Computational Microelectronics
L7 (Pre-recorded)

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1D nonlinear Poisson equation

Poisson equation

- Source-free Poisson equation
  - When the net charge density vanishes, we have a special form of the Poisson equation:

$$\nabla \cdot [\epsilon(\mathbf{r})\nabla\phi] = 0$$

  - Now we want to keep the net charge density.

$$\nabla \cdot [\epsilon(\mathbf{r})\nabla\phi] = -\rho(\mathbf{r})$$

- Charges inside semiconductor

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

  - Hole density, $p(\mathbf{r})$
  - Electron density, $n(\mathbf{r})$
  - Doping density, $N_{dop}^{+}(\mathbf{r})$: Positive for donors and negative for acceptors

At equilibrium,

- We have special expressions for charge densities:
  - Hole density, $p(\mathbf{r}) = n_{int}(\mathbf{r}) \exp\left(-\frac{q\phi(\mathbf{r})}{k_B T}\right)$
  - Electron density, $n(\mathbf{r}) = n_{int}(\mathbf{r}) \exp\left(\frac{q\phi(\mathbf{r})}{k_B T}\right)$
  - By adopting these expressions, we have the nonlinear Poisson equation:

$$\nabla \cdot [\epsilon(\mathbf{r})\nabla\phi] + qn_{int}(\mathbf{r}) \exp\left(-\frac{\phi(\mathbf{r})}{V_T}\right) - qn_{int}(\mathbf{r}) \exp\left(\frac{\phi(\mathbf{r})}{V_T}\right) + qN_{dop}^{+}(\mathbf{r}) = 0$$

Discretization

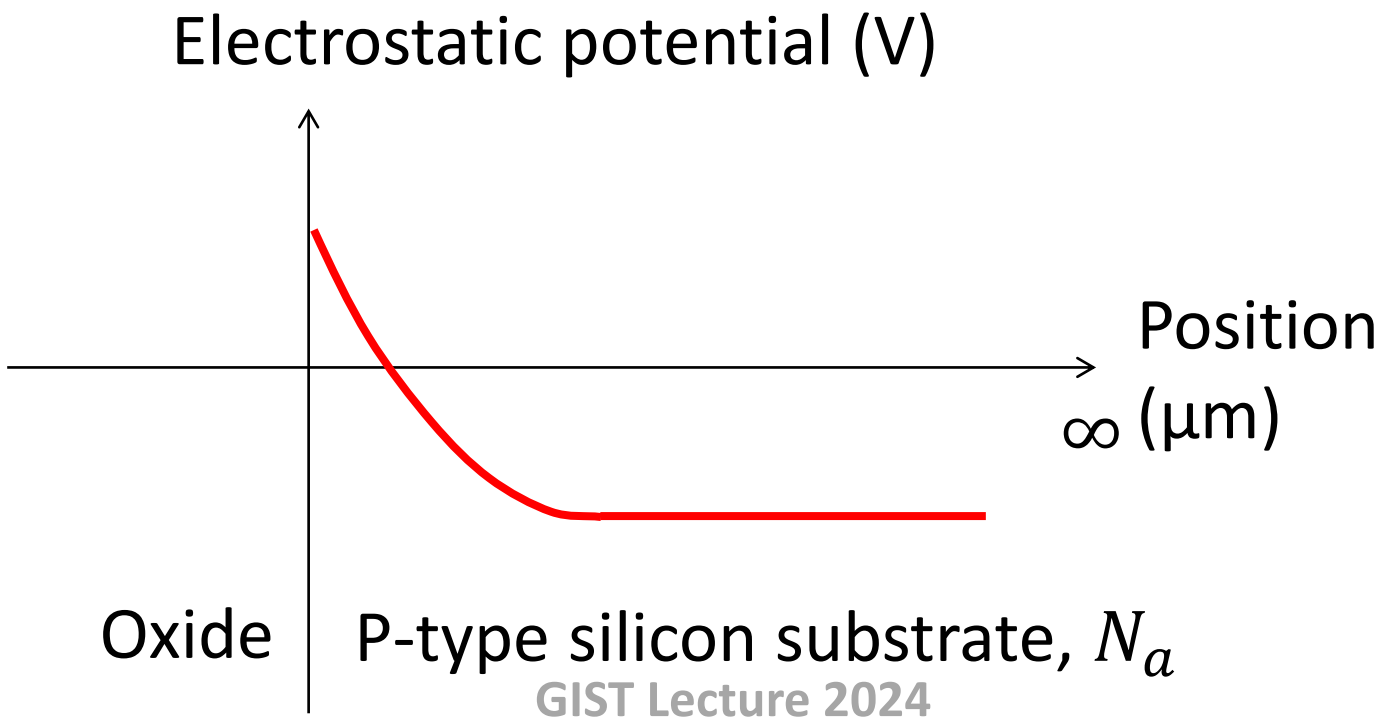
- When the nonlinear Poisson equation is considered,
  - We have additional terms related to $\int_{x_{i-0.5}}^{x_{i+0.5}} \rho(\mathbf{r})dx$.
  - Simple treatment for this integration:

