# Lecture 1 - Electronic structure of semiconductors

February 7, 2007

## Contents:

1. Electronic structure of semiconductors
2. Electron statistics
3. Thermal equilibrium

## Reading assignment:

del Alamo, Ch. 1

## Announcements:

Tomorrow's recitation slot will be used as lecture. This will be in exchange for lecture slot in May that will be used as recitation.

# Key questions

- What makes semiconductors so special?
- How do electrons arrange themselves (in energy) in an electronic system?
- What is the formal definition of thermal equilibrium? What are some of its consequences?

# 1. Semiconductors as solids

□ Semiconductors are crystalline solids

*Crystalline solid* = elemental atomic arrangement, or *unit cell*, repeated ad infinitum in space in three dimensions.

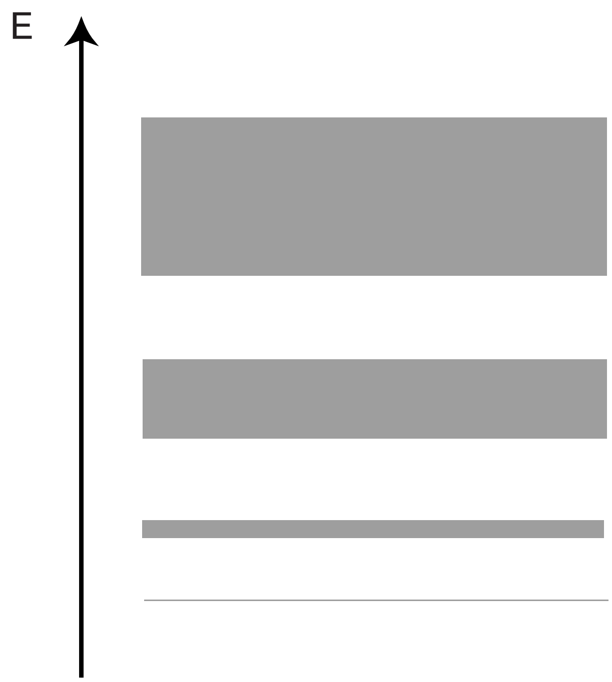
- Si lattice constant: 0.54 $nm$
- Si atomic spacing: 0.24 $nm$
- Si atomic density: $5.0 \times 10^{22}$ $cm^{-3}$

Semiconductors held together by *covalent bonding* ⇒ 4 valence electrons shared with 4 neighbours ⇒ low energy situation.

| IIB | IIIA | IVA | VA | VIA |
|---|---|---|---|---|
| | 5 B | 6 C | 7 N | 8 O |
| | 13 Al | 14 Si | 15 P | 16 S |
| 30 Zn | 31 Ga | 32 Ge | 33 As | 34 Se |
| 48 Cd | 49 In | 50 Sn | 51 Sb | 52 Te |

□ Solid is electronic system with *periodic potential*

Fundamental result of solid-state physics: *quantum states cluster in bands leaving bandgaps* (regions without allowed states) *in between.*

