Computational Microelectronics L4 (Pre-recorded)

Sung-Min Hong

smhong@gist.ac.kr

Semiconductor Device Simulation Laboratory, GIST

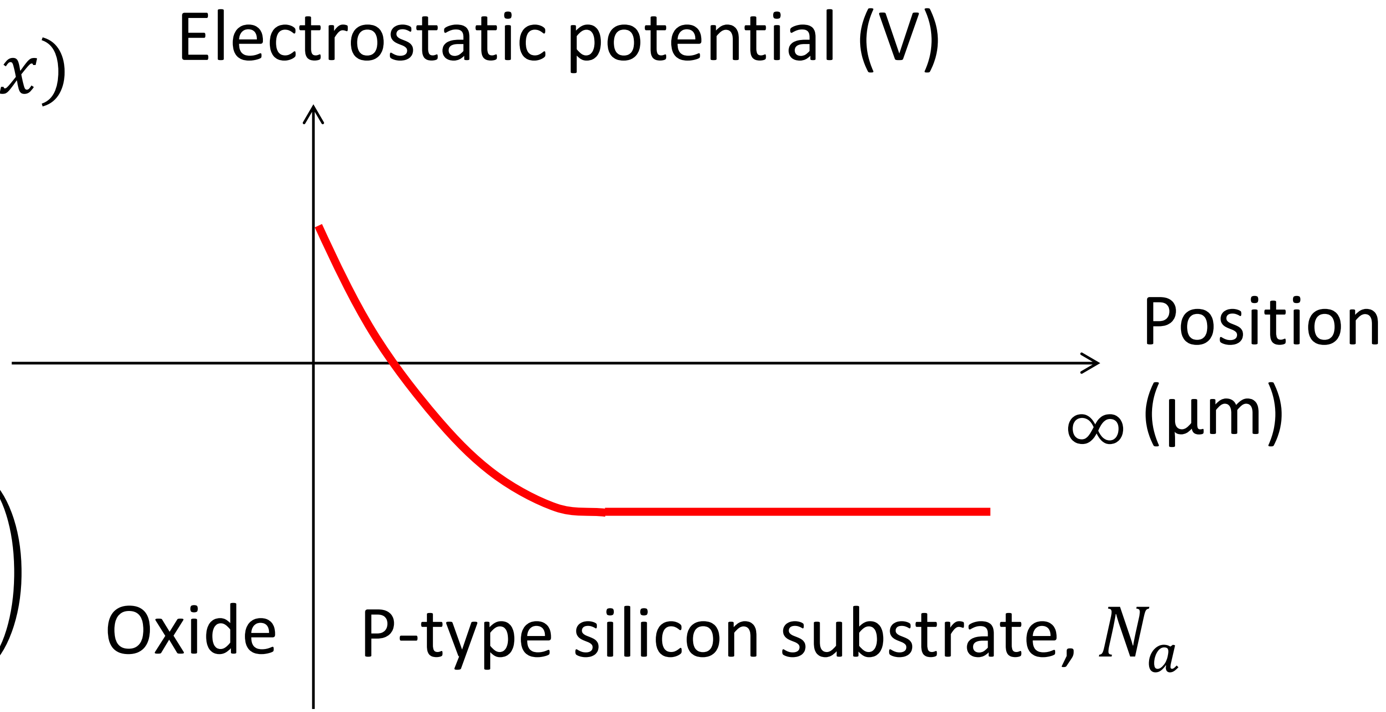
MOS capacitor

MOS capacitor

- Problem specification
  - P-type silicon substrate, N_a
  - Interface at $x = 0$
  - Semi-infinite substrate
  - Electrostatic potential, $\phi(x)$

$$n(x) = n_{int} \exp\left(\frac{q\phi(x)}{k_B T}\right)$$

$$p(x) = n_{int} \exp\left(-\frac{q\phi(x)}{k_B T}\right)$$



Quantities of interest

- We want to know
  - The electrostatic potential at the interface, $\phi(x = 0)$
  - More precisely,
$$\phi_s = \phi(x = 0) - \phi(x = \infty)$$
- At $x = \infty$,
  - The electrostatic potential at the substrate, $\phi(x = \infty) = \phi_\infty$, satisfies
$$N_a = n_{int} \exp\left(-\frac{q}{k_B T}\phi_\infty\right) - n_{int} \exp\left(\frac{q}{k_B T}\phi_\infty\right)$$
  - The electric field vanishes at the substrate,
$$\left.\frac{d\phi}{dx}\right|_\infty = 0$$

