



山东大学  
SHANDONG UNIVERSITY

# 基础物理 II 固体理论导引

Lecturer: 张晨

Office: N5-227-1

Email: [chenzhang@sdu.edu.cn](mailto:chenzhang@sdu.edu.cn)

Website:

[faculty.sdu.edu.cn/zhangc/zh\\_CN/index.htm](http://faculty.sdu.edu.cn/zhangc/zh_CN/index.htm)

# What can we get from solid state physics?



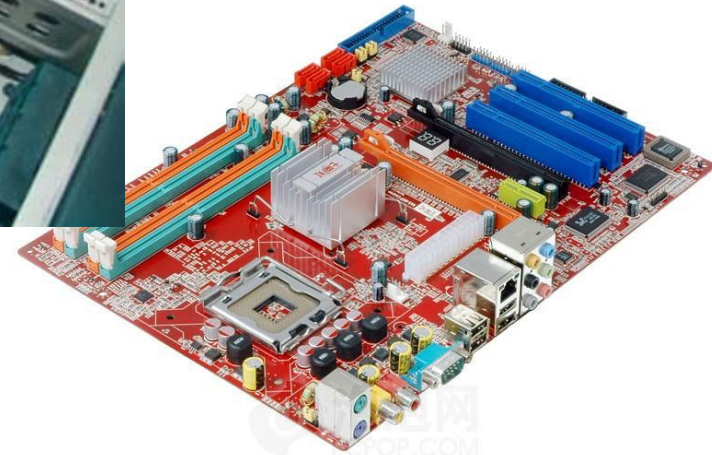
Dielectric materials



Semiconductor



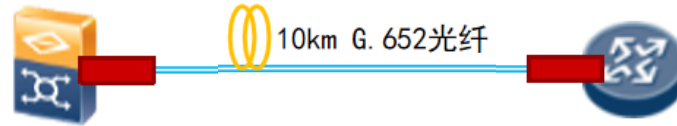
Magnetic materials



Metal

# What can we get from solid state physics?

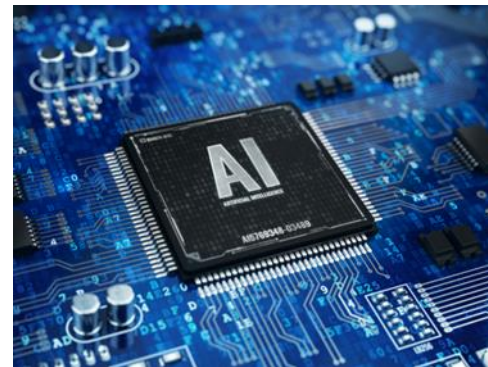
5G communication network



Laser, detector, and multiplexer chips



AI chips: new architecture,  
new materials

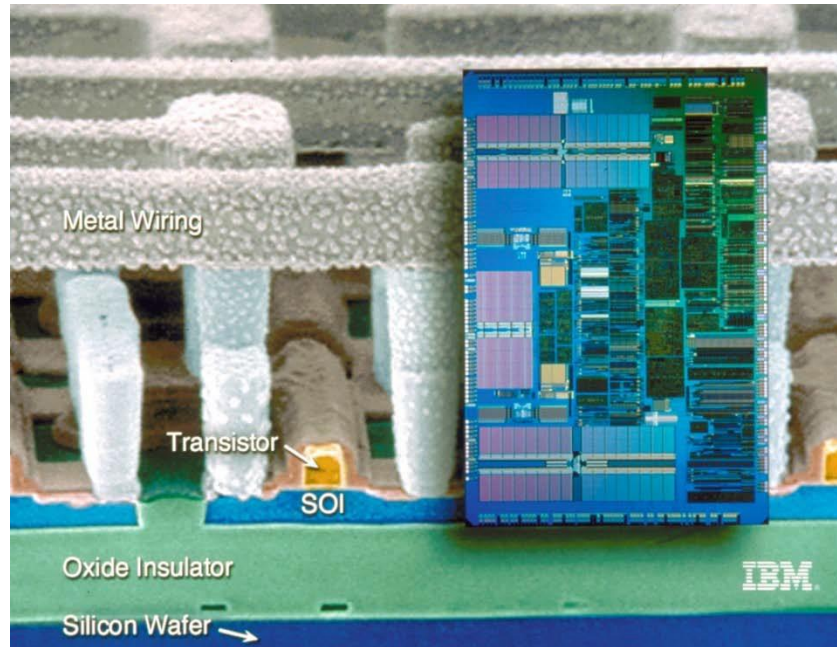


Wearable chips:



# Chapter 6 Electronic Properties of Semiconductors

1. Intrinsic semiconductors (本征半导体)
2. Extrinsic semiconductors (非本征半导体) and PN junction (PN结)



Silicon is the most important semiconductor in today's electronics

SOURCE: Courtesy of IBM



# Typical Semiconductors



200 mm and 300 mm Si wafers.

[SOURCE: Courtesy of MEMC, Electronic Materials, Inc.]