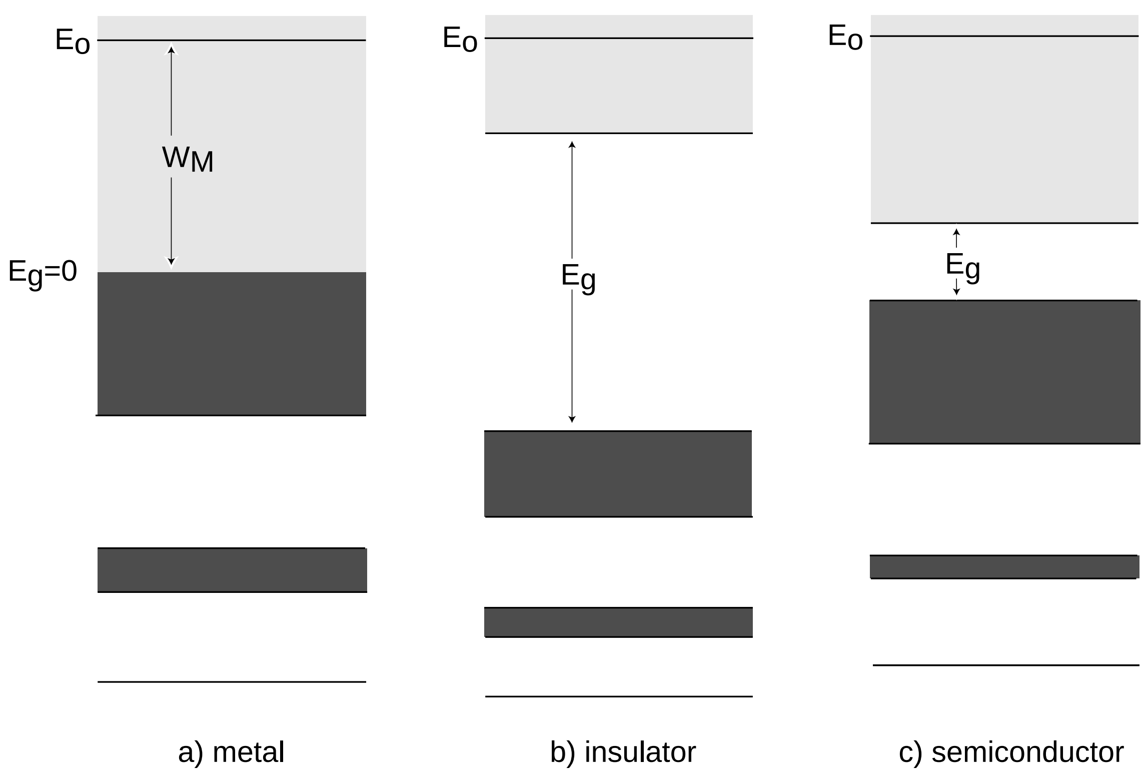


□ Electronic structure of semiconductors

There are many more quantum states than electrons in a solid.

Quantum states filled with one electron per state starting from lowest energy state (*Pauli exclusion principle*).

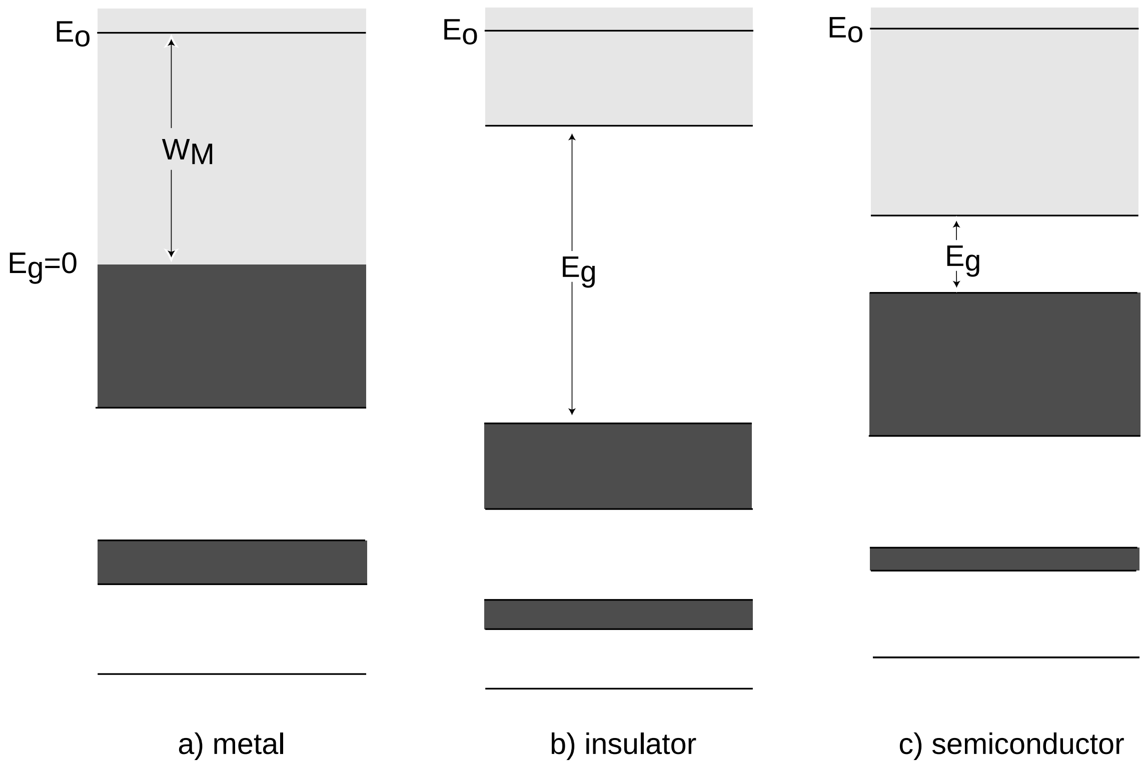
Different solids have different band structures. At 0 $K$:




Distinct feature of semiconductors:

At 0 $K$, filling ends up with full band separated by $1-3\ eV$ bandgap from next empty band.

