Lecture10

Sung-Min Hong (smhong@gist.ac.kr)

Semiconductor Device Simulation Lab.

School of Electrical Engineering and Computer Science

Gwangju Institute of Science and Technology

GIST Lecture on October 7, 2020

Poisson equation in 2D

- Poisson equation in 2D (xy-plane)
  - For a function, $\phi(x,y)$, the Poisson equation reads
$$\frac{\partial}{\partial x}\left[\epsilon(x,y)\frac{\partial \phi}{\partial x}\right]+\frac{\partial}{\partial y}\left[\epsilon(x,y)\frac{\partial \phi}{\partial y}\right]=-\rho$$
  - The boundary conditions are the same.

Initial guess at equilibrium

- How can we set the initial guess?
  - A rule of thumb
  - For semiconductor regions, apply the local charge balance.

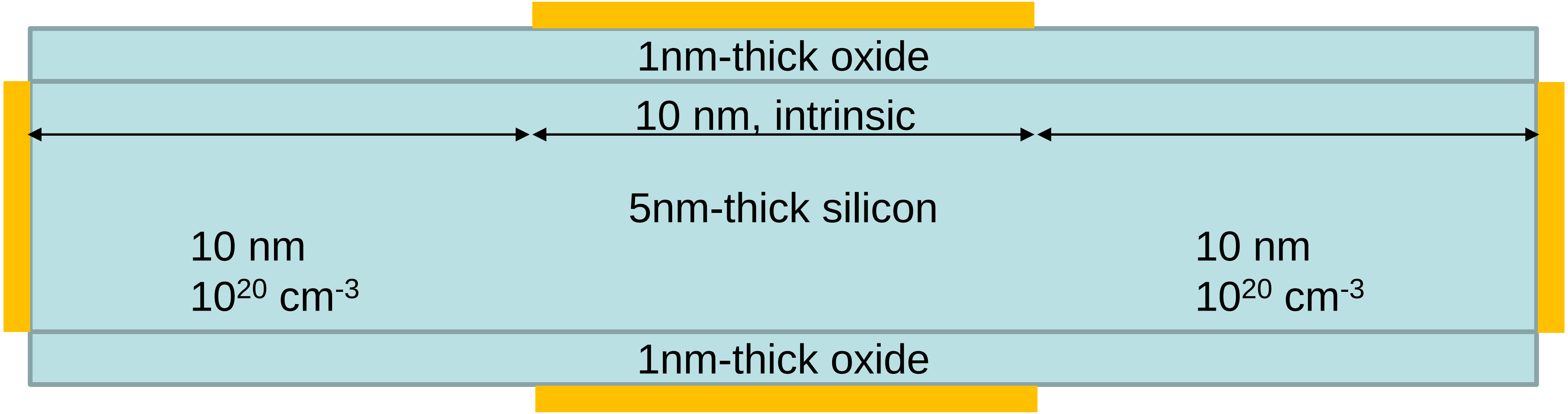
$$N^{+} + n_{int} e^{-\frac{\phi}{V_T}} - n_{int} e^{\frac{\phi}{V_T}} = 0$$

(Yes, it was the Homework#7.)

  - For insulator regions, leave it zero.