$$\epsilon(x_{i+0.5})\frac{\phi(x_{i+1})-\phi(x_i)}{x_{i+1}-x_i}-\epsilon(x_{i-0.5})\frac{\phi(x_i)-\phi(x_{i-1})}{x_i-x_{i-1}}$$
$$+q\left(n_{int}\exp\left(-\frac{q\phi(x_i)}{k_BT}\right)-n_{int}\exp\left(\frac{q\phi(x_i)}{k_BT}\right)+N_{dop}^{+}(x_i)\right)(x_{i+0.5}$$
$$-x_{i-0.5})=0$$

  - This expression is used to construct the i-th row of b vector.

Only silicon region

- In general, we must consider the oxide layer and the gate contact.
  - For simplicity, consider only the silicon region.
  - It is assumed that the surface potential, $\phi_s = \phi(x = 0) - \phi_\infty$, is known.



Once again, nonlinearity

- There are N unknown variables, $\phi_0, \phi_1, \ldots, \phi_{N-1}$.
  - 1) Evaluate the following equation at $N-2$ points, $x_1, x_2, \ldots, x_{N-2}$.

$$\epsilon(x_{i+0.5})\frac{\phi(x_{i+1})-\phi(x_i)}{x_{i+1}-x_i}-\epsilon(x_{i-0.5})\frac{\phi(x_i)-\phi(x_{i-1})}{x_i-x_{i-1}}$$
$$+q\left(n_{int}\exp\left(-\frac{q\phi(x_i)}{k_BT}\right)-n_{int}\exp\left(\frac{q\phi(x_i)}{k_BT}\right)+N_{dop}^{+}(x_i)\right)(x_{i+0.5}$$
$$-x_{i-0.5})=0$$

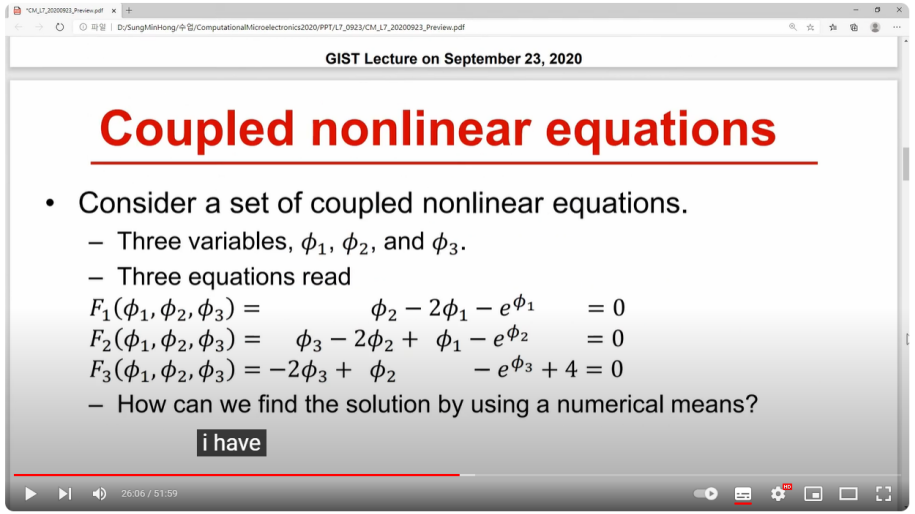
  - 2) Apply the boundary condition at 2 points, x_0 and x_{N-1}.

