

## Lecture 2 - Carrier Statistics in Equilibrium

September 5, 2002

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1. Conduction and valence bands, bandgap, holes
2. Intrinsic semiconductor
3. Extrinsic semiconductor
4. Conduction and valence band density of states

### Reading assignment:

del Alamo, Ch. 2, §§2.1-2.4 (2.4.1)

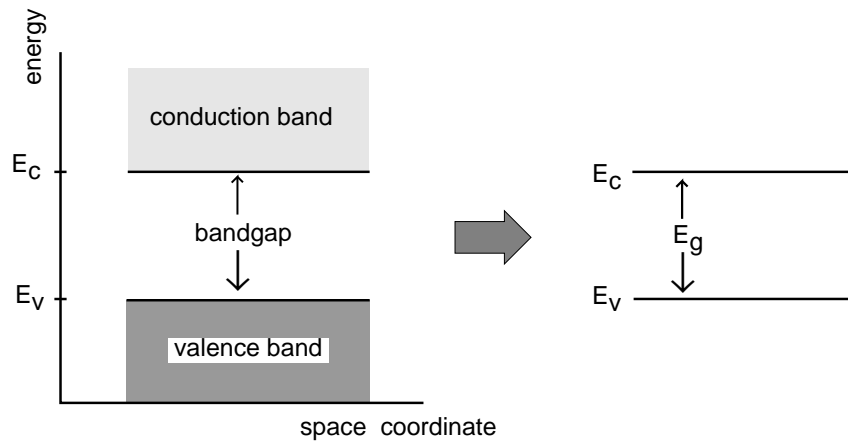
### Announcement:

Go to <http://weblab.mit.edu> and register. Put "6.720 student" in the Description field.

## Key questions

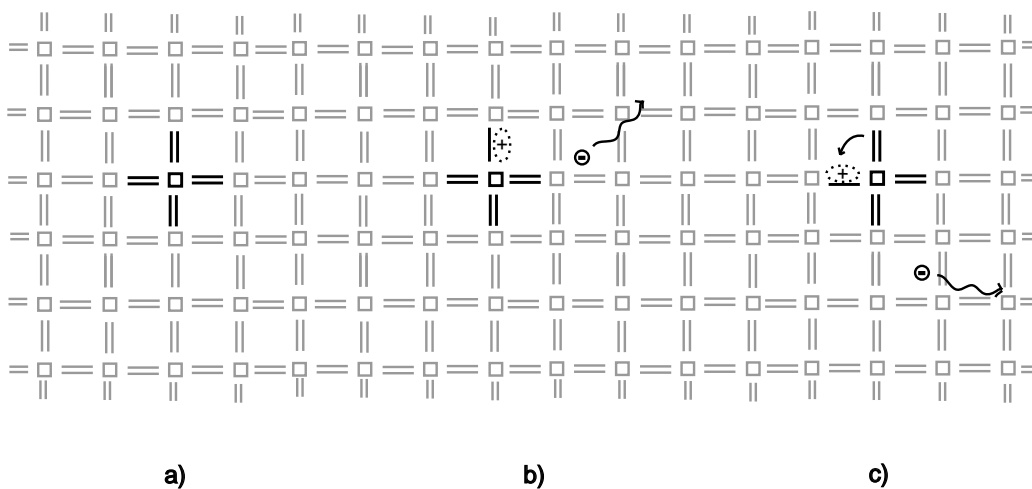
- What are these "energy band diagrams"?
- What are these "holes"?
- In a perfectly pure semiconductor, how many electrons and holes are there?
- Can one engineer the electron and hole concentrations in a semiconductor?