(Modified) Poisson equation

- Poisson equation

$$\frac{d^2\phi}{dx^2} = -\frac{q}{\epsilon_{si}}[p(x) - n(x) - N_a]$$

  - Multiplying $\frac{d\phi}{dx}dx$, we have

$$\frac{d\phi}{dx}d\left(\frac{d\phi}{dx}\right) = -\frac{q}{\epsilon_{si}}\left[n_{int}\exp\left(-\frac{q\phi}{k_B T}\right) - n_{int}\exp\left(\frac{q\phi}{k_B T}\right) - N_a\right]d\phi$$

  - By using N_a,

$$\frac{d\phi}{dx}d\left(\frac{d\phi}{dx}\right) = -\frac{q}{\epsilon_{si}}n_{int}$$

$$\times\left[\exp\left(-\frac{q\phi}{k_B T}\right) - \exp\left(\frac{q\phi}{k_B T}\right) - \exp\left(-\frac{q\phi_\infty}{k_B T}\right) + \exp\left(\frac{q\phi_\infty}{k_B T}\right)\right]d\phi$$

Change of variable

- After simple manipulation,
  - It can be simplified with $\bar{\phi} = \phi - \phi_\infty$:

$$\frac{d\phi}{dx} d\left(\frac{d\phi}{dx}\right) = -\frac{q}{\epsilon_{si}} n_{int}$$

$$\sim \frac{N_a}{n_{int}}$$

$$\times \left[\boxed{\exp\left(-\frac{q\phi_\infty}{k_B T}\right)}\left\{\exp\left(-\frac{q\bar{\phi}}{k_B T}\right) - 1\right\} - \boxed{\exp\left(\frac{q\phi_\infty}{k_B T}\right)}\left\{\exp\left(\frac{q\bar{\phi}}{k_B T}\right) - 1\right\}\right] d\bar{\phi}$$

$$\sim \frac{n_{int}}{N_a}$$

Integration from 0 to ∞

- Then, $\frac{d\phi}{dx}$ and $\bar{\phi}$ vanish at the substrate.
  - The integrated equation reads

$$\frac{1}{2}\left(\left.\frac{d\phi}{dx}\right|_0\right)^2 = -\frac{q}{\epsilon_{si}} n_{int}$$
$$\times\left[\exp\left(-\frac{q\phi_\infty}{k_B T}\right)\left\{-\frac{k_B T}{q}\exp\left(-\frac{q\phi_s}{k_B T}\right)+\frac{k_B T}{q}-\phi_s\right\}\right.$$
$$\left.-\exp\left(\frac{q\phi_\infty}{k_B T}\right)\left\{\frac{k_B T}{q}\exp\left(\frac{q\phi_s}{k_B T}\right)-\frac{k_B T}{q}-\phi_s\right\}\right]$$

(Note that $\phi_s = \bar{\phi}(0)$)