Why is this significant?




No conduction is possible in a full band ⇒ insulators and semiconductors do not conduct at 0 $K$.

Conduction requires a partially filled band ⇒ metals conduct at 0 $K$.

*But* in semiconductors at finite temperatures, some electrons populate next band above bandgap ⇒ conduction becomes possible.

What is the law that regulates electron ocupation of states as a function of energy and temperature?

## 2. Electron statistics

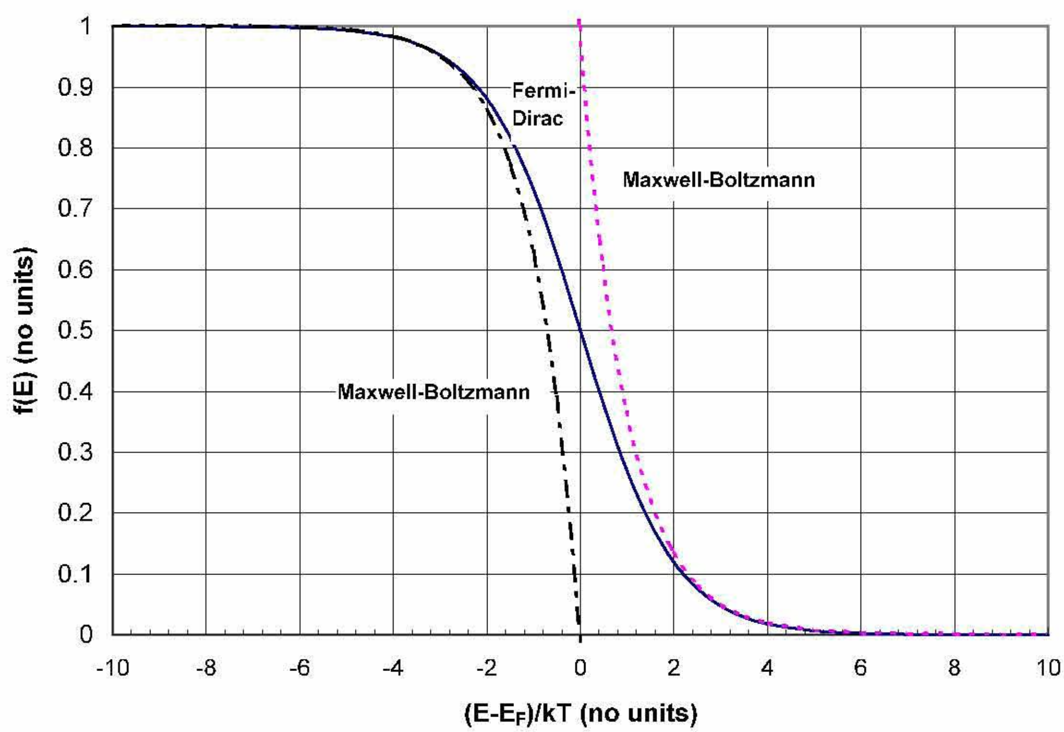
At finite temperature, state occupation probability by electron determined by **Fermi-Dirac distribution function**:

$$f(E) = \frac{1}{1 + \exp\frac{E-E_F}{kT}}$$

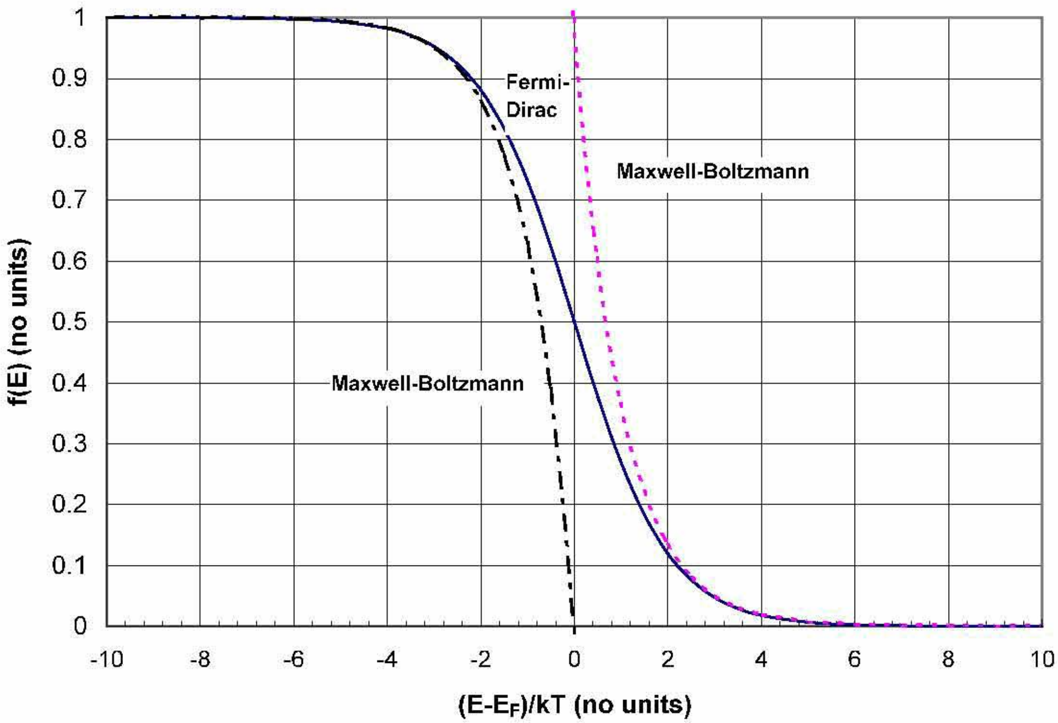
$E_F \equiv$ *Fermi energy* $\equiv$ energy for which occupation probability is 50%

