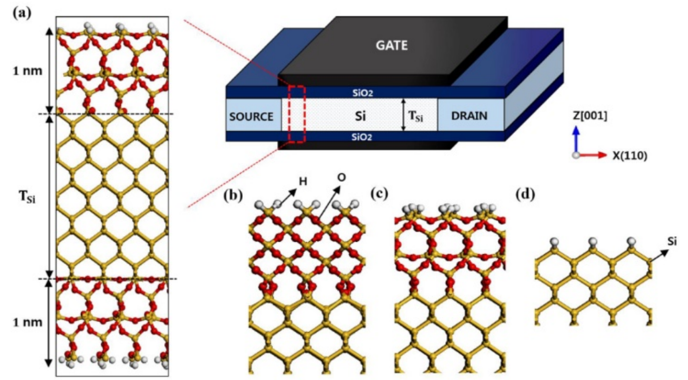
Lecture 11 – 27/11/2024

- Metal-semiconductor junction: Schottky vs Ohmic contact
- Basic features of a heterojunction
- Formation of an insulating layer: case of SiO_2 on silicon
- Absorption
    - General insights into the light absorption process



Summary Lecture 10

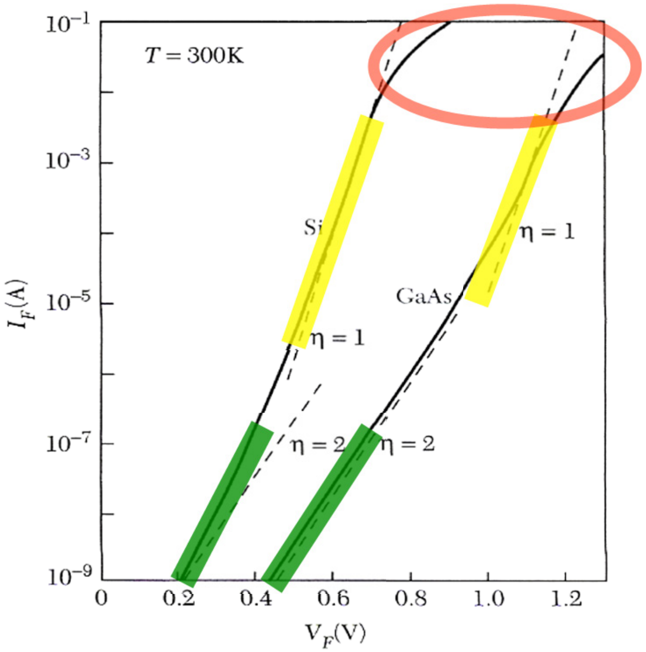
$$r \approx \frac{1}{\tau}\frac{n_i^2(e^{eV/k_BT}-1)}{2n_i+p+n} \quad \text{and} \quad J_{g,r} = e\int_{-x_p}^{x_n} r\,dx$$

$\Rightarrow$

Reverse bias: $J_g = -\frac{en_i}{2\tau_e}W$

Forward bias: $J_r = \frac{en_i}{2\tau_e}W_{eff}$ with $W_{eff} = W\,e^{eV/2k_BT}$

Experimental I-V curves:



$\eta = 1$ when diffusion current dominates

$\eta = 2$ when recombination current dominates

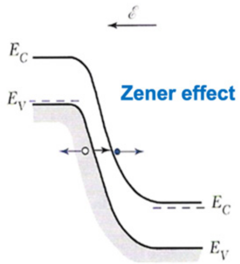
$\Rightarrow \quad I \propto \exp\left(\frac{eV}{\eta KT}\right)$

Series resistance @ high current: potential drop IR_S

$\Rightarrow \quad I \propto \exp\left(\frac{e(V-IR_S)}{\eta KT}\right)$

Summary Lecture 10

- **Highly doped: Zener diode** (tunneling-based)

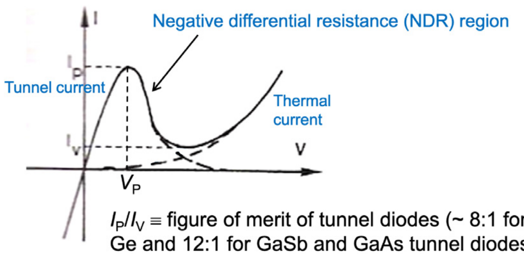


Breakdown condition: $\exists E_{max} = E_c$ such that impact ionization occurs

- **Lightly doped: Avalanche diode** (breakdown-based)

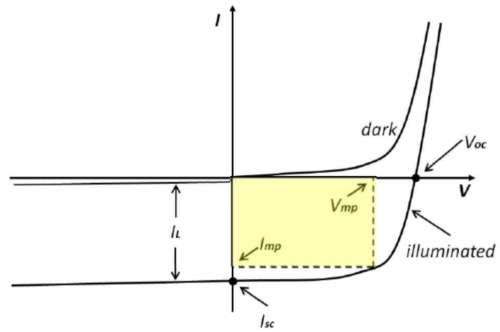
$$V_{B_{av}} = \frac{\epsilon_r \epsilon_0 E_c^2}{2e}(N_B)^{-1}$$

- **Highly doped: Tunnel diode** (tunneling-based)



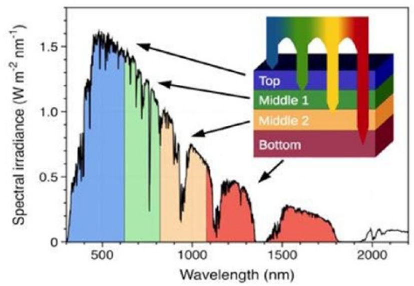
$I_P/I_V \equiv$ figure of merit of tunnel diodes (~ 8:1 for Ge and 12:1 for GaSb and GaAs tunnel diodes)

Application: solar cells



P = *IV* < 0 (produces power)