$$\phi_0=\phi_s+\phi_\infty$$
$$\phi_{N-1}=\phi_\infty$$

  - It is nonlinear!

Newton-Raphson method

- Newton method for multiple variables
  - For a single variable, ϕ, we calculate $f(\phi)$. Its derivative, $\frac{df}{d\phi}$, is useful.
  - For two variables, ϕ and ψ, we calculate $f(\phi,\psi)$ and $g(\phi,\psi)$. Partial derivatives are $\frac{\partial f}{\partial \phi}$, $\frac{\partial f}{\partial \psi}$, $\frac{\partial g}{\partial \phi}$, and $\frac{\partial g}{\partial \psi}$. How can we arrange them to calculate $\delta\phi$ and $\delta\psi$?
  - Watch my video [CM2020] L6.5 from 26:06.
  - Key lesson:
  - Partial derivatives construct A.
  - Then, solve $\mathrm{Ax} = \mathrm{b}$.



The i–th row

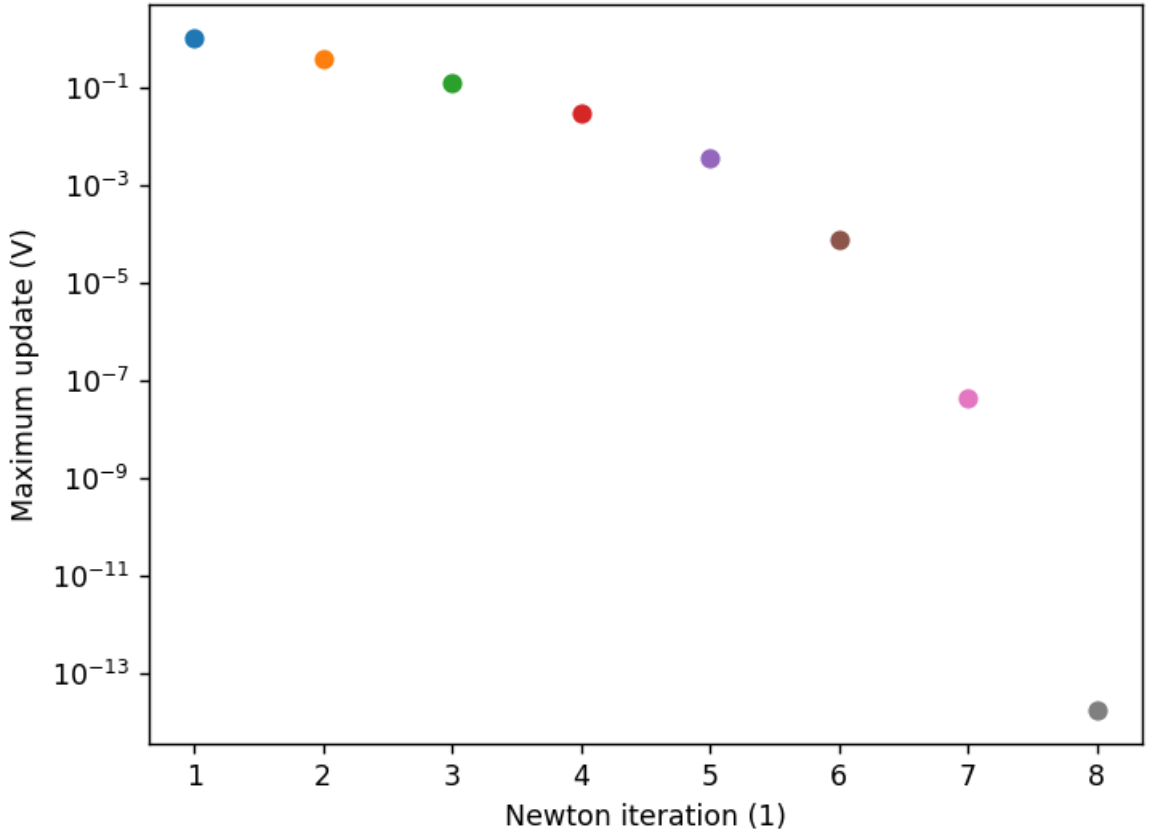
- Consider a case of $1 \leq i \leq N-2$.
  - Then, $(i, i+1)$ component becomes $\epsilon(x_{i+0.5}) \frac{1}{x_{i+1}-x_i}$.
  - The diagonal, (i, i), component becomes

