#### Lecture5

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#### Poisson equation

Fixed-source case

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

– The net charge density,  $\rho(x)$ , is given by

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

p(x): Hole density, n(x): Electron density,  $N_{dop}^+(x)$ : Net doping density

- Calculating p(x) and n(x) is not a trivial task.
- Let us assume that all mobile carriers are depleted.

$$\left| \frac{d}{dx} \left| \epsilon(x) \frac{d}{dx} \phi(x) \right| = -q N_{dop}^{+}(x)$$

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#### **Double-gate MOS**

- Real engineering problem
  - A silicon layer (whose thickness is  $t_{si}$ ) surrounded by two oxide layers (whose thickness is  $t_{ox}$ )

$$\phi(0) = 0 \text{ V}$$

$$\epsilon_{ox} = 3.9 \epsilon_{o}$$

$$\epsilon_{si} = 11.7 \epsilon_{o}$$

$$\epsilon_{ox} = \phi(a)$$

$$\epsilon_{ox} = 0 \text{ V}$$

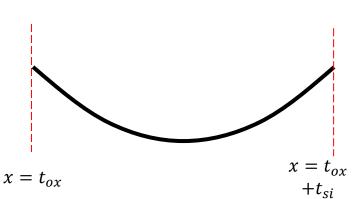
- The silicon layer is doped with p-type dopants. The doping density is  $N_{acc}$ . Since the p-type dopant provides a hole, the dopant itself is negatively charged.  $N_{dop}^+ = -N_{acc}$ .

## **Analytic solution (1)**

#### Qualitative analysis

- Due to the mirror symmetry, the electrostatic potential is also mirror symmetric.
- Inside the oxide layer, the electrostatic potential must be linear.
- Inside the silicon layer, the Poisson equation reads  $(N_{acc} > 0)$

$$\frac{d}{dx} \left[ \frac{d}{dx} \phi(x) \right] = \frac{q N_{acc}}{\epsilon_{si}}$$



# **Analytic solution (2)**

#### Solution

Integrating the Poisson equation inside the silicon layer,

$$\left. \frac{d\phi}{dx} \right|_{x=t_{ox}+t_{si}} - \frac{d\phi}{dx} \right|_{x=t_{ox}} = \frac{qN_{acc}}{\epsilon_{si}} t_{si}$$

We know that

$$\left. \frac{d\phi}{dx} \right|_{x=t_{ox}} = \frac{\phi(t_{ox})}{3t_{ox}}$$

- The electrostatic potential at  $x = t_{ox}$  is given by

$$\phi(t_{ox}) = -\frac{3t_{ox}qN_{acc}t_{si}}{2\epsilon_{si}}$$

### **Scaling**

#### A suitable form

- The original form

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

- However, the values of  $\epsilon(x)$  and dx in the SI unit is very small.
- Equivalently, we will use the following form:

$$(\Delta x) \frac{d}{dx} \left[ \frac{\epsilon(x)}{\epsilon_0} \frac{d}{dx} \phi(x) \right] = (\Delta x) \frac{q N_{acc}(x)}{\epsilon_0}$$

- The discretized version at  $x = x_i$  is

$$\frac{\epsilon(x_{i+0.5})}{\epsilon_0}\phi_{i+1} - \frac{\epsilon(x_{i+0.5}) + \epsilon(x_{i-0.5})}{\epsilon_0}\phi_i + \frac{\epsilon(x_{i-0.5})}{\epsilon_0}\phi_{i-1} = (\Delta x)^2 \frac{qN_{acc}(x_i)}{\epsilon_0}$$

## **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
Deltax = 0.1e-9; % 0.1 nm spacing
N = 61; % 6 nm thick
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
```

## 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, contains the doping effect.

```
b = zeros(N,1);
for ii=interface1:interface2
   i f
           (ii==interface1) b(ii,1) = Deltax*Deltax*q*Nacc/eps0*0.5;
   elseif (ii==interface2) b(ii,1) = Deltax*Deltax*g*Nacc/eps0*0.5;
   else
                              b(ii,1) = Deltax*Deltax*q*Nacc/eps0;
   end
end
                          -0.002
                          -0.004
                          -0.006
                          -0.008
                           -0.01
                          -0.012
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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:  $\phi > 0$ ?

$$E_i$$
 -----

 $E_F = 0 \text{ eV}$ 

 $E_V$