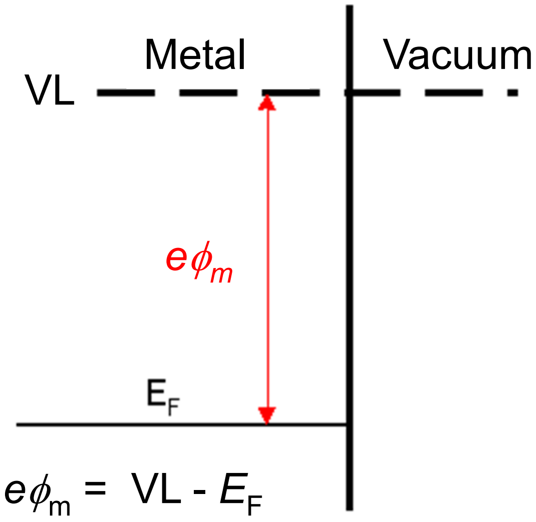
Conversion efficiency: $\eta = \frac{I_{mp}V_{mp}}{P_{in}}$



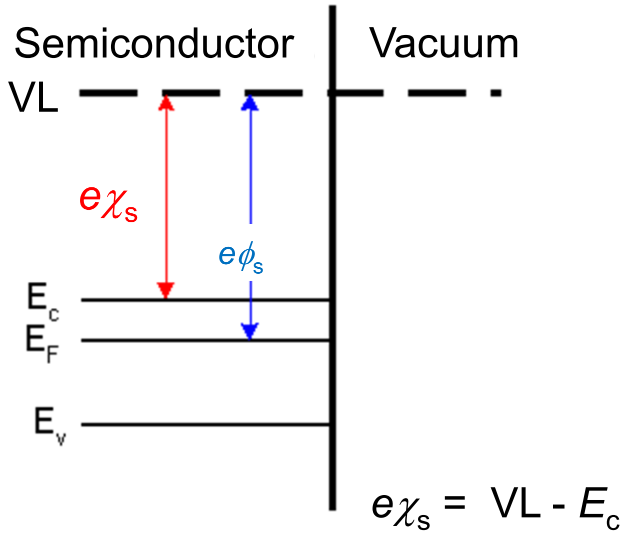
Higher solar cell efficiency

Work function and electron affinity

VL: vacuum level



Work function of a metal



Work function of a semiconductor and its electron affinity

Metals with small work function

	Li	Na	K	Rb	Cs	Fr
(eV)	2.3	2.3	2.2	2.2	1.8	1.8

Metals with large work function

	Cr	Fe	Ni	Al	Cu	Ag	Au	Pt
(eV)	4.6	4.4	4.4	4.3	4.4	4.3	4.8	5.3

Electron affinity

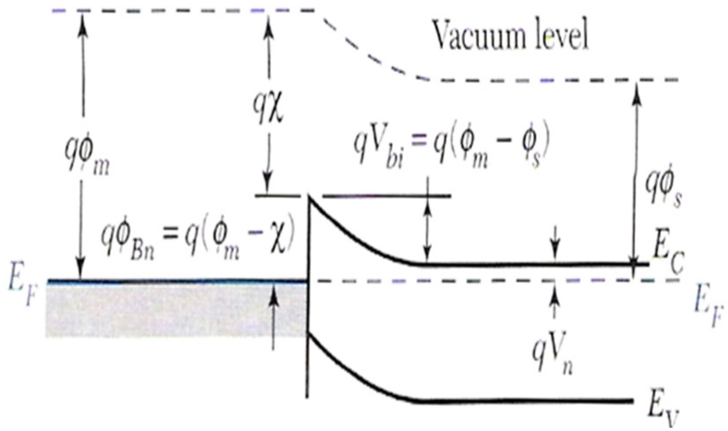
	Si	Ge	GaP	GaAs	GaSb	SiO_2
(eV)	4.01	4.13	4.3	4.07	4.06	1.1

Metal-semiconductor junction

At thermal equilibrium

Vacuum level continuous and // to the band edges ⇒ Creation of a depletion region

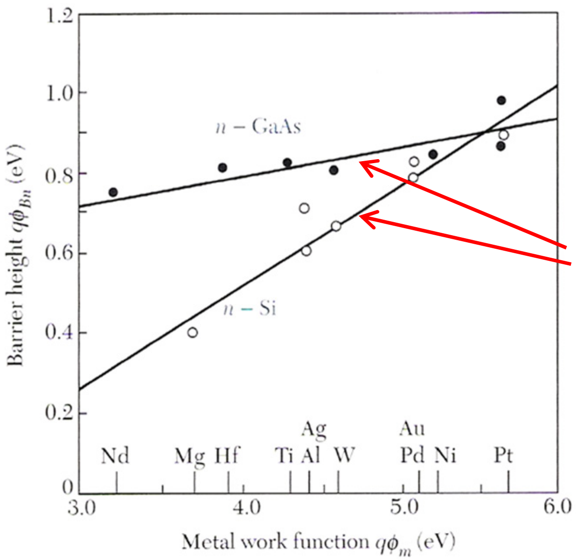
Metal-semiconductor junction



$\phi_m > \phi_s$

$e\phi_{Bn} = e(\phi_m - \chi)$

$eV_{bi} = e\phi_{Bn} - eV_n$ with $eV_n = E_C - E_F$
due to equalization of the Fermi levels

