Lecture6

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0 V? What does it mean?

- Electrostatic potential, $\phi(\mathbf{r})$
  - Let us assume that it is 0 V at a certain point.Then, what is its meaning?
  - Misconception) That point has the same electrostatic potential with the ground.
  - We have to realize that the applied voltages at contacts are *<u>NOT</u>* the electrostatic potential.
- What's the matter with $\phi(\mathbf{r})$?
  - In the computational electronics, it is very important to understand the meaning of $\phi(\mathbf{r})$ exactly.

Ambiguity

- Global shift of the potential
  - Since the electric field is given by $\mathbf{E}(\mathbf{r}) = -\nabla\phi(\mathbf{r})$, a global shift of the potential does not introduce different physics.
- We must answer two questions:
  - Which quatity is described by the electrostatic potential? (Especially, in the semiconductor device simulator)
  - What is the reference of the electrostatic potential?

Widely adopted convention

- Answer #1
  - By the electrostatic potential, we want to point out the intrinsic Fermi level of the reference material.
  - For example, when the reference material is silicon,

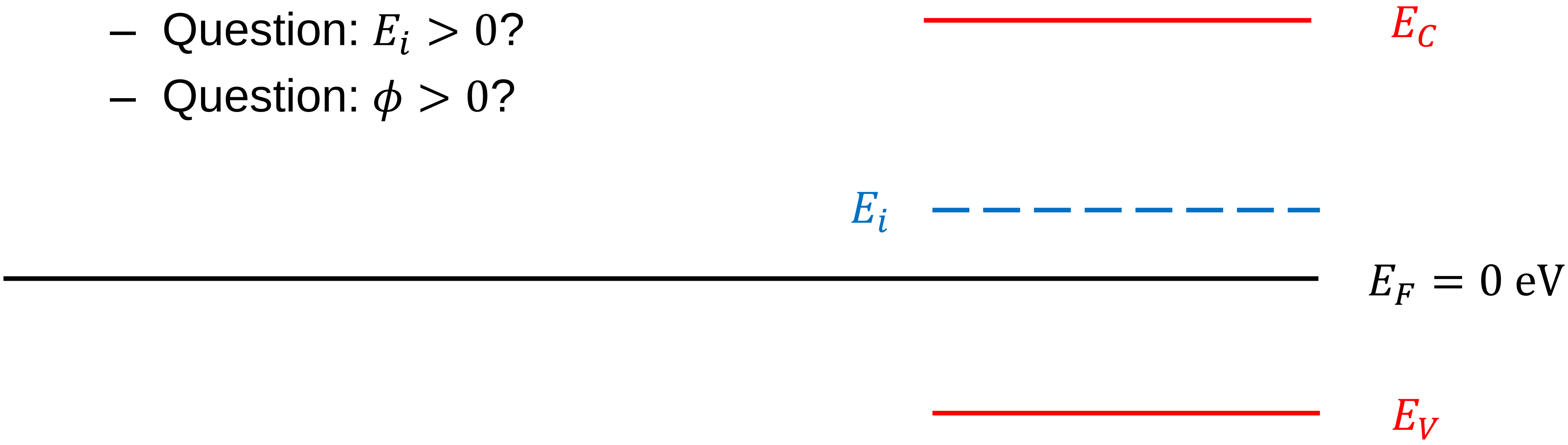
$$E_i(\mathbf{r}) = -q\phi(\mathbf{r})$$

$E_i(\mathbf{r})$: Intrinsic Fermi level of silicon in this example

- Answer #2
  - The reference energy is the Fermi level at equilibrium.
  - Therefore, the Fermi potential at equilibrium is 0 V.

Diagram

- First, there is the Fermi level, E_F.
  - Now, the conduction band minimum (E_C) and the valence band maximum (E_V) are identified.
  - Using them, the intrinsic Fermi level (E_i) is found.
  - Question: $E_i > 0$?
  - Question: $\phi > 0$?