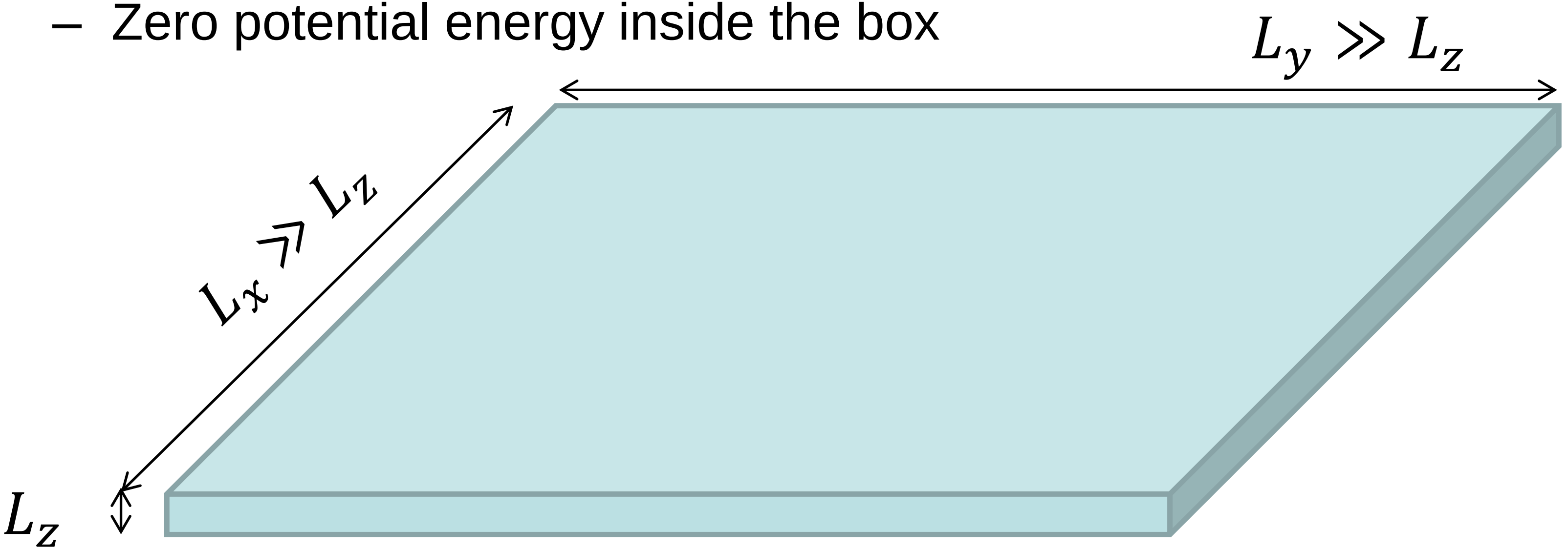
Homework#10

- Due: AM08:00, October 12 (Next Monday)
- Problem#1
  - Calculate the electrostatic potential at V_G = 0 V and V_G = 1.1 V .



Thin and wide box

- Consider a thin and wide box. (3D infinite potential well)
  - Length along the confinement direction, L_z
  - At all six surfaces, the wavefunction vanishes.
  - Zero potential energy inside the box



Eigen-energy?

- Hamiltonian operator

$$H = -\frac{\hbar^2}{2m_{xx}}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_{yy}}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_{zz}}\frac{\partial^2}{\partial z^2}$$

  – We can find the following solution:

$$\psi_{l,m,n}(x,y,z) = A_{l,m,n}\sin\left(\frac{l\pi}{L_x}x\right)\sin\left(\frac{m\pi}{L_y}y\right)\sin\left(\frac{n\pi}{L_z}z\right)$$

  – Of course, the eigen-energy is given by

$$E_{l,m,n} = \frac{\hbar^2}{2m_{xx}}\frac{l^2\pi^2}{L_x^2} + \frac{\hbar^2}{2m_{yy}}\frac{m^2\pi^2}{L_y^2} + \frac{\hbar^2}{2m_{zz}}\frac{n^2\pi^2}{L_z^2}$$

Fermi-Dirac distribution

- Let us assume that there is a state whose eigen-energy is $E_{l,m,n}$.
  - Still, the Fermi level is located at 0 eV.
  - Then, the Fermi-Dirac distribution is given by

$$f_{FD} = \frac{1}{1 + \exp\left(\frac{E_{l,m,n}}{k_B T}\right)}$$

Total number?

- Number of electrons at a certain state
  - For a state with (l, m, n), the number of electrons is $2 \times f_{FD}\left(E_{l,m,n}\right)$. The factor of 2 is due to the spin degeneracy.
- There are many states.
  - The total number is given by

$$2 \times \sum_{l=1}^{\infty} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} f_{FD}\left(E_{l,m,n}\right)$$

MATLAB example (1)

- Let us consider $L_x = L_y = 100\ \mathrm{nm}$ and $L_z = 5\ \mathrm{nm}$.
  - In practical sense, L_z is reasonable. L_x and L_y are somewhat large.
  - Also, assume that $m_{xx} = m_{yy} = 0.19\, m_0$ and $m_{zz} = 0.91\, m_0$.
  - First, define some constants.

```
h = 6.626176e-34; % Planck constant, J s
hbar = h / (2*pi); % Reduced Planck constant, J s
q = 1.602192e-19; % Elementary charge, C
m0 = 9.109534e-31; % Electron rest mass, kg
k_B = 1.380662e-23; % Boltzmann constant, J/K
T = 300.0; % Temperature, K
```

MATLAB example (2)

- What is the number?
  - Set the box size and the masses.

```
Lx = 100e-9; Ly = 100e-9; Lz = 5e-9; % Lenghs, m
mxx = 0.19; myy = 0.19; mzz = 0.91; % Masses, m0
```

  - Calcultate the total number. How large is it?

```
lmax = 50; mmax = 50; nmax = 50;
totalNumber = 0;
for l=1:lmax
   for m=1:mmax
      for n=1:nmax
         E = (hbar*pi)^2/2/m0*(1/mxx*(l/Lx)^2 + 1/myy*(m/Ly)^2 + 1/mzz*(n/Lz)^2);
         totalNumber = totalNumber + 2/(1+exp(E/(k_B*T)));
      end
   end
end
```