Relation between ϕ_s and $d\phi/dx|_0$

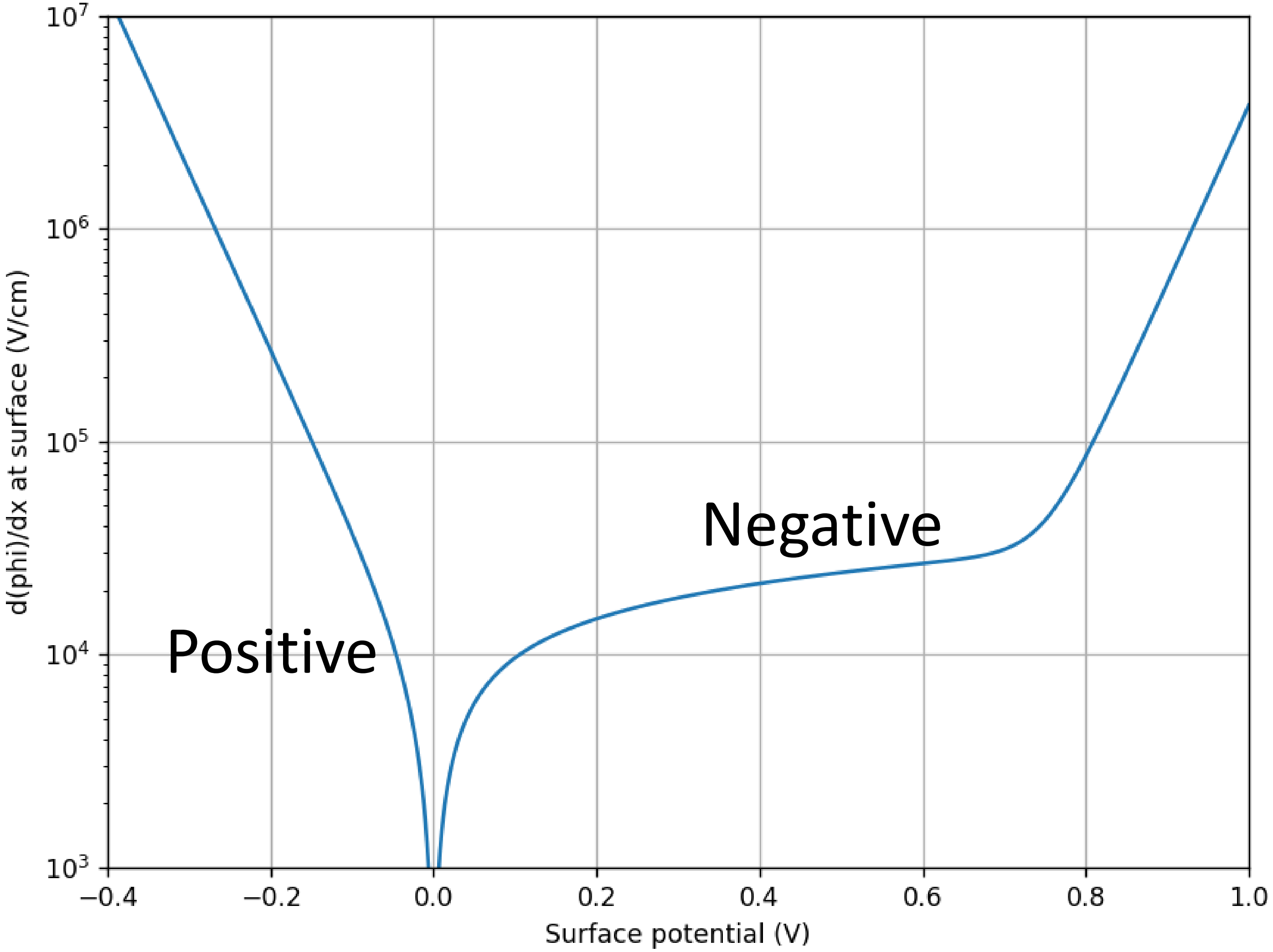
- Then,
  - Now, ϕ_s and $\left.\frac{d\phi}{dx}\right|_0$ related through

$$\left(\left.\frac{d\phi}{dx}\right|_0\right)^2 = \frac{2k_BT}{\epsilon_{si}} n_{int} \times \left[\exp\left(-\frac{q\phi_\infty}{k_BT}\right)\left\{\exp\left(-\frac{q\phi_s}{k_BT}\right) - 1 + \frac{q\phi_s}{k_BT}\right\} + \exp\left(\frac{q\phi_\infty}{k_BT}\right)\left\{\exp\left(\frac{q\phi_s}{k_BT}\right) - 1 - \frac{q\phi_s}{k_BT}\right\}\right]$$

Draw $d\phi/dx|_0$ as a function of ϕ_s

- It is straightforward to draw it.
  - N_a = 4X10^{15} cm^{-3}
  - Parameters

q = 1.602192X10^{-19} C
n_{int} = 1.075X10^{10} cm^{-3}
k_B = 1.38065X10^{-23} J/K
T = 300 K



Approximated expressions

- Negative ϕ_s

$$\left(\left.\frac{d\phi}{dx}\right|_0\right)^2 \approx \frac{2k_BT}{\epsilon_{si}} n_{int} \left[\exp\left(-\frac{q\phi_\infty}{k_BT}\right)\exp\left(-\frac{q\phi_s}{k_BT}\right)\right]$$