Electron density (1)

- Effective density-of-states of the conduction band, N_C
  - For example, N_C of silicon at 300 K is about 2.86X10^{19} cm^{-3}.
- Electron density
  - Assume the Boltzmann statistics.
  - At equilibrium, the electron density can be obtained by

$$n(\mathbf{r}) = N_C \exp\left(\frac{E_F - E_C}{k_B T}\right)$$

E_F: Fermi level, E_C: Conduction band minimum

k_B: Boltzmann constant, T: Temperature

  - At 300 K, $k_B T \approx 25.85\ \mathrm{meV}$.

Electron density (2)

- Remember that $E_F = 0$. Then,

$$n(\mathbf{r}) = N_C \exp\left(-\frac{E_C}{k_B T}\right)$$

  - Also, the energy difference between E_C and E_i is a given constant.

$$n(\mathbf{r}) = N_C \exp\left(-\frac{E_C}{k_B T}\right) = N_C \exp\left(-\frac{E_C - E_i + E_i}{k_B T}\right)$$

  - Using $E_i = -q\phi$, we can obtain

$$n(\mathbf{r}) = N_C \exp\left(-\frac{E_C - E_i}{k_B T}\right) \exp\left(\frac{q\phi}{k_B T}\right) = n_i \exp\left(\frac{q\phi}{k_B T}\right)$$

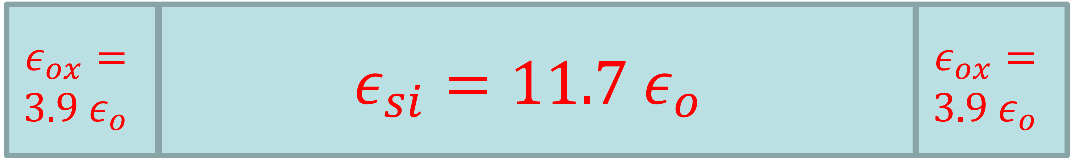
Gate potential

- Let us assume that $V_G = 0\ \mathrm{V}$.
  - However, the electrostatic potential is **NOT** 0 V at that point.
  - For the gate metal, the workfunction is known. The workfunction is the energy difference between the vacuum level and the Fermi level.
  - Therefore, when the workfunction is 4.3 eV, the vacuum level is located at 4.3 eV, because the Fermi level is the energy reference.
  - Moreover, the energy difference between the vacuum level and the intrinsic Fermi level of silicon is given. (About 4.63 eV)
  - Then, the intrinsic Fermi level of silicon is located at -0.33 eV.
  - Finally, the electrostatic potential is 0.33 V.

Double-gate MOS revisited

- Now apply the realistic boundary condition.
  - With the gate metal whose workfunction is 4.3 eV, the boundary value of the electrostatic potential is 0.33374 V.

$\phi(0)$ = 0.33374 V



$\phi(a)$ = 0.33374 V

$x = 0$ $\quad x = t_{ox}$ $\quad x = t_{ox} + t_{si}$ $\quad x = a = 2t_{ox} + t_{si}$

  - Solve the same problem. Neglect the carrier densities.
  - After the solution is obtained, estimate the electron density by using $n(\mathbf{r}) = n_i \exp\left(\frac{q\phi}{k_B T}\right)$.

MATLAB example (1)

- Step-by-step procedure
  - First, 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
Deltax = 0.1e-9; % 0.1 nm spacing
N = 61; % 6 nm thick
x = Deltax*transpose([0:N-1]); % real space, m
interface1 = 6; % At x=0.5 nm
interface2 = 56; % At x=5.5 nm
eps_si = 11.7; eps_ox = 3.9; % Relative permittivity
Nacc = 1e24; % 1e18 /cm^3
ni = 1.075e16; % 1.075e10 /cm^3
```

MATLAB example (2)

- Step-by-step procedure (continued)
  - Next, set the matrix, A. (Five cases)