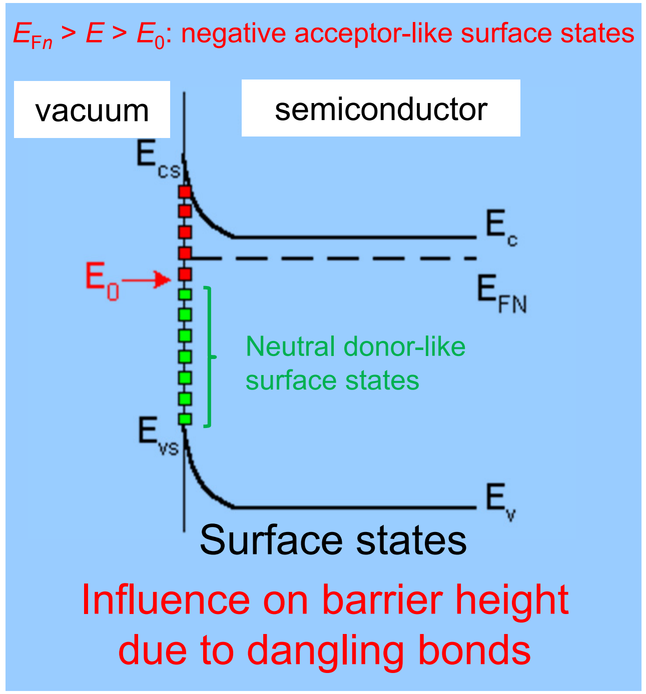


Role of surface states

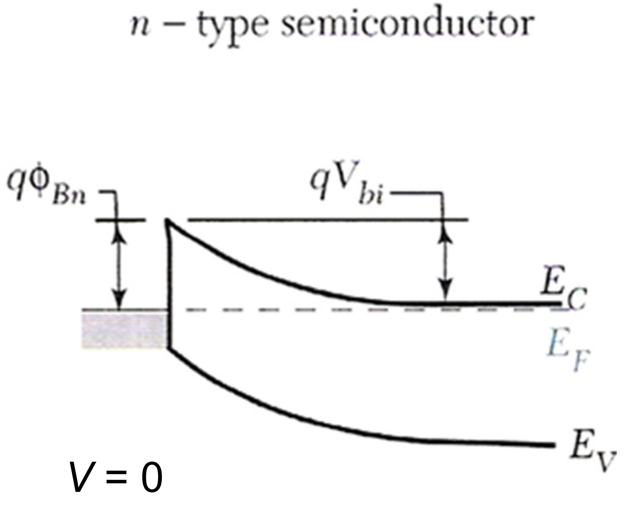
⇒

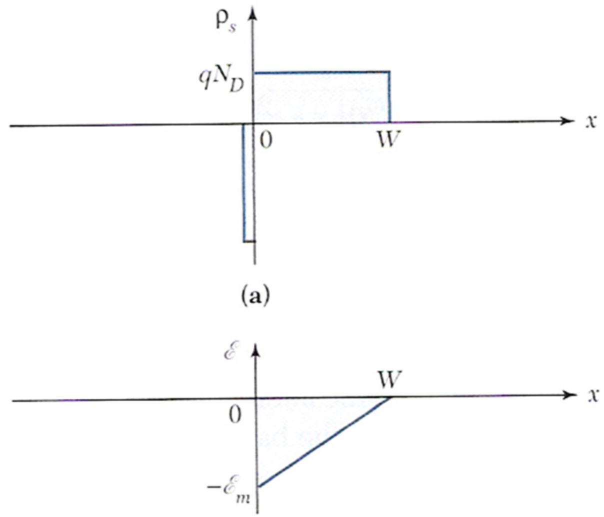
Different slopes despite a similar electron affinity close to 4 eV (cf. slide #4)!

In practice, the Fermi level at the interface is "pinned" by surface states and the actual Schottky barrier height becomes independent of the metal work function



Metal-semiconductor junction





Surface charge density

Surface state density per unit of energy

$$\sigma = -eN_{ss}(E_F - E_0)$$

Electrical neutrality

$$-\sigma = eN_D W$$

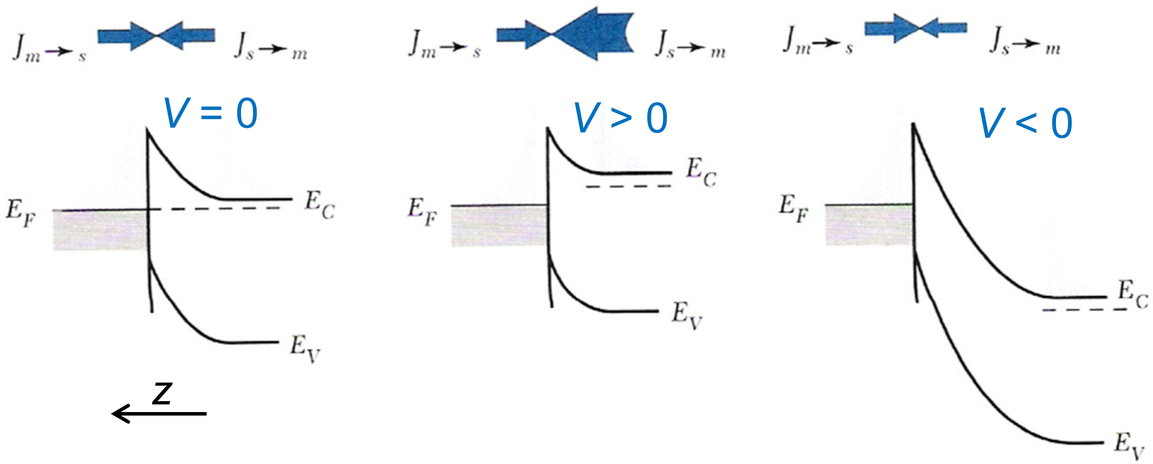
Potential drop across the depletion region

$$V_{bi} = -\frac{\sigma W}{2\varepsilon},$$ use of Poisson's equation + boundary conditions

Details to be seen in the series

Metal-semiconductor junction

Schottky diode (thermionic emission theory)



$J(V) = J_{s\to m} + J_{m\to s}$, at equilibrium $J_{s\to m} = -J_{m\to s}$ but when a potential V is applied, a dissymmetry arises between the metal and the semiconductor (change in barrier height) $\Rightarrow$ rectifying behavior of the diode

$J_{s\to m} = e\dfrac{n(0)}{2}\langle v_z\rangle$ with $\langle v_z\rangle = \left(\dfrac{2k_B T}{\pi m^*}\right)^{0.5}$ (derived from Boltzmann velocity distribution) and $n(0) = N_C \exp\left(-\dfrac{q\phi_B}{k_B T}\right)$

$J(V) = J_S\left[\exp\left(\dfrac{qV}{k_B T}\right) - 1\right]$ with $J_S = A^* T^2 \exp\left(-\dfrac{q\phi_B}{k_B T}\right)$ A^* is the effective Richardson constant

J_S based on the majority carrier properties (unipolar device)

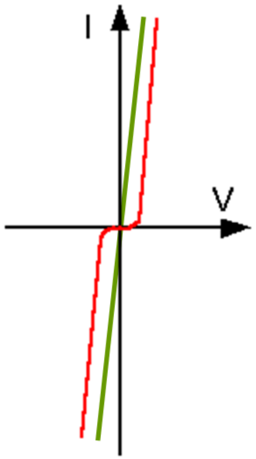
Ohmic contact $\Rightarrow$ the barrier height must be low enough

Details to be seen in the series

Metal-semiconductor junction

Ohmic contact

Very thin barrier



Contact resistance

$$R_C = \left(\frac{\partial J}{\partial V}\right)^{-1}_{V=0} = \frac{k_B}{eA^*T}\exp\left(\frac{q\phi_B}{k_B T}\right)$$

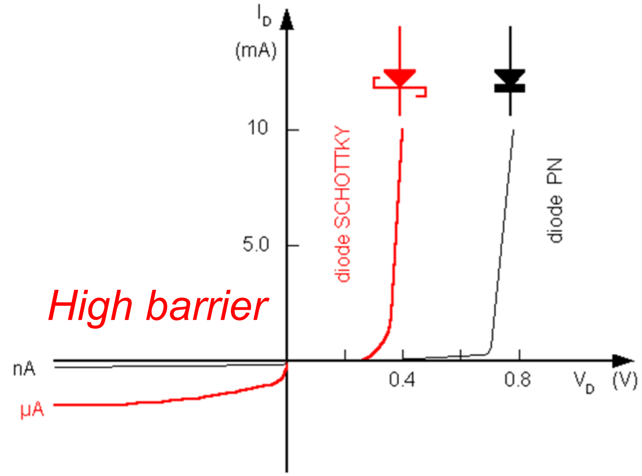
$\Rightarrow$ small Schottky barrier height required

- Low barrier height $\Rightarrow$ non-rectifying M-S contact
- Heavy doping conditions $\rightarrow$ barrier thickness relatively thin $\rightarrow$ **tunneling** becomes the dominating process for current transport (over the thermionic one)

Tunneling current $I \propto \exp\left[-2W\left(2m^*\left(q\phi_B - qV\right)/\hbar^2\right)^{1/2}\right]$ with $W^2 \sim \frac{2\varepsilon}{eN_D}\left(\phi_B - V\right)$

$R_C \sim \exp\left[\frac{4\left(m^*\varepsilon\right)^{1/2}\phi_B}{\hbar N_D^{1/2}}\right] \propto \exp\left[\frac{\phi_B}{N_D^{1/2}}\right]$, strong dependence on the doping level

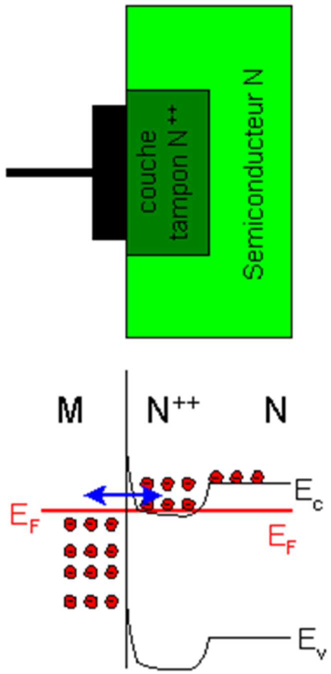
Schottky diode



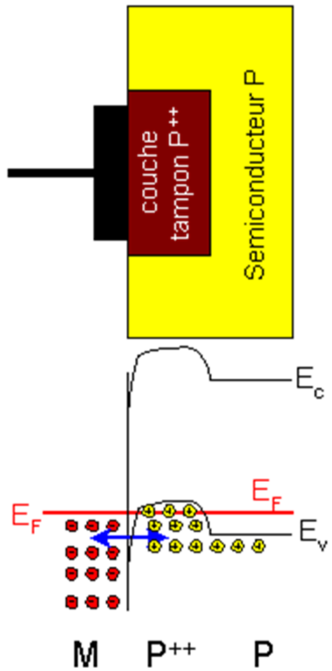
Ohmic contact

- Negligible contact resistance vs series resistance of the semiconductor
- Transfer of the requested current at the contact level will occur with a small potential drop vs potential drop occurring in the active region of the device

