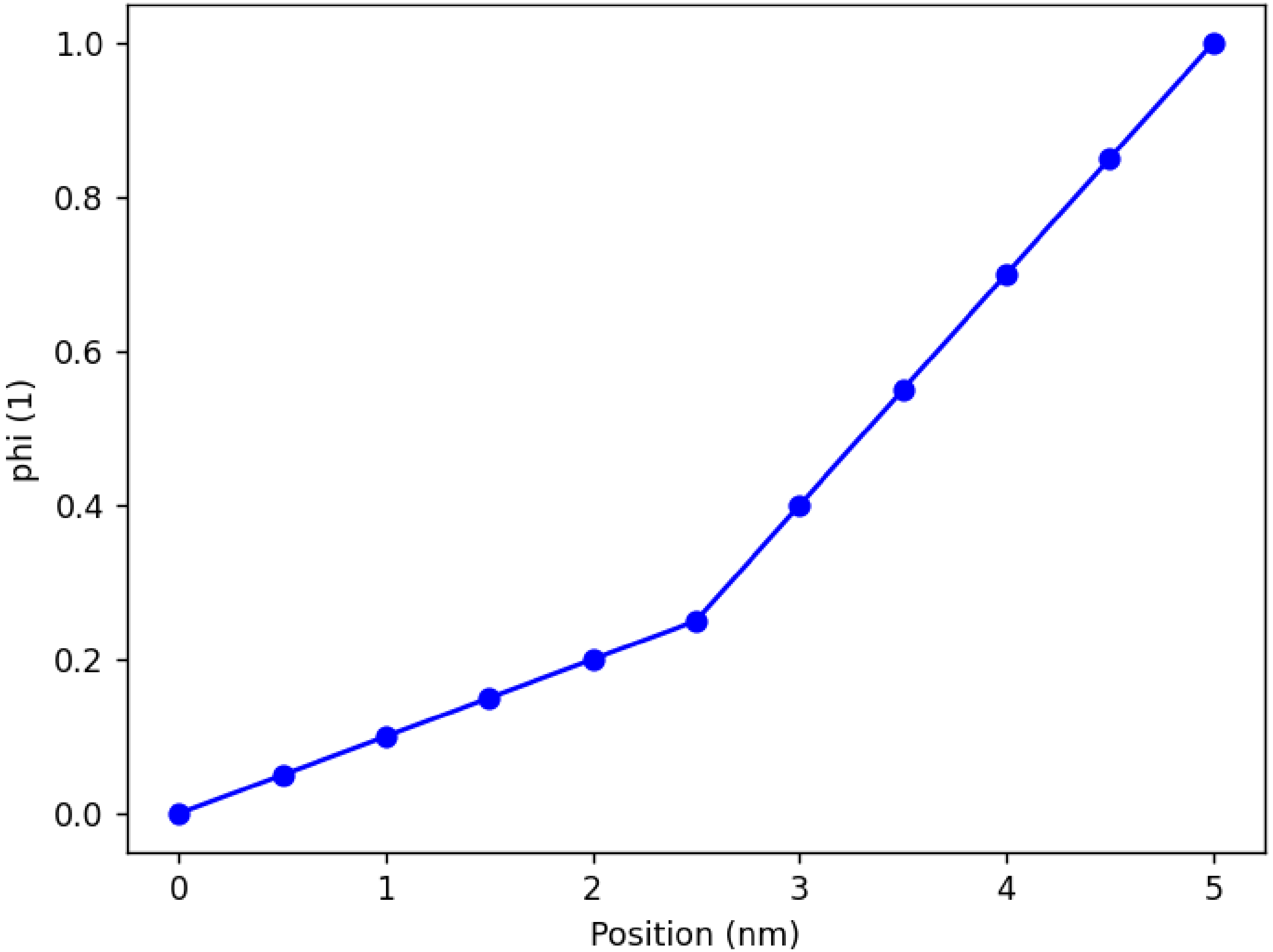
- At x_2 (the middle point), two layers ($\epsilon_1 = 11.7\,\epsilon_0$ and $\epsilon_2 = 3.9\,\epsilon_0$) meet.
  - Equations at x_1, x_2, and x_3 (together with boundary conditions at x_0 and x_4) are given by

$$\mathrm{Ax} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ \epsilon_1 & -2\epsilon_1 & \epsilon_1 & 0 & 0 \\ 0 & \epsilon_1 & -\epsilon_2 - \epsilon_1 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_2 & -2\epsilon_2 & \epsilon_2 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \phi(x_0) \\ \phi(x_1) \\ \phi(x_2) \\ \phi(x_3) \\ \phi(x_4) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \mathrm{b}$$

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

Its solution

- Potential, ϕ



Homework#6

- Due: AM08:00, October 8
- Problem#1
  - Draw the potential, ϕ, by solving the source-free Poisson equation under the following conditions:
  - The first layer (from -1.0 nm to 0 nm) has a relative permittivity of 3.9.
  - The second layer (from 0 nm to 2.5 nm) has a relative permittivity of 11.7.
  - ϕ at -1.0 nm is 1.7 V. ϕ at -2.5 nm is -0.5 V.

Thank you for your attention!