```
A = zeros(N,N);
A(1,1) = 1.0;
for ii=2:N-1
   if     (ii< interface1) A(ii,ii-1) = eps_ox; A(ii,ii) = -2*eps_ox;      A(ii,ii+1) = eps_ox;
   elseif (ii==interface1) A(ii,ii-1) = eps_ox; A(ii,ii) = -eps_ox-eps_si; A(ii,ii+1) = eps_si;
   elseif (ii< interface2) A(ii,ii-1) = eps_si; A(ii,ii) = -2*eps_si;      A(ii,ii+1) = eps_si;
   elseif (ii==interface2) A(ii,ii-1) = eps_si; A(ii,ii) = -eps_si-eps_ox; A(ii,ii+1) = eps_ox;
   elseif (ii> interface2) A(ii,ii-1) = eps_ox; A(ii,ii) = -2*eps_ox;      A(ii,ii+1) = eps_ox;
   end
end
A(N,N) = 1.0;
```

MATLAB example (3)

- The vector, b, has the correct boundary values.

```
b = zeros(N,1);
b(1,1) = 0.33374;
for ii=interface1:interface2
   if     (ii==interface1) b(ii,1) = Deltax*Deltax*q*Nacc/eps0*0.5;
   elseif (ii==interface2) b(ii,1) = Deltax*Deltax*q*Nacc/eps0*0.5;
   else                    b(ii,1) = Deltax*Deltax*q*Nacc/eps0;
   end
end
b(N,1) = 0.33374;
```

- Get the solution, phi.

```
phi = A \ b;
```

MATLAB example (4)

- Using `phi`, the electron density is estimated.

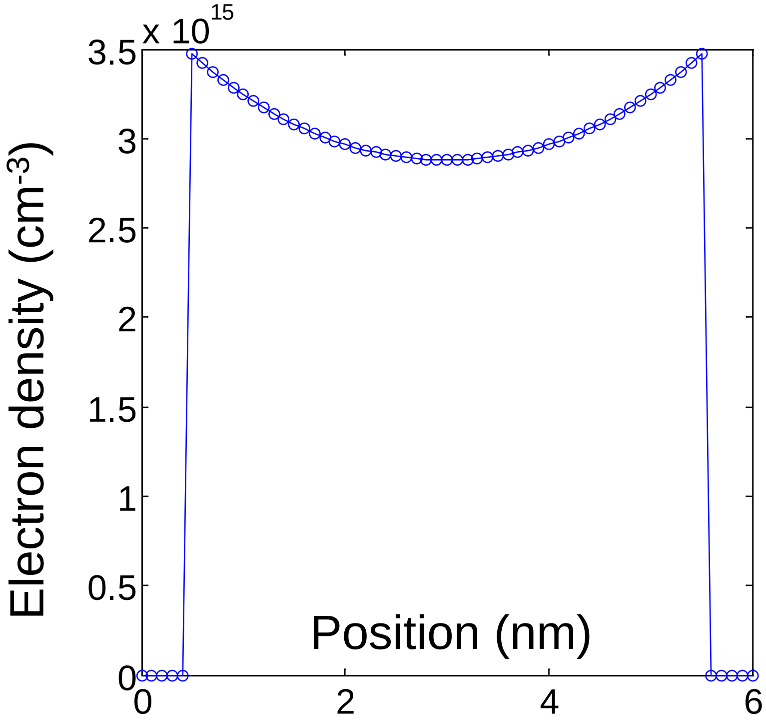
```
elec = zeros(N,1);
for ii=interface1:interface2
   elec(ii,1) = ni * exp(q*phi(ii,1)/(k_B*T));
end
```

- Plot it!

```
plot(x/1e-9,elec*1e-6);
```

MATLAB example (5)

- Graph with $N_{acc} = 10^{18}\ \mathrm{cm}^{-3}$



Homework#4

- Due: AM08:00, October 1
- Problem#1
  - Write your own code for the double-gate structure.
  - The electrostatic potential is obtained under the depletion approximation. (The initial potential)
  - The electron density is calculated by assuming $n_i \exp\left(\frac{q\phi}{k_B T}\right)$.
  - Then, using the electron density, re-calculate the potential. (The updated potential)
  - Check their difference for several gate voltages from 0 V to 1 V. (The voltage step is 0.1 V. 11 points in total.)