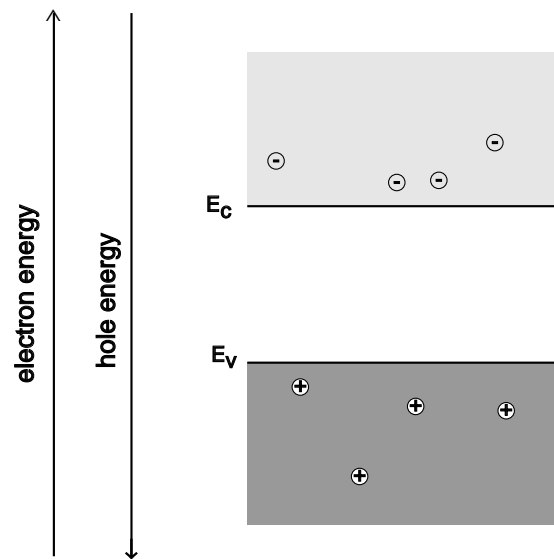
# 1. Conduction and valence bands, bandgap, holes



Conduction and valence bands:

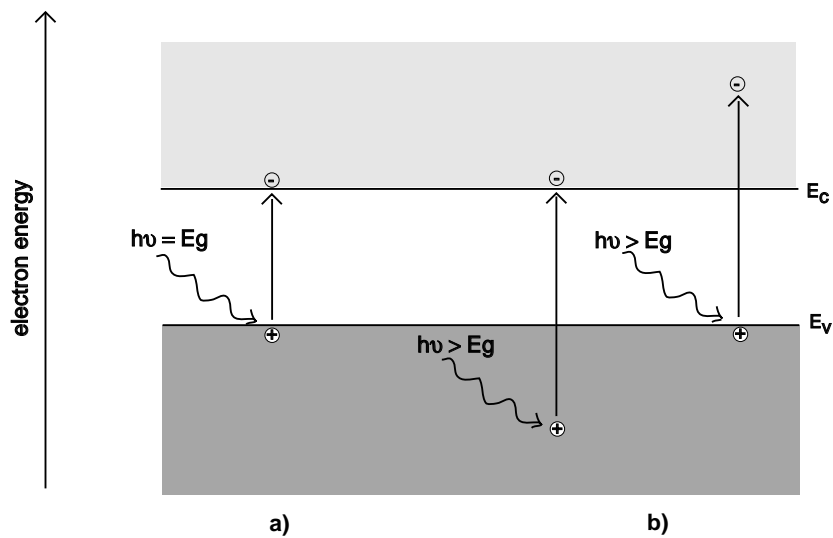
- *bonding electrons* occupy states in valence band
- "*free*" electrons occupy states in conduction band
- *holes*: empty states in valence band
- CB electrons and VB holes can move around: "*carriers*"





Elements of energy band diagrams:

- at edges of bands, kinetic energy of carriers is zero
- electron energies increase upwards
- hole energies increase downwards



## 2. Intrinsic semiconductor

Define *intrinsic semiconductor*, or "ideal" semiconductor:

- perfectly crystalline (no perturbations to periodic lattice)
- perfectly pure (no foreign atoms)
- no surface effects

Question: *How many electrons and holes are there in an intrinsic semiconductor in thermal equilibrium?*

Answer requires fairly elaborate model [lecture 3], but key dependencies can be readily identified.

Define:

$n_o \equiv$  equilibrium (free) electron concentration in conduction band [ $cm^{-3}$ ]

$p_o \equiv$  equilibrium hole concentration in valence band [ $cm^{-3}$ ]

Certainly in intrinsic semiconductor:

$$n_o = p_o = n_i$$

$n_i \equiv$  intrinsic carrier concentration [ $cm^{-3}$ ]

Key dependencies of  $n_i$ :

- *Temperature:*

$$T \uparrow \Rightarrow n_i$$

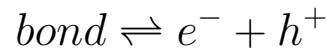
- *Bandgap:*

$$E_g \uparrow \Rightarrow n_i$$

What is detailed form of dependencies?

Use analogy of chemical reactions.

Electron-hole formation can be thought of as chemical reaction:



similar to water decomposition reaction:



*Law-of-mass action* relates concentration of reactants and reaction products. For water:

$$K = \frac{[H^{+}][OH^{-}]}{[H_2O]} \sim \exp\left(-\frac{E}{kT}\right)$$

$E$  is energy consumed or released in reaction.