$$k \equiv \textit{Boltzmann constant} = 8.62 \times 10^{-5}\ eV/K$$

$$kT \equiv \textit{thermal energy} = 25.9\ meV\ @\ 300\ K$$



Properties of Fermi-Dirac distribution function:




- for $E \ll E_F$: $f(E) \simeq 1$
- for $E \gg E_F$: $f(E) \simeq 0$
- width of transition around $E_F \simeq 3kT$ (20% criterium)
- symmetry: $f(E_F + E_1) = 1 - f(E_F - E_1)$
- Maxwell-Boltzmann approximation:

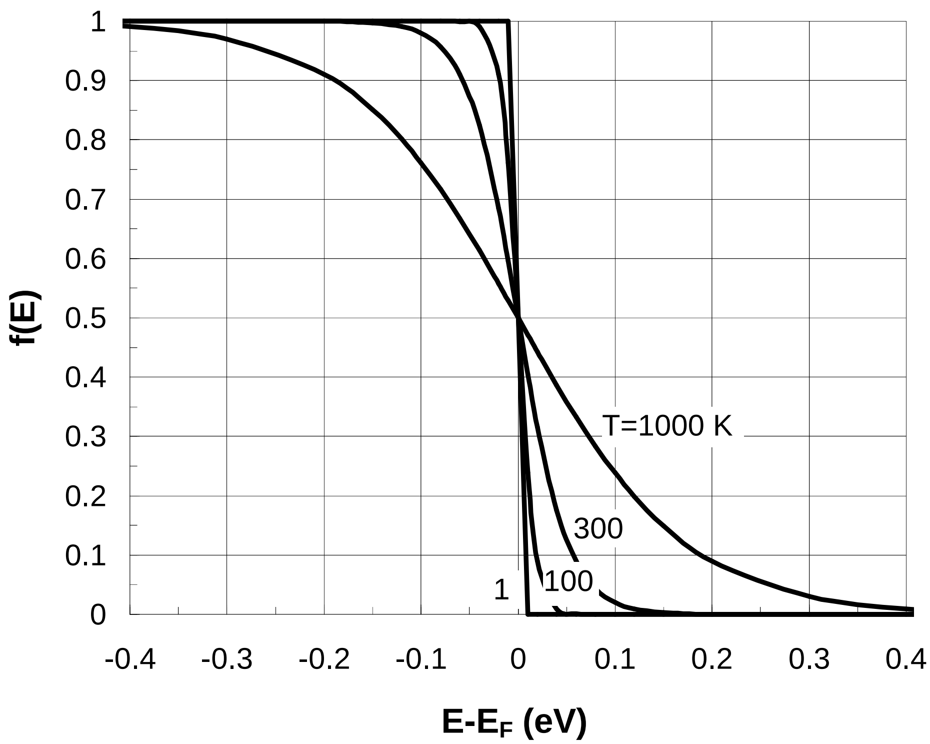
  For $E - E_F \gg kT$:

$$f(E) \simeq \exp - \frac{E - E_F}{kT}$$

  For $E - E_F \ll kT$:

$$f(E) \simeq 1 - \exp \frac{E - E_F}{kT}$$

Temperature dependence of Fermi-Dirac distribution function:

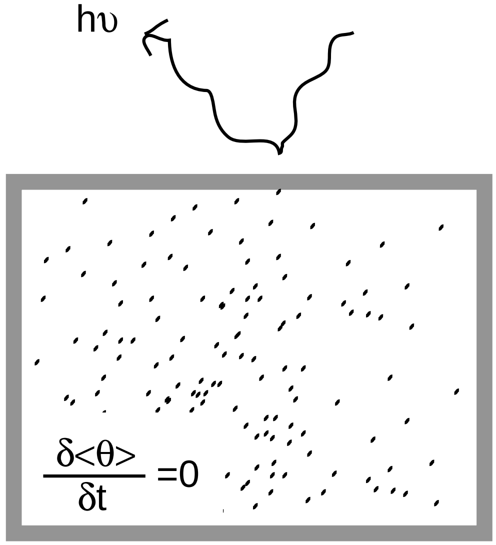



In general, $E_F$ function of T.

## 3. Thermal equilibrium

A particle system is in thermal equilibrium if:

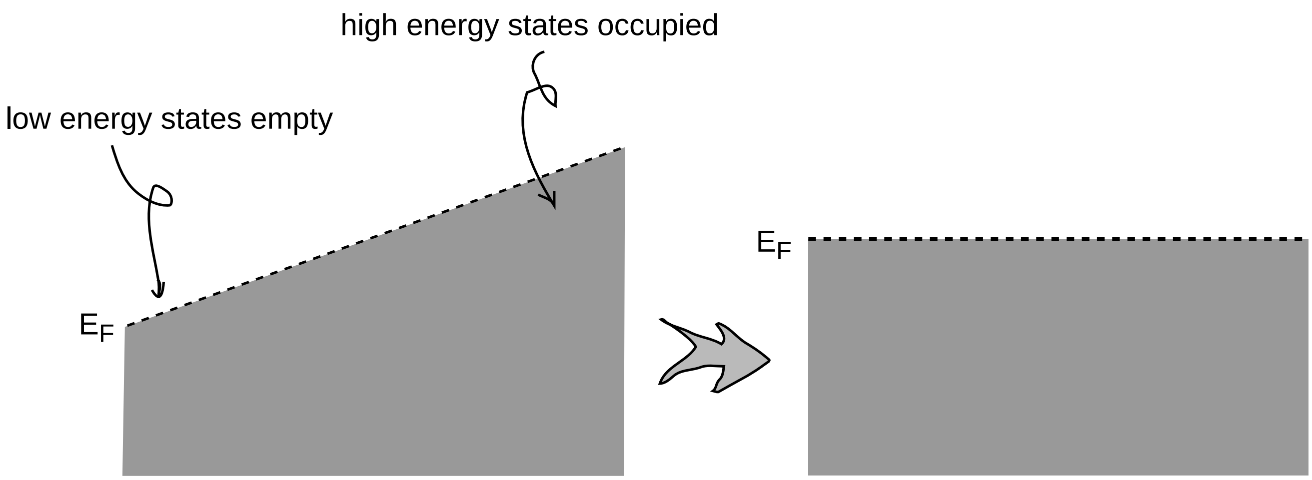
- it is *closed*: no energy flow through boundaries of system
- it is in *steady-state*: time derivatives of all ensemble averages (global and local) are zero




Thermal equilibrium important because all systems evolve towards TE after having been perturbed.

In order to know how a system evolves, it is essential to know where it is going.

□ In thermal equilibrium, $E_F$ constant throughout system



## Key conclusions

- In solids, electron states cluster in bands separated by bandgaps.
- Distinct feature of semiconductors: at $0\ K$, quantum state filling ends up with full band separated from next empty band by $1-3\ eV$ bandgap $\Rightarrow$ at around $300\ K$, some electrons populate next band above bandgap.
- Occupation probability of quantum systems in thermal equilibrium governed by *Fermi-Dirac distribution function*:

$$f(E) = \frac{1}{1 + \exp \frac{E - E_F}{kT}}$$

- System in *thermal equilibrium*: isolated from outside world + in steady state.
- In thermal equilibrium, $E_F$ is independent of position.
- Order of magnitude of key parameters:
  - atomic density of Si: $N_{Si} \sim 5 \times 10^{22}\ cm^{-3}$
  - bandgap of Si: $E_g \sim 1\ eV$
  - thermal energy: $kT \sim 26\ meV$ @ 300K

## Self-study

- Concept of *blackbody radiation*.
- Concept of *vacuum energy*.
- Concept of *density of states*.
- Understand how can the Fermi energy change with temperature.
- *Maxwell-Boltzmann distribution function*.