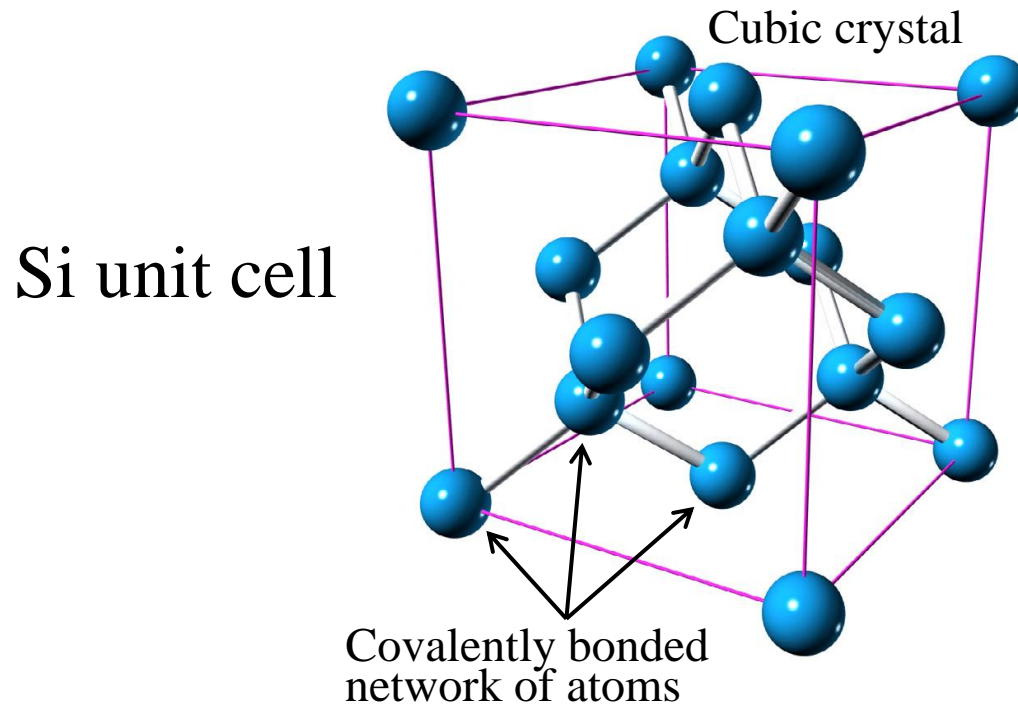
GaAs ingots and wafers. GaAs is used in high speed electronic devices, and optoelectronics.

[SOURCE: Courtesy of Sumitomo Electric Industries, Ltd.]



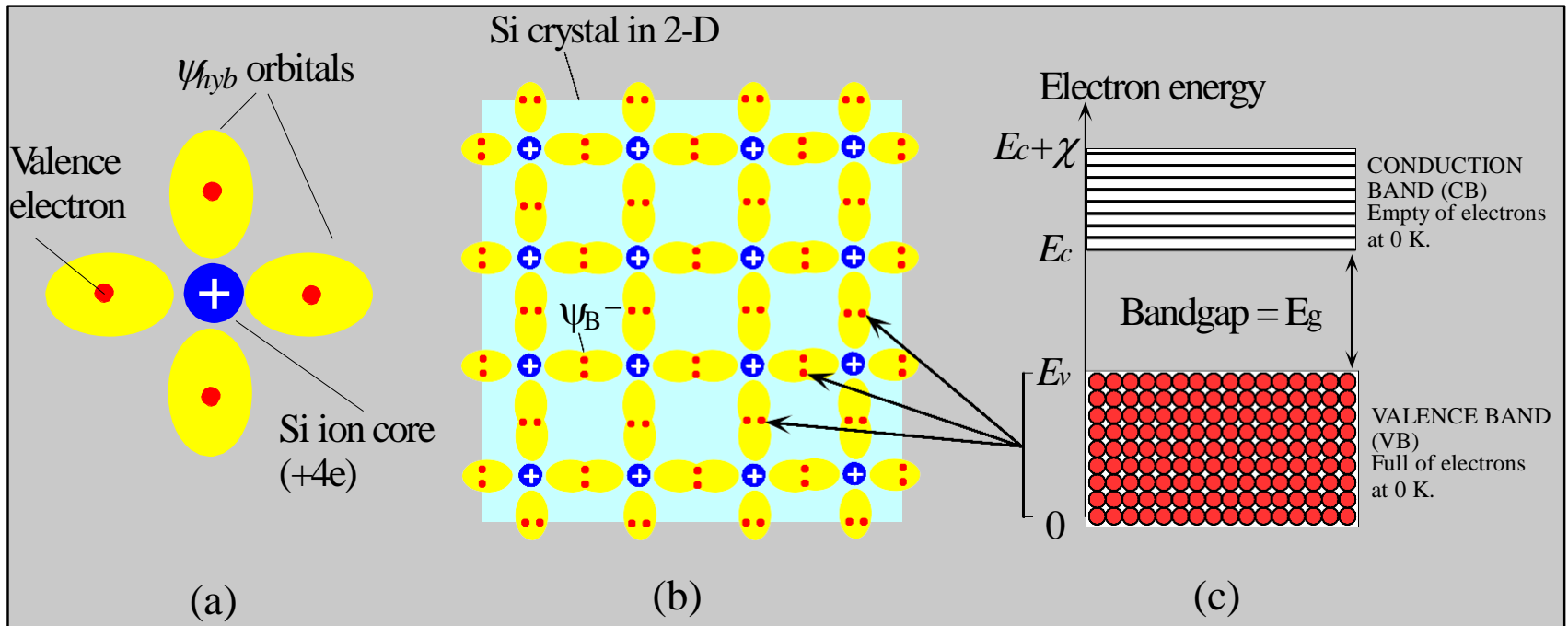
# Crystal structure of Si

**Intrinