Lecture16

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Drift-diffusion model

- We have to solve these equations.
  - The Poisson equation

$$\nabla \cdot \mathbf{D} = \rho = +q(p - n + N^+)$$

  - Electron/hole continuity

$$\frac{\partial n}{\partial t} = -\nabla \cdot \mathbf{F}_n = \frac{1}{q} \nabla \cdot \mathbf{J}_n$$

$$\frac{\partial p}{\partial t} = -\nabla \cdot \mathbf{F}_p = -\frac{1}{q} \nabla \cdot \mathbf{J}_p$$

  - Electron/hole current density

$$\mathbf{J}_n = +q\mu_n n\mathbf{E} + qD_n \nabla n$$

$$\mathbf{J}_p = +q\mu_p p\mathbf{E} - qD_p \nabla p$$

Continuity equation

- By using the current density,
  - The electron continuity can be simplified as

$$\frac{\partial n}{\partial t} = -\nabla \cdot \mathbf{F}_n = \frac{1}{q}\nabla \cdot (+q\mu_n n\mathbf{E} + qD_n\nabla n\ )$$

- Steady-state
  - Time derivative vanishes.

$$\nabla \cdot (+q\mu_n n\mathbf{E} + qD_n\nabla n\ ) = 0$$

N^+NN^+ structure

- 600-nm-long version (Long)
  - 100 nm: Highly doped ($5x10^{17}$ cm^{-3})
  - 400 nm: Lowly doped ($2x10^{15}$ cm^{-3})
  - 100 nm: Highly doped ($5x10^{17}$ cm^{-3})
- 60-nm-long version (Short)
  - 10 nm: Highly doped ($5x10^{19}$ cm^{-3})
  - 40 nm: Lowly doped ($2x10^{17}$ cm^{-3})
  - 10 nm: Highly doped ($5x10^{19}$ cm^{-3})

Boundary condition

- 600-nm-long version (Long)
  - At $x = 0$ nm or 600 nm, the electrostatic potential is given by the charge neutrality condition.

$$5 \times 10^{17}\ \mathrm{cm}^{-3} \approx n_{int} \exp\left(\frac{\phi}{V_T}\right)$$

  - Here, V_T is the thermal voltage.
  - Therefore, the electrostatic potential at the boundary points is

$$\phi = V_T \log\left(\frac{5 \times 10^{17}\ \mathrm{cm}^{-3}}{n_{int}}\right)$$

Nonliear Poisson equation (1)

- Set up the structure.

```
q = 1.602192e-19; % Elementary charge, C
eps0 = 8.854187817e-12; % Vacuum permittivity, F/m
k_B = 1.380662e-23; % Boltzmann constant, J/K
T = 300.0; % Temperature, K
thermal = k_B*T/q; % Thermal voltage, V
Deltax = 1e-9; % 1 nm spacing
N = 601; % 600-nm-long structure
x = Deltax*transpose([0:N-1]); % real space, m
x_12 = 101; % At x=100 nm
x_23 = 501; % At x=500 nm
eps_si = 11.7; eps_ox = 3.9; % Relative permittivity
Ndon = 2e21*ones(N,1); % 2e15 /cm^3
Ndon(1:x_12,1) = 5e23; % 5e17 /cm^3
Ndon(x_23:N,1) = 5e23; % 5e17 /cm^3
ni = 1.075e16; % 1.075e10 /cm^3
coef = Deltax*Deltax*q/eps0;
```

Nonliear Poisson equation (2)

- `Jaco` and `res` should be constructed.

```
res = zeros(N,1);
Jaco = sparse(N,N);
res(1,1) = phi(1,1) – thermal*log(Ndon(1,1)/ni);
Jaco(1,1) = 1.0;
for ii=2:N-1
   res(ii,1) = eps_si*(phi(ii+1,1)-2*phi(ii,1)+phi(ii-1,1));
   Jaco(ii,ii-1) =    eps_si;
   Jaco(ii,ii  ) = -2*eps_si;
   Jaco(ii,ii+1) =    eps_si;
end
res(N,1) = phi(N,1) - thermal*log(Ndon(N,1)/ni);
Jaco(N,N) = 1.0;
for ii=2:N-1
   res(ii,1) = res(ii,1) - coef*(-Ndon(ii,1)+ni*exp(phi(ii,1)/thermal));
   Jaco(ii,ii) = Jaco(ii,ii) - coef*ni*exp(phi(ii,1)/thermal)/thermal;
end
```

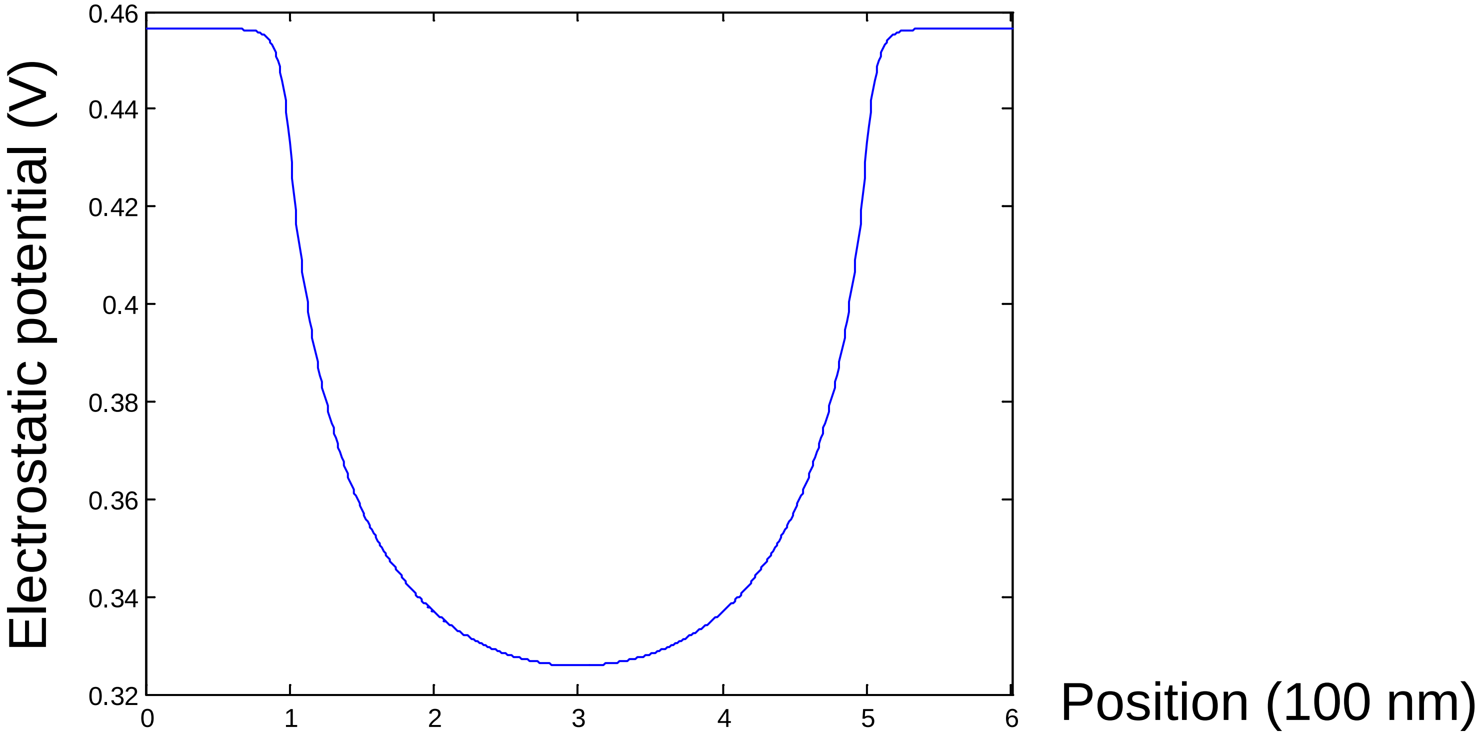
Nonliear Poisson equation (3)

- Full code

```
(Defining variables. Copy-and-paste)
phi = zeros(N,1);
phi(:,1) = thermal*log(Ndon(:,1)/ni);
for newton=1:10
   (Jaco and res are constructed here. Copy-and-paste)
   update = Jaco \ (-res);
   phi = phi + update;
   norm(update,inf)
end
plot(x,phi);
```

Long structure

- Result of `plot(x,phi)`



Next step

- 1D, steady-state
  - The electrostatic potential, ϕ, is given.

$$\frac{d}{dx}\left(-q\mu_n n \frac{d\phi}{dx} + qD_n \frac{dn}{dx}\right) = 0$$

  - Moreover, μ_n and D_n are assumed to be constant.
  - They have the following relation (Einstein relation)

$$D_n = \frac{k_B T}{q}\mu_n = V_T \mu_n$$

- A naïve approach to discretize the above equation

Integration

- The equation is integrated from $x_{i-0.5}$ to $x_{i+0.5}$.
  - Then, we have

$$J_{n,i+0.5} - J_{n,i-0.5} = 0$$

  - Remember that

$$J_{n,i+0.5} = -q\mu_n n_{i+0.5} \left.\frac{d\phi}{dx}\right|_{i+0.5} + qD_n \left.\frac{dn}{dx}\right|_{i+0.5}$$

  - By using the Einstein relation,

$$J_{n,i+0.5} = -q\mu_n \left(n_{i+0.5} \left.\frac{d\phi}{dx}\right|_{i+0.5} - V_T \left.\frac{dn}{dx}\right|_{i+0.5} \right)$$

Discretized form

- Continuity equation after integration
  - It is written as

$$n_{i+0.5} \left.\frac{d\phi}{dx}\right|_{i+0.5} - V_T \left.\frac{dn}{dx}\right|_{i+0.5} - n_{i-0.5} \left.\frac{d\phi}{dx}\right|_{i-0.5} + V_T \left.\frac{dn}{dx}\right|_{i-0.5} = 0$$

  - How can we discretize the above equation? One possibility is…

$$n_{i+0.5} = \frac{n_{i+1} + n_i}{2}$$

$$\left.\frac{d\phi}{dx}\right|_{i+0.5} = \frac{\phi_{i+1} - \phi_i}{\Delta x}$$

$$\left.\frac{dn}{dx}\right|_{i+0.5} = \frac{n_{i+1} - n_i}{\Delta x}$$

Contribution to Jacobian

- Consider the flux, $J_{n,i+0.5}$ (Divided by $-q\mu_n$)
  - It is written as

$$n_{i+0.5}\left.\frac{d\phi}{dx}\right|_{i+0.5}-V_T\left.\frac{dn}{dx}\right|_{i+0.5}$$

  - Its contributions to the Jacobian matrix are

$$-\frac{1}{q\mu_n}\frac{\partial J_{n,i+0.5}}{\partial n_{i+1}}=\frac{1}{2}\left.\frac{d\phi}{dx}\right|_{i+0.5}-V_T\frac{1}{\Delta x}$$

$$-\frac{1}{q\mu_n}\frac{\partial J_{n,i+0.5}}{\partial n_{i}}=\frac{1}{2}\left.\frac{d\phi}{dx}\right|_{i+0.5}+V_T\frac{1}{\Delta x}$$

Notes

- It is noted that $J_{n,i+0.5}$ is used both for x_i-centered integration and x_{i+1}-centered one.
  - Therefore, we will construct it once and apply it to two equations.

- Boundary condition
  - At boundary points, the electron density is equal to the donor density.
  - For the 600-nm-long structure,

$$5 \times 10^{17}\ \mathrm{cm}^{-3} \approx n$$

Continuity equation (1)

- The code is based on the previous nonlinear Poisson equation solver.
- First, the electron density is calculated from $n = n_{int} \exp \frac{\phi}{V_T}$.

```
elec = zeros(N,1);
elec = ni*exp(phi/thermal);
plot(x,elec,'r');
hold on;
```

Continuity equation (2)

- Now, the continuity equation is constructed.

```
res_elec = zeros(N,1);
Jaco_elec = sparse(N,N);
for ii=1:N-1 % edge-wise construction
   n_av = 0.5*(elec(ii+1,1)+elec(ii,1));
   dphidx = (phi(ii+1,1)-phi(ii,1))/Deltax;
   delecdx = (elec(ii+1,1)-elec(ii,1))/Deltax;
   Jn = n_av * dphidx – thermal * delecdx;
   res_elec(ii,1) = res_elec(ii,1) + Jn;
   Jaco_elec(ii,ii+1) = Jaco_elec(ii,ii+1) + 0.5*dphidx – thermal / Deltax;
   Jaco_elec(ii,ii  ) = Jaco_elec(ii,ii  ) + 0.5*dphidx + thermal / Deltax;
   res_elec(ii+1,1) = res_elec(ii+1,1) - Jn;
   Jaco_elec(ii+1,ii+1) = Jaco_elec(ii+1,ii+1) - 0.5*dphidx + thermal / Deltax;
   Jaco_elec(ii+1,ii  ) = Jaco_elec(ii+1,ii  ) - 0.5*dphidx - thermal / Deltax;
end
```

Continuity equation (3)

- Boundary condition

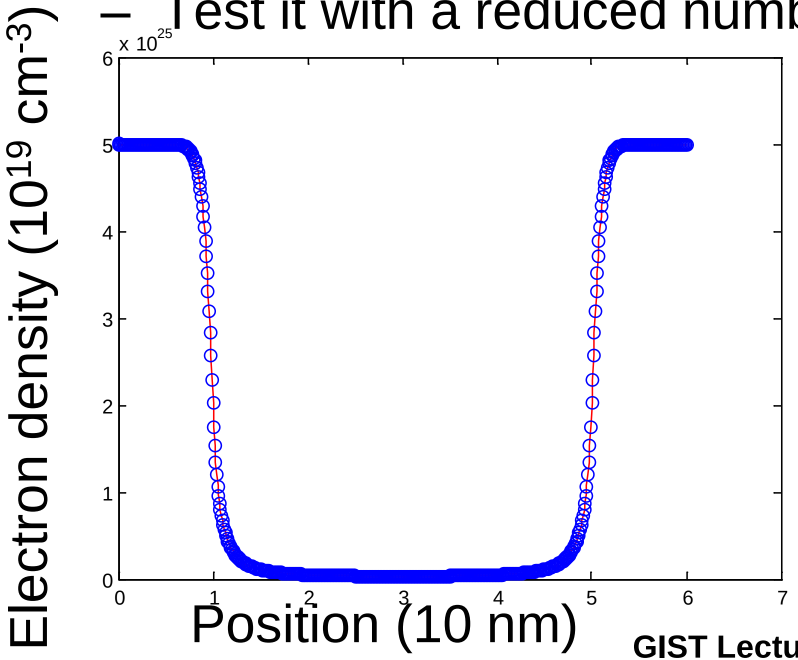
```
res_elec(1,1) = elec(1,1) – Ndon(1,1);
Jaco_elec(1,:) = 0.0;
Jaco_elec(1,1) = 1.0;
res_elec(N,1) = elec(N,1) - Ndon(N,1);
Jaco_elec(N,:) = 0.0;
Jaco_elec(N,N) = 1.0;
```

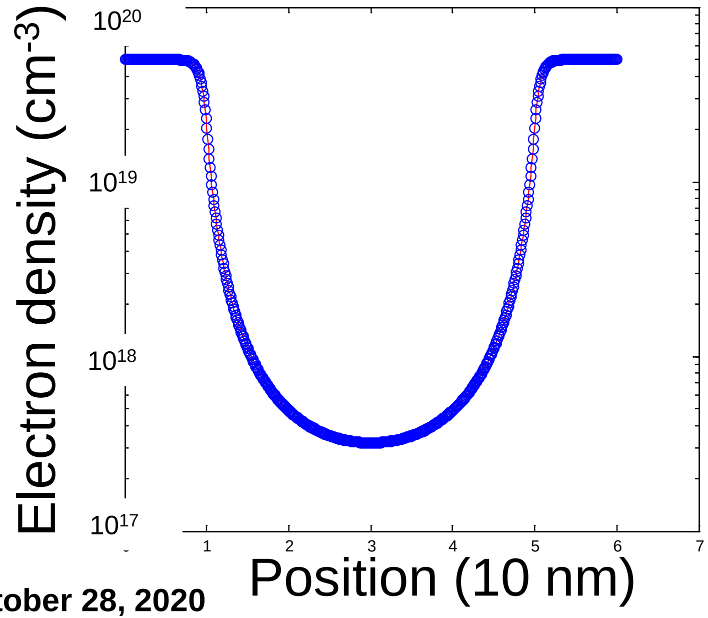
- Obtain the result.
  - Since it is a linear equation of n, only one solution step is sufficient.

```
update_elec = Jaco_elec \ (-res_elec);
elec = elec + update_elec;
plot(x,elec,’o’);
```

Short structure

- Result of `plot(x,elec)`
  - Red line (Nonlinear Poisson) vs circle (Continuity equation)
  - Test it with a reduced number of points.





Homework#14

- Due: AM08:00, November 2 (Next Monday)
- Problem#1
  - Consider a PN junction at equilibrium.
  - In both regions (PN), the doping density is 10^{17} /cm^3.
  - First, solve the nonlinear Poisson equation.
  - Then, solve the drift-diffusion equations. (Since you have the solution, your residue should be quite small!)