$$-\epsilon(x_{i+0.5}) \frac{1}{x_{i+1}-x_i} - \epsilon(x_{i-0.5}) \frac{1}{x_i - x_{i-1}} + q\left(-\frac{q}{k_B T} n_{int} \exp\left(-\frac{q\phi(x_i)}{k_B T}\right) - \frac{q}{k_B T} n_{int} \exp\left(\frac{q\phi(x_i)}{k_B T}\right)\right)(x_{i+0.5} - x_{i-0.5})$$

  - Also, $(i, i-1)$ component becomes $\epsilon(x_{i-0.5}) \frac{1}{x_i - x_{i-1}}$.

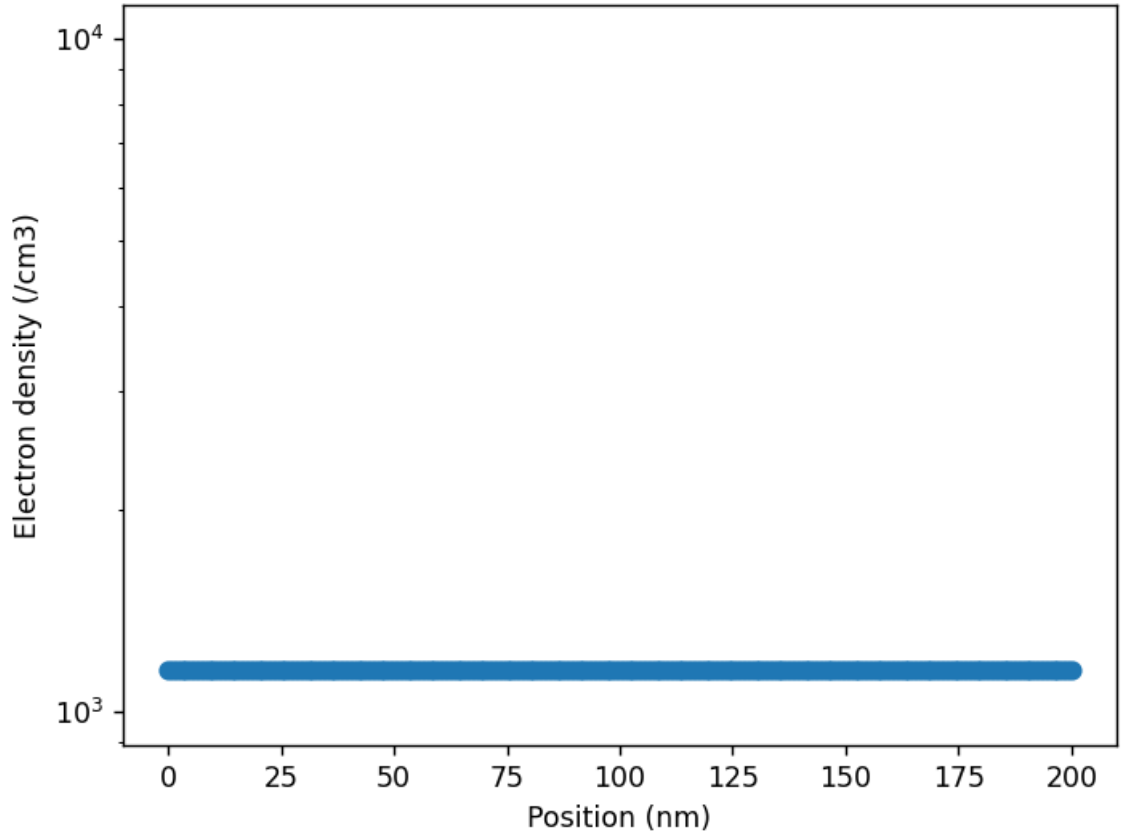
Convergence criterion

- By solving $\mathrm{Ax} = \mathrm{b}$, we obtain a vector of $\delta\phi$.
  - When every entry of this vector becomes sufficiently small, we can stop the Newton-Raphson iterations.



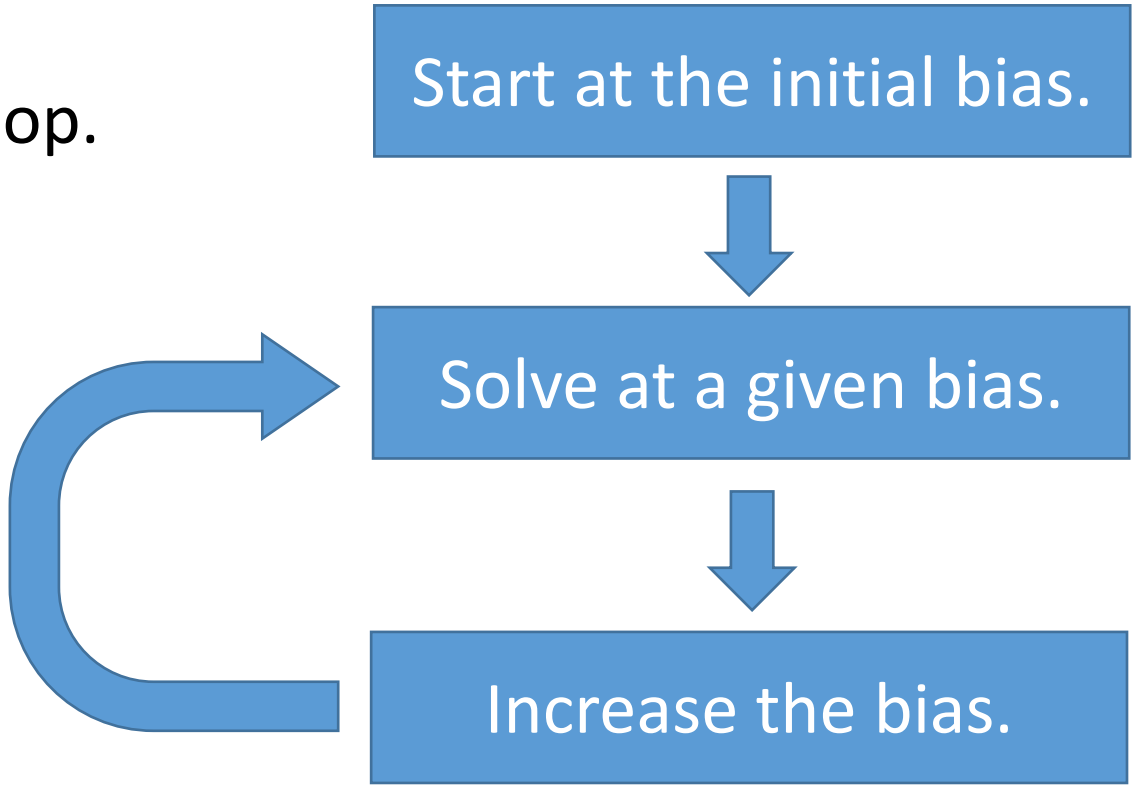
Flatband condition

- It means that ϕ_s = 0.0 V.
  - Also, the p-type doping concentration is 10^{17} cm^{-3}.
  - Use Δx = 1 nm. N is 201.



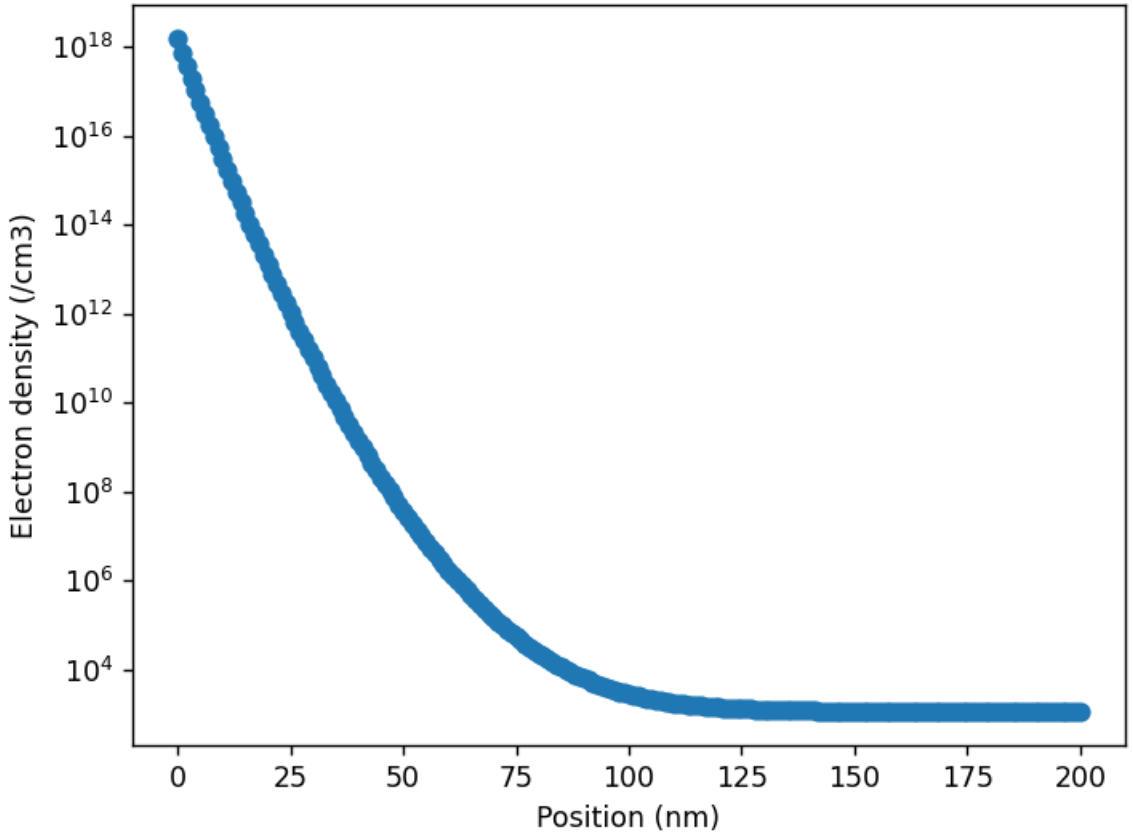
Bias ramping

- Ramp up the surface potential, ϕ_s. (The term, "bias," is usually used for terminal quantities. In this lecture, we instead increase ϕ_s, only for simplicity.)
  - Simply add an outermost loop.



Electron density at ϕ_s = 0.9 V

- Now, strong inversion
  - The electron density at x = 0 is 1.5X10^{18} cm^{-3}.
  - Numerically integrated electron density is 2.3X10^{11} cm^{-2}.



Homework#7

- Due: AM08:00, October 8
- Problem#1
  - Now, we have two methods to calculate semiconductor charges. One is an analytic expression studied in L4. The other is a numerical approach studied in L7. When the p-type doping concentration is $4X10^{17}$ cm^{-3}, compare two results.

Thank you for your attention!