Lecture 21 - The Si surface and the Metal-Oxide-Semiconductor Structure

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Reading assignment:

del Alamo, Ch. 8, §§8.1-8.2 (8.2.1-8.2.2)

Seminar:

Key questions

• How does the surface of a semiconductor look like at the atomic level?

• If one assembles a metal-oxide-semiconductor structure and allows equilibrium to be established, what is the final situation?

• How does this picture change for different choices of metal work function?
1. Semiconductor Surface

At a surface, perfect crystalline periodicity of solid comes to an abrupt end. What happens?

☐ *Ideal semiconductor surface*

Semiconductor comes to an end, but bulk properties unaffected → bonding arrangement at surface unchanged from bulk.

Zero carrier current normal to surface; other than that, carriers unaffected by surface.
Real surface

In ideal surface, four-fold coordination of atoms cannot be preserved \(\Rightarrow\) broken bonds \(\Rightarrow\) surface is very reactive.

Surface can lower its energy by:

- **surface contamination**: absorption of O, C, and other foreign atoms and molecules
- **surface reconstruction**: surface atoms bond among themselves.
Example of surface reconstruction: 7x7 (111) Si surface:

[courtesy of R. Martel and P. Avouris, IBM]
Passivated surface

"Coating" of semiconductor surface with passivating layer so that bulk bonding prevails for surface atoms.

Most important passivating material: SiO₂ - one of the keys of the microelectronics revolution:

- amorphous dielectric: only short-range order
- natural product of Si oxidation ("Si rusts!")
- exceptional chemistry
- nearly ideal interface with Si

Wide energy gap of SiO₂ prevents carriers from escaping from semiconductor.
Residual surface roughness in modern Si/SiO\textsubscript{2} structures: \( \sim 2 \) monolayers.

[courtesy of D. Buchanan, IBM]
2. Ideal Metal-Oxide-Semiconductor structure in thermal equilibrium

MOS structures pervasive in modern microelectronics:

- heart of MOSFETs (from which CMOS is made)
- heart of DRAMs, Flash memories
- MOS structure everytime a metal line runs over a dielectric-coated semiconductor

MOS understanding is portable ⇒ view it as generic sandwich of highly conducting material/dielectric/semiconductor (better name MIS)

- Al/SiO₂/Si (early MOSFETs)
- n⁺-polySi/SiO₂/Si (modern MOSFETs)
- Al/Si₃N₄/Si (metal lines on Si)
- WSi/AlGaAs/InGaAs (modern high-frequency transistors)
Energy band diagram (p-type substrate)

Insulator does not allow charge exchange between metal and semiconductor ⇒ to attain thermal equilibrium, need wire that connects metal and semiconductor.

\[ q\phi_{bi} = W_S - W_M \]

Note: large band discontinuities at insulator-semiconductor interface.
Other possible band arrangements depending on relative values of $W_S$ and $W_M$:
\( \square \) General relations for MOS electrostatics

- no charge in dielectric
- overall charge neutrality:
  \[ Q_g = -Q_s \]
- field inside dielectric uniform:
  \[ \mathcal{E}_{ox} = -\frac{Q_s}{\varepsilon_{ox}} \]
- normal component of displacement vector conserved at semiconductor/dielectric interface:
  \[ \varepsilon_s \mathcal{E}_s = \varepsilon_{ox} \mathcal{E}_{ox} \]
Hence field at semiconductor surface:

$$\mathcal{E}_s = -\frac{Q_s}{\varepsilon_s}$$

Total potential difference across structure:

$$\phi_{bi} = \phi_s + \phi_{ox}$$

-drop across semiconductor, $\phi_s$, called *surface potential*

-drop in oxide:

$$\phi_{ox} = x_{ox} \mathcal{E}_{ox}$$

Define *oxide capacitance per unit area*:

$$C'_{ox} = \frac{\varepsilon_{ox}}{x_{ox}}$$

All together, total potential build-up across MOS:

$$\phi_{bi} = \phi_s - \frac{Q_s}{C'_{ox}}$$

Key relationship between $\phi_s$ and $Q_s$. 
\[ \text{Depletion} \]

Do depletion approximation:
Integrated semiconductor charge:

\[ Q_s \simeq -qN_A x_d \]

Field at semiconductor surface:

\[ \mathcal{E}_s \simeq \frac{qN_A x_d}{\epsilon_s} \]

Field in insulator:

\[ \mathcal{E}_{ox} \simeq \frac{qN_A x_d}{\epsilon_{ox}} \]

Surface potential:

\[ \phi_s \simeq \frac{qN_A x_d^2}{2\epsilon_s} \]

Everything in terms of \( x_d \), but don’t know \( x_d \)!
Demand $\phi_{bi}$ be the right amount from energy considerations:

$$\phi_{bi} = \frac{1}{q}(W_S - W_M) = \phi_s + \phi_{ox} \simeq \frac{qN_Ax_d^2}{2\epsilon_s} + \frac{qN_Ax_d}{C_{ox}}$$

Solve for $x_d$:

$$x_d \simeq \frac{\epsilon_s}{C_{ox}}\left(\sqrt{1 + \frac{4\phi_{bi}}{\gamma^2}} - 1\right)$$

Where $\gamma$ is body-factor coefficient:

$$\gamma = \frac{1}{C_{ox}\sqrt{2\epsilon_s qN_A}}$$

Key dependencies: $\phi_{bi} \uparrow \rightarrow x_d \uparrow$

$$N_A \uparrow \rightarrow x_d \downarrow$$
Body-factor coefficient, $\gamma$:

$$
\gamma = \frac{1}{C_{ox}} \sqrt{2 \epsilon_s q N_A}
$$

$\gamma$ depends on:

- doping of body
- capacitance of insulator

$\Rightarrow$ relative magnitude of depletion capacitance and oxide capacitance.

In well designed MOSFETs, $\gamma \sim 0.1 - 1 \ V^{1/2}$. 
\[ Q_s = Q_d + Q_i \]
Key conclusions

• Si/SiO₂ interface nearly ideal: most Si bonds satisfied but interface about two monolayers rough.

• Most typical equilibrium case of MOS structure: depletion region next to Si/SiO₂ interface; other possible cases: accumulation or inversion.

• Surface potential, \( \phi_s \): total potential build-up across semiconductor.

• General relationships for MOS electrostatics:
  
  – overall charge neutrality: \( Q_g = -Q_s \)
  
  – continuity of normal displacement vector at semiconductor/insulator interface: \( \varepsilon_s \mathcal{E}_s = \varepsilon_{ox} \mathcal{E}_{ox} \)
  
  – total potential difference must add up to \( \phi_{bi} \): \( \phi_{bi} = \phi_s - \frac{Q_s}{C_{ox}} \)

• Order of magnitude of key parameters of Si at 300K:
  
  – Body factor coefficient: \( \gamma \sim 0.1 - 1 \, V^{1/2} \) (depends on doping level of semiconductor and insulator capacitance).