- Positive, but small ϕ_s

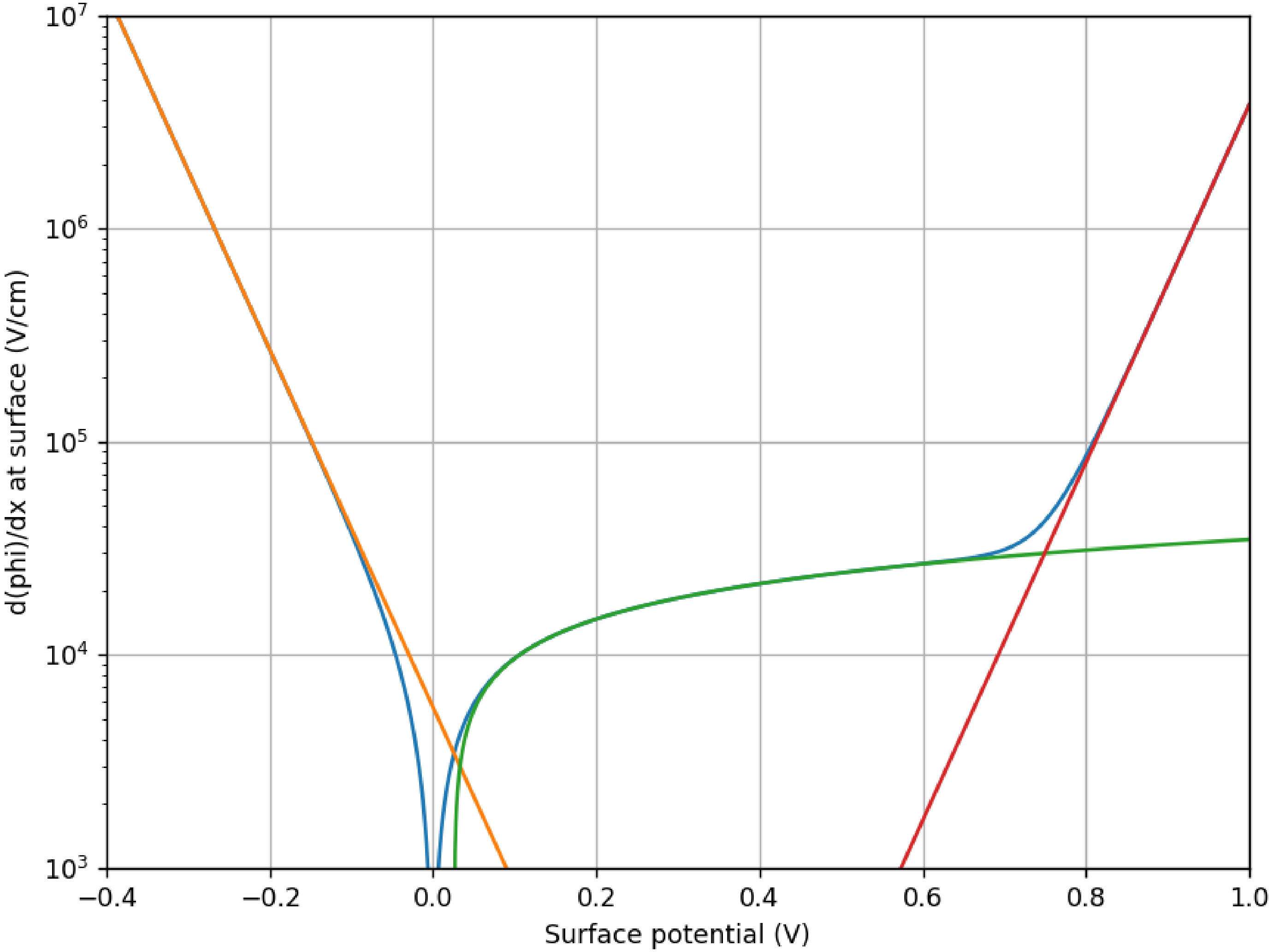
$$\left(\left.\frac{d\phi}{dx}\right|_0\right)^2 \approx \frac{2k_BT}{\epsilon_{si}} n_{int} \left[\exp\left(-\frac{q\phi_\infty}{k_BT}\right)\frac{q\phi_s}{k_BT}\right]$$

- Sufficiently large ϕ_s

$$\left(\left.\frac{d\phi}{dx}\right|_0\right)^2 \approx \frac{2k_BT}{\epsilon_{si}} n_{int} \left[\exp\left(\frac{q\phi_\infty}{k_BT}\right)\exp\left(\frac{q\phi_s}{k_BT}\right)\right]$$

Draw approximate expressions.