Ohmic contacts



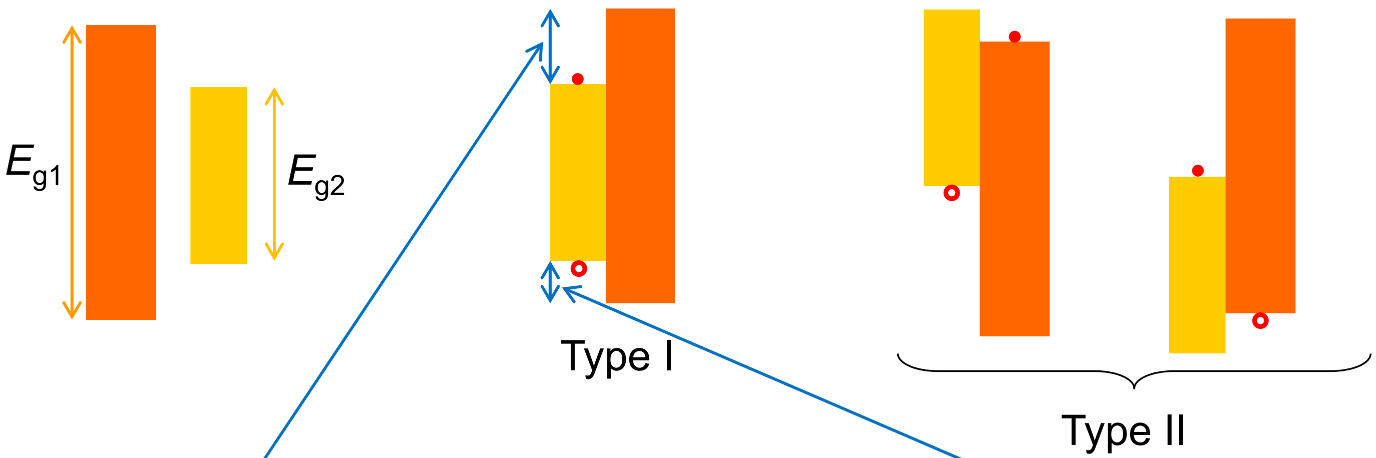
n-type semiconductor



p-type semiconductor

Heterostructures: band offsets

Different configurations



In III-V semiconductor compounds sharing the same anion: $\Delta V_{VB} \approx 0.3 \times \Delta E_g$

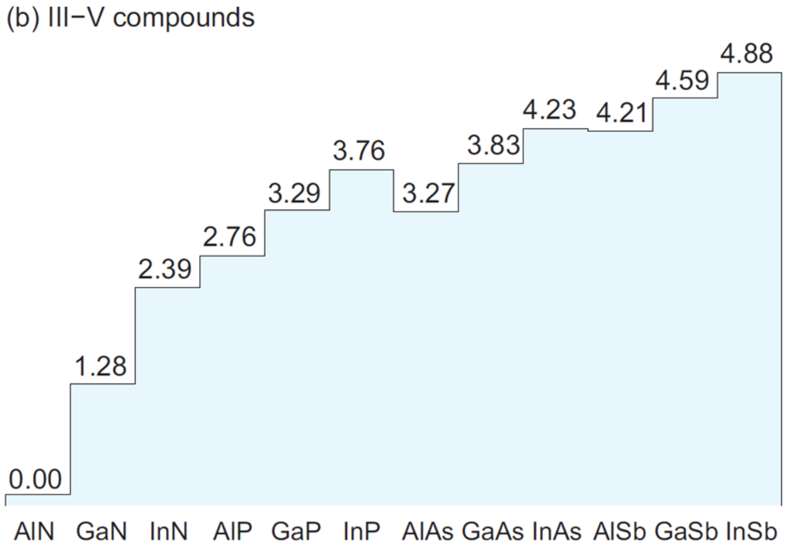
Valence band offset

$\Rightarrow \Delta V_{CB} \approx 0.7 \times \Delta E_g$

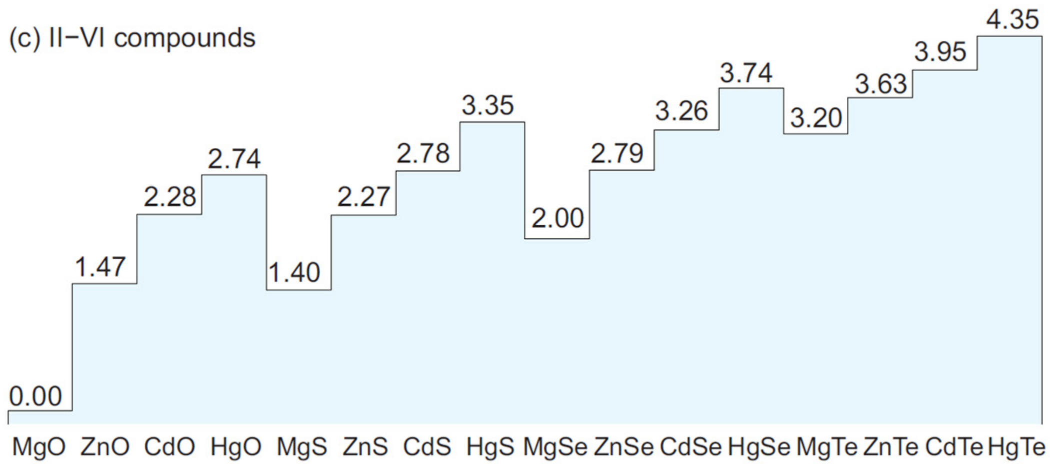
Conduction band offset

Heterostructures: band offset

Valence band offset (VBO)

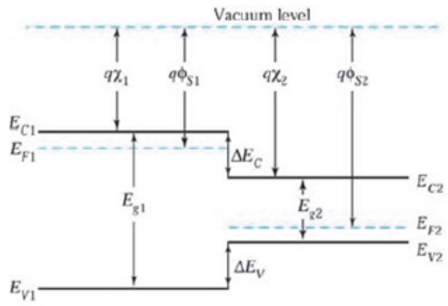


The quoted values are all expressed in eV!

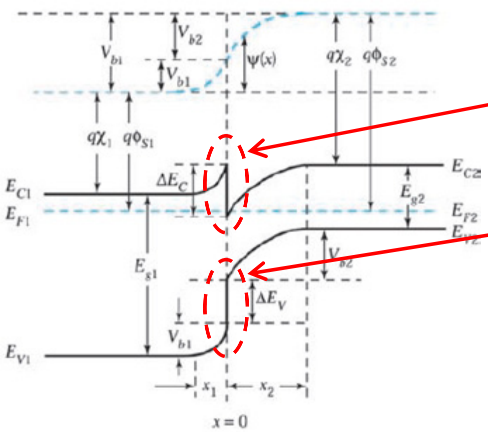


- VBOs can be computed not only for binary compounds but also ternary alloys using the rules detailed in **Lecture 1**

Heterostructures: band offset



(a)



(b)

$q\phi_{si}$: work functions; $q\chi_i$: electron affinities

Vacuum level continuous and // to the band edges

Band alignment (case of a type I heterojunction)