This is a "*thermally activated*" process  $\Rightarrow$  rate of reaction limited by need to overcome energy barrier  $E$  (*activation energy*).

In analogy, for electron-hole formation:

$$K = \frac{n_o p_o}{[bonds]} \sim \exp\left(-\frac{E_g}{kT}\right)$$

$[bonds]$  is concentration of unbroken bonds.

Note: activation energy is  $E_g$ .

In general, relatively few bonds are broken. Hence:

$$[bonds] \gg n_o, p_o$$

and

$$[bonds] \simeq constant$$

Then:

$$n_o p_o \sim \exp\left(-\frac{E_g}{kT}\right)$$

Two important results:

- First,

$$n_i \sim \exp\left(-\frac{E_g}{2kT}\right)$$

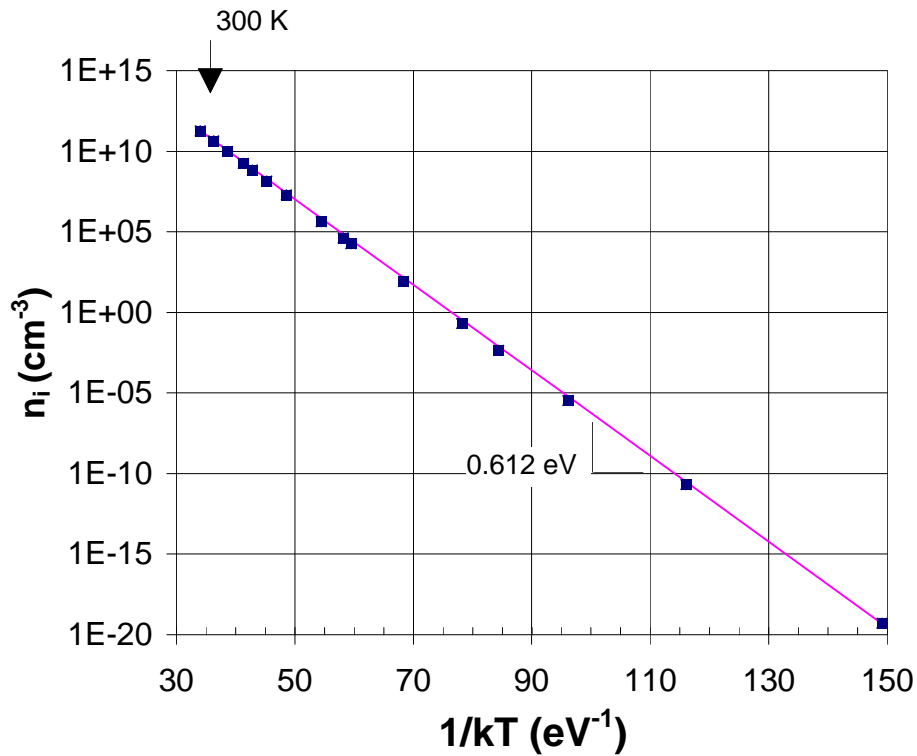
As expected:  $T \uparrow \Rightarrow n_i \uparrow$

$$E_g \uparrow \Rightarrow n_i \downarrow$$

To get prefactor, need detailed model [lecture 3].



Arrhenius plot for Si [experiments of Misiakos and Tsamakis, 1993]:



In Si at  $300 \text{ K}$ ,  $n_i \simeq 1.1 \times 10^{10} \text{ cm}^{-3}$ .