- Approximate expressions are reasonably good.



Calculate ϕ_s at a given $d\phi/dx|_0$

- For example, calculate ϕ_s corresponding to -1 MV/cm .
  - Function to become zero

$$\left(\left.\frac{d\phi}{dx}\right|_0\right)^2 - \frac{2k_BT}{\epsilon_{si}} n_{int} \left[\exp\left(-\frac{q\phi_\infty}{k_BT}\right)\left\{\exp\left(-\frac{q\phi_s}{k_BT}\right) - 1 + \frac{q\phi_s}{k_BT}\right\} + \exp\left(\frac{q\phi_\infty}{k_BT}\right)\left\{\exp\left(\frac{q\phi_s}{k_BT}\right) - 1 - \frac{q\phi_s}{k_BT}\right\}\right]$$

Derivative

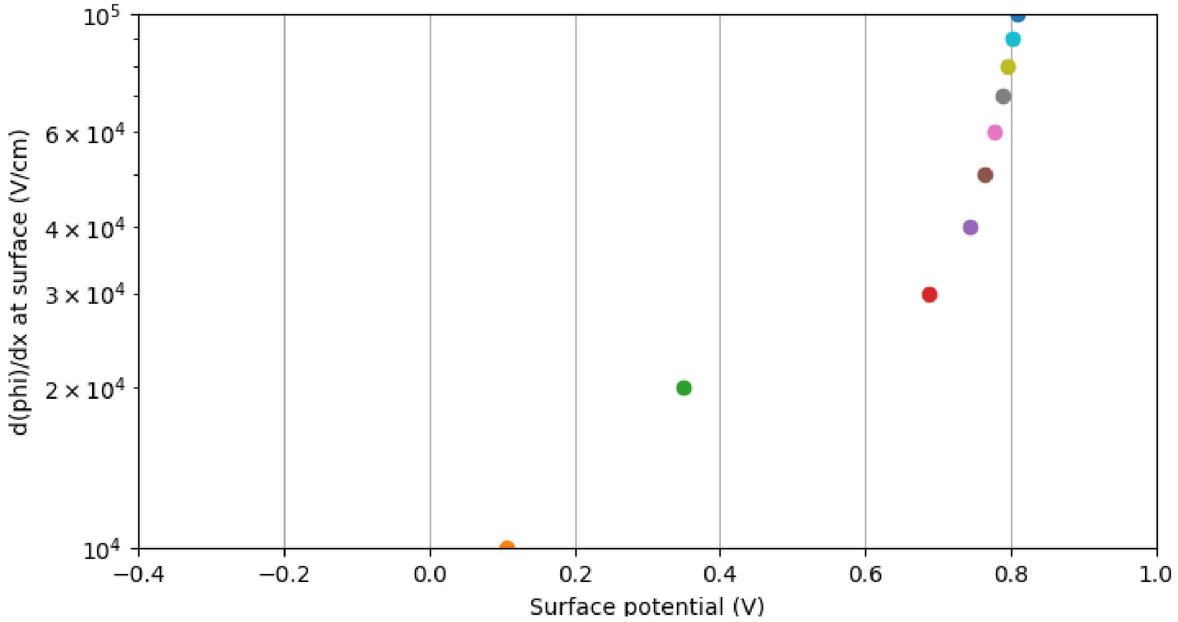
- For example, calculate ϕ_s corresponding to -1 MV/cm .
  - Derivative of the function

$$-\frac{2q}{\epsilon_{si}} n_{int} \left[\exp\left(-\frac{q\phi_\infty}{k_B T}\right) \left\{ -\exp\left(-\frac{q\phi_s}{k_B T}\right) + 1 \right\} + \exp\left(\frac{q\phi_\infty}{k_B T}\right) \left\{ \exp\left(\frac{q\phi_s}{k_B T}\right) - 1 \right\} \right]$$

- We can implement the Newton method.
  - Once again, be careful about too large update.
  - For example, the maximum update can be limited up to $\frac{k_B T}{q}$.

Homework#4

- Due: AM08:00, September 19
- Problem#1
  - Consider a MOS capacitor with N_a = 4X10^{15} cm^{-3}. Calculate the surface potential at $\left.\frac{d\phi}{dx}\right|_0$ = -10 kV/cm, -20 kV/cm, …, -100 kV/cm (10 cases) by using the Newton method. Specify the number of iterations.



Thank you for your attention!