1. We draw the energy bands before "physically" connecting them, including the position of E_F
2. At thermal equilibrium, E_F is constant throughout the structure
3. *The bandgap is conserved throughout the structure $\Rightarrow$ it is material and position dependent physical quantity*
4. *Strong curvature of the bands in the space charge region with a singularity occurring for one of the bands while an abrupt jump occurs for the other one (imposed by condition (2) and the continuity of the vacuum level (// to the band edges))*
5. Extension of the curved regions highly depends on the doping level (extent of depleted region as in the bulk case for a single material)
6. *The singularity is increased for a forward biased junction whereas it is decreased (cancelled) for a reverse biased junction*

Basic insights into the formation of SiO_2 films

Key features of SiO_2

Insulating material (dielectric) commonly used in the semiconductor industry for surface passivation that offers a tunable capacitance

- Band gap ~9-10 eV (exact value still debated)[1]
- Resistivity ~10^{15} Ω.cm
- Dielectric strength ~10 MV/cm (≡ maximum sustainable electric field without breakdown)
- Capacitance (per unit area) $C_o = \frac{\varepsilon_{ox}}{d}$ with *d* the oxide thickness

Specific case of silicon

SiO_2 films are mostly formed via thermal oxidation of silicon through the chemical reactions:

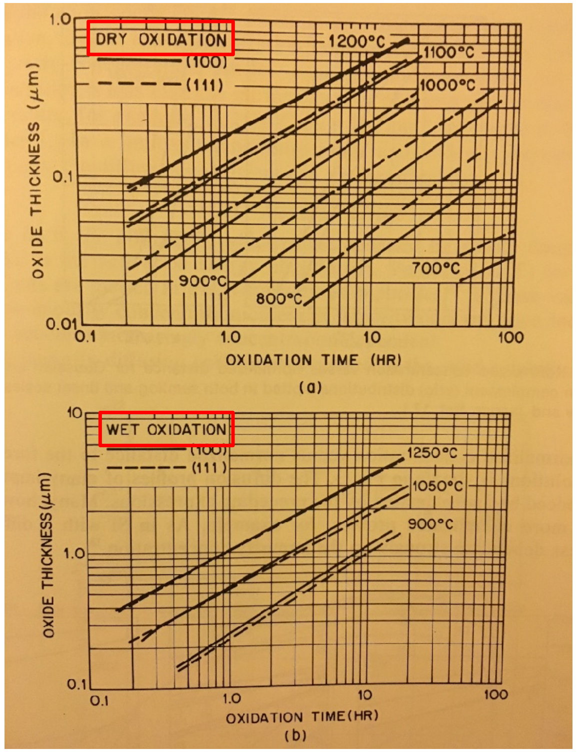
Si(solid) + O_2(dry oxygen) → SiO_2(solid) — Dry oxidation

or Si(solid) + $2H_2O$(steam) → SiO_2(solid) + $2H_2$ — Wet oxidation

[1] F. Messina *et al.*, Phys. Rev. Lett. **105**, 116401 (2010)

Basic insights into the formation of SiO_2 films

Experimental results of SiO_2 thickness as a function of the reaction time and temperature for two silicon substrate orientations

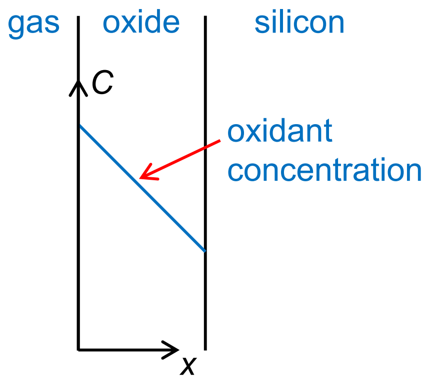


- For short reaction times, the oxide thickness *d* varies linearly as a function of time *t*
- *For* prolonged oxidation, *d* varies as $t^{1/2}$

⇒ inherited from the fact that the flux of the oxidant across the oxide layer can be described by a 1D diffusion process given by Fick's law and that the concentration of the oxidant within the oxide layer is linear.[1]

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2}$$

where *C* is the impurity concentration and *D* is the diffusion coefficient



3rd employee of Intel and 3rd CEO of Intel

[1]B. S. Deal and A. S. Grove, J. Appl. Phys. **36**, 3770 (1965) (> 3000 citations)

Basic insights into the formation of SiO_2 films

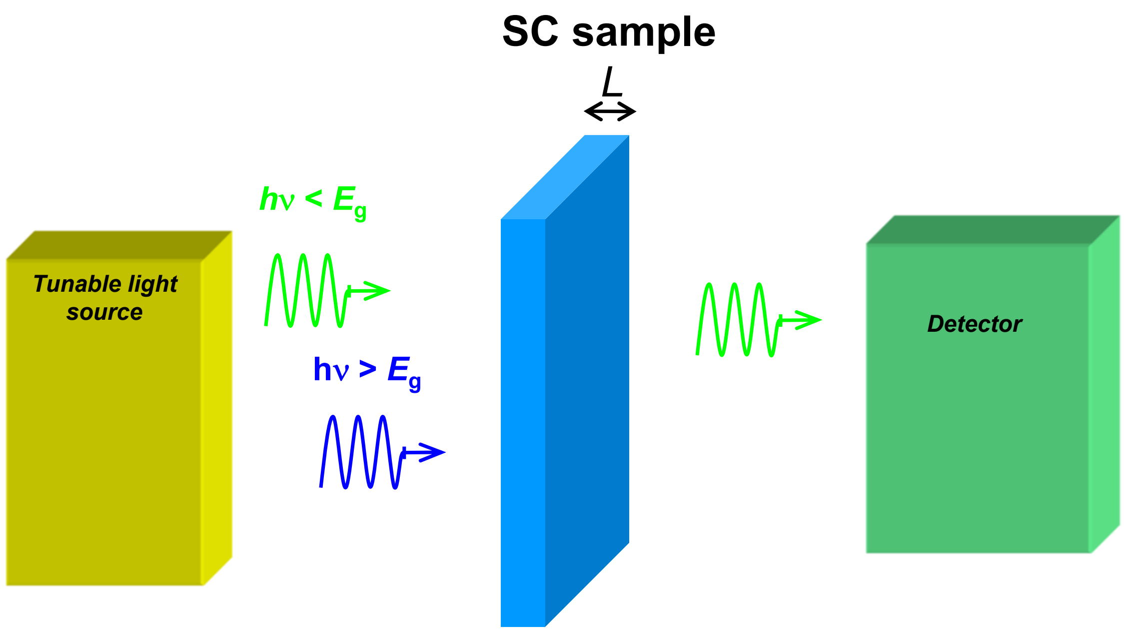
Experimental results of SiO_2 thickness as a function of the reaction time and temperature for two silicon substrate orientations

- At a given temperature, the oxidation rate in steam is about 5 to 10 times higher than for dry oxygen
- The oxidation rates show pronounced dependence on crystal orientation when decreasing the temperature
- The crystal orientation ((100) vs (111), which are the two most common orientations for silicon wafers with the (100) orientation being the CMOS compatible one) does not seem to play a role as far as the oxidation rate is concerned for temperatures in excess of 1200°C
- For lower temperatures while for dry oxygen growth the oxidation rate is faster for the (111) orientation, the reverse situation is achieved for steam growth
- The Si (100) orientation prevails in the industry. It exhibits a reasonably fast oxidation rate under steam growth (at 1250°C, 400 nm after 10' and ~1 μm after 1 hour))

Absorption

Absorption in semiconductors

Experimental evidence



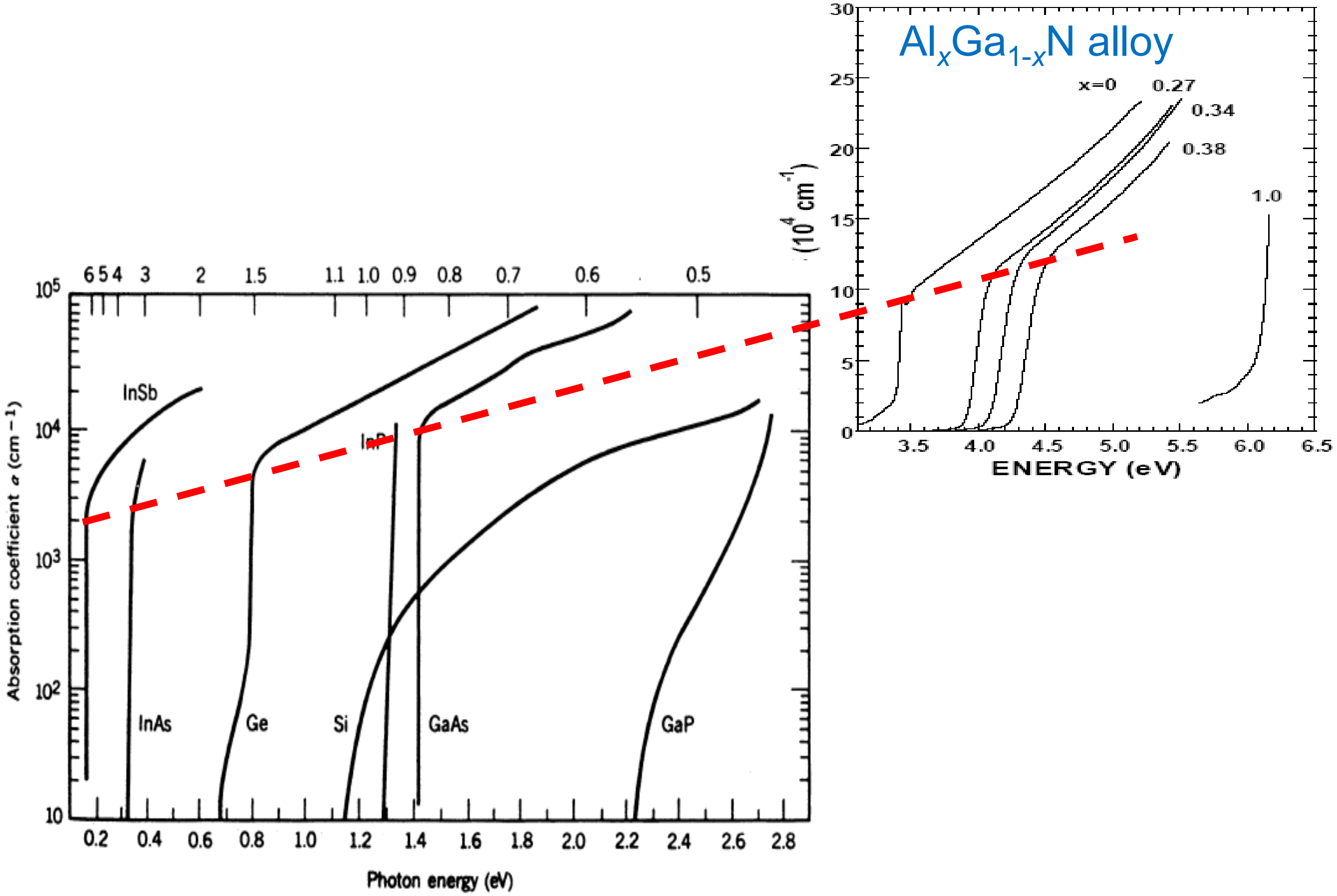
If one neglects surface reflection, then for $h\nu > E_g$

$$I_{\text{transmitted}} = I_{\text{initial}} \exp(-\alpha L)$$

α is the absorption coefficient

(usually expressed in cm^{-1})

Absorption: experimental considerations



The absorption coefficient at the (direct) band gap increases together with the energy of the band gap

Absorption in diamond

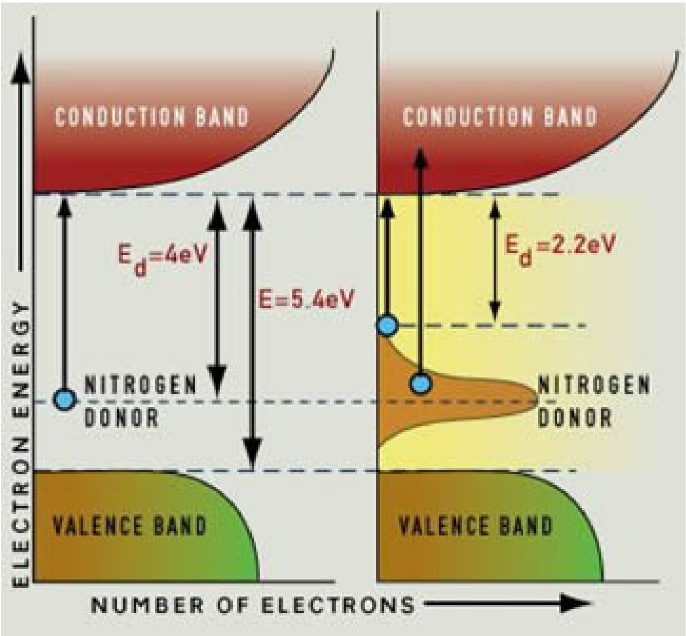
Band gap ~ 5.4-5.5 eV
(~225 nm)

C:N	yellow
C:B	blue

N and B are dopants acting as donors and acceptors, respectively

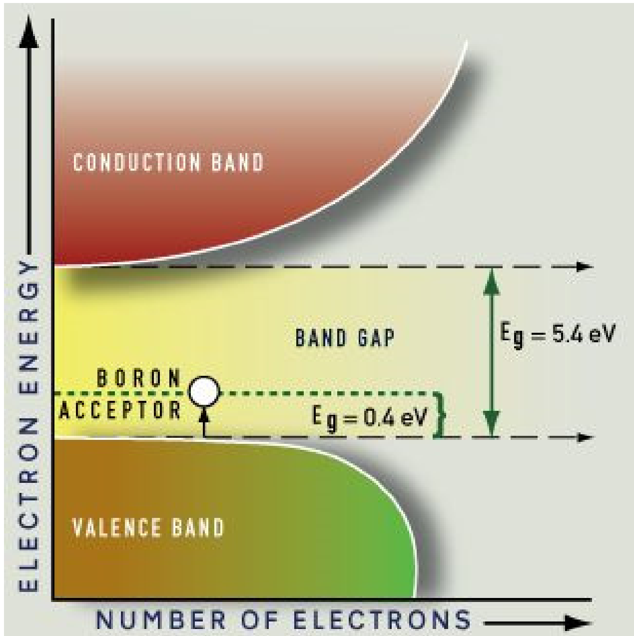
Absorption in diamond

C:N



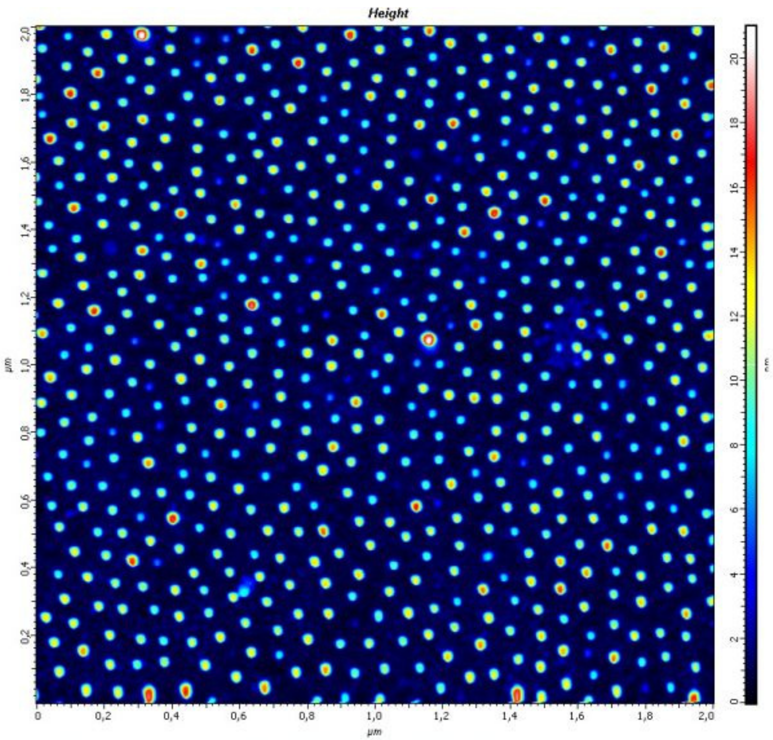
E = 2.2 eV ≈ 563 nm

C:B

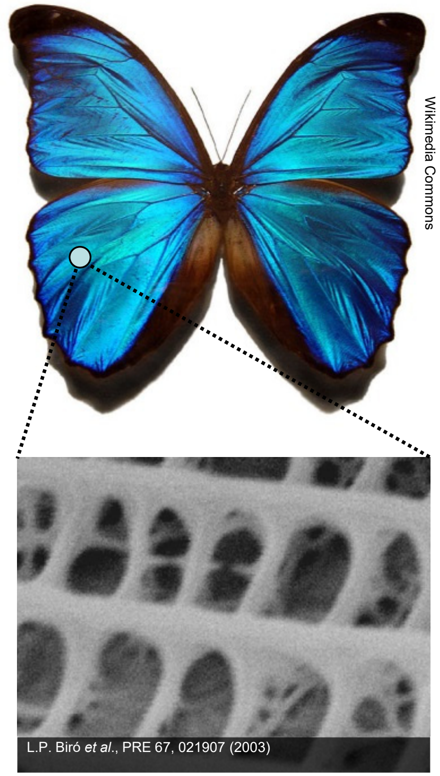


The absorption tapers off throughout the visible light energies in C:B diamond

Other origins of colored materials



http://webexhibits.org/causesofcolor



Photonic bandgap