- Second important result:

$$n_o p_o = n_i^2$$

*Equilibrium np product in a semiconductor at a certain temperature is a constant specific to the semiconductor.*

### 3. Extrinsic semiconductor

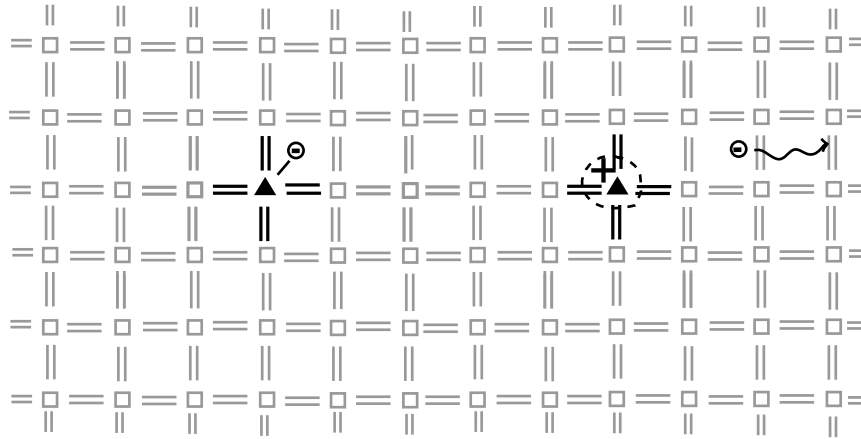
Can electron and hole concentrations be engineered?

Insert *dopants* in substitutional positions in the lattice:

- **Donors:** introduce electrons to conduction band without introducing holes to valence band
- **Acceptors:** introduce holes to valence band without introducing electrons to conduction band

If any one carrier type overwhelms  $n_i \Rightarrow$  extrinsic semiconductor

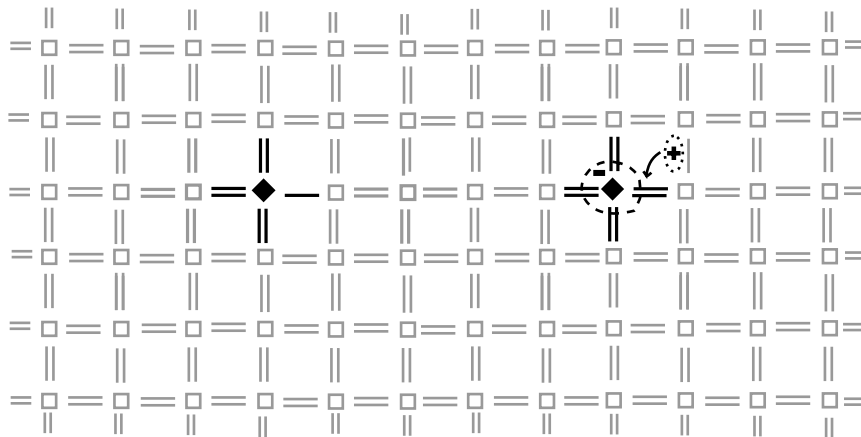
Donor in Si, atom from column V (As, P):



a) neutral donor

b) ionized donor

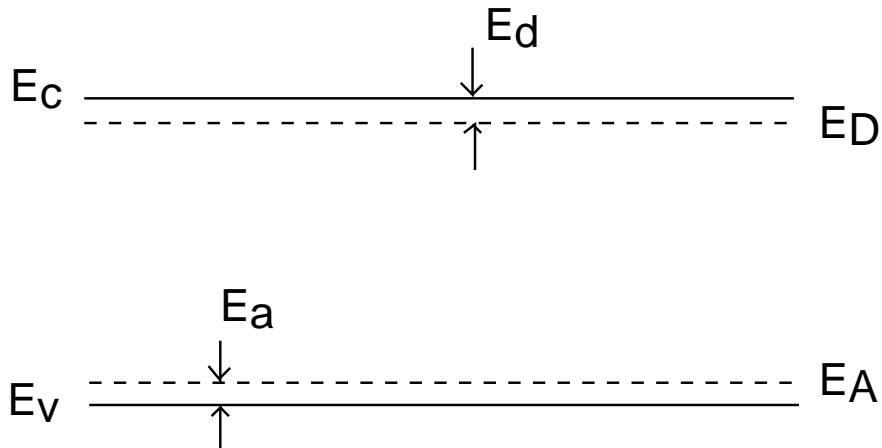
Acceptor in Si, atom from column III (B):



a) neutral acceptor

b) ionized acceptor

Representation of donor and acceptor states in energy band diagram:



$E_d, E_a \sim 40 - 60 \text{ meV}$ , for common dopants

□ Near room temperature, all dopants are ionized:

$$N_D^+ \simeq N_D$$

$$N_A^- \simeq N_A$$

Typical doping levels:

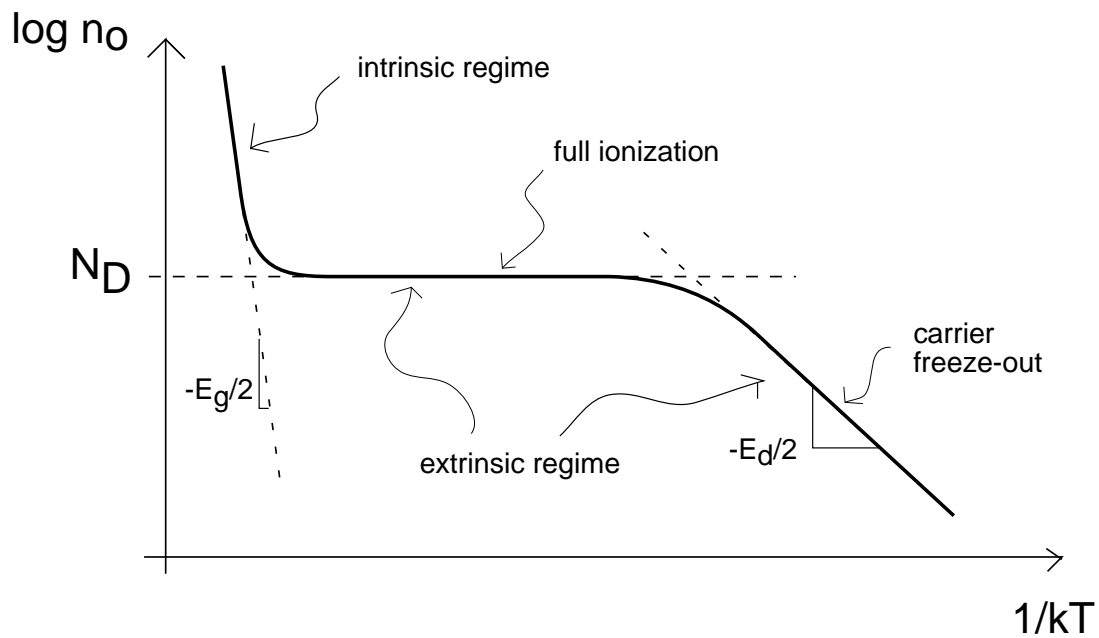
$$N_A, N_D \sim 10^{15} - 10^{20} \text{ cm}^{-3}$$

## □ n-type semiconductor

$$n_o \simeq N_D$$

$$p_o \simeq \frac{n_i^2}{N_D}$$

These equations are valid at intermediate temperatures.

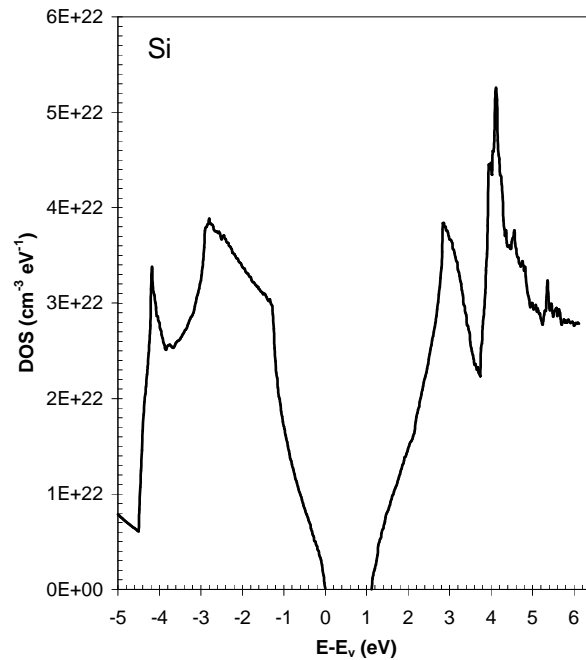


## □ p-type semiconductor

$$p_o \simeq N_A$$

$$n_o \simeq \frac{n_i^2}{N_A}$$

## 4. Conduction and valence band density of states

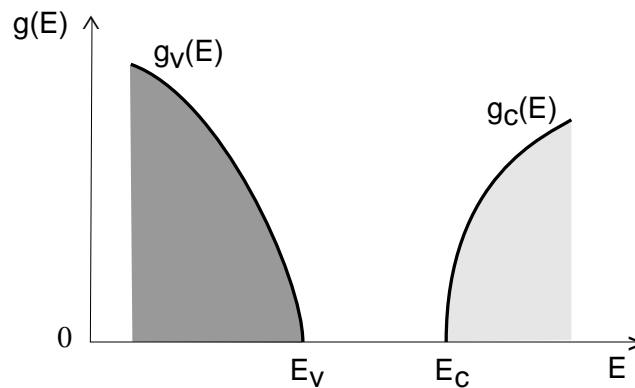


[Calculations by M. Fischetti, IBM]

Close to edges:

$$g_c(E) \propto \sqrt{E - E_c} \quad E \geq E_c$$

$$g_v(E) \propto \sqrt{E_v - E} \quad E \leq E_v$$



Common expressions for DOS:

$$g_c(E) = 4\pi \left( \frac{2m_{de}^*}{h^2} \right)^{3/2} \sqrt{E - E_c} \quad E \geq E_c$$

$$g_v(E) = 4\pi \left( \frac{2m_{dh}^*}{h^2} \right)^{3/2} \sqrt{E_v - E} \quad E \leq E_v$$

$m_{de}^*$   $\equiv$  density of states electron effective mass

$m_{dh}^*$   $\equiv$  density of states hole effective mass

Three comments:

- $m_{de}^*$ ,  $m_{dh}^*$  values given in terms of  $m_o$ , electron rest mass  
*i.e.* for Si at 300 K,  $m_{de}^* = 1.09m_o$ ,  $m_{dh}^* = 1.15m_o$

$$m_o = 5.69 \times 10^{-16} \text{ eV} \cdot \text{s}^2 / \text{cm}^2$$

- other "effective masses" defined: conductivity, longitudinal, transversal, light-hole, heavy-hole, etc; only DOS  $m^*$  should be used to compute DOS
- values of DOS  $m^*$  are definition sensitive

## Key conclusions

- Concept of *(free) electron*: electron in conduction band.
- Concept of *hole*: empty state in valence band.
- *Intrinsic semiconductor*: ideally pure semiconductor.

$$n_o = p_o = n_i \sim \exp\left(-\frac{E_g}{2kT}\right)$$

- To first order, for a given semiconductor  $n_o p_o$  is a constant that only depends on  $T$ :

$$n_o p_o = n_i^2$$

- Equilibrium carrier concentrations can be engineered through *shallow dopants*  $\Rightarrow$  *extrinsic semiconductor*.

– n-type semiconductor:

$$n_o \simeq N_D, \quad p_o \simeq \frac{n_i^2}{N_D}$$

– p-type semiconductor:

$$p_o \simeq N_A, \quad n_o \simeq \frac{n_i^2}{N_A}$$

- Around edges, conduction and valence bands in semiconductors feature  $DOS \sim \sqrt{E}$ .
- Order of magnitude of key parameters for Si at 300 K:
  - intrinsic carrier concentration:  $n_i \sim 10^{10} \text{ cm}^{-3}$
  - typical doping level range:  $N_D, N_A \sim 10^{15} - 10^{20} \text{ cm}^{-3}$



## Self study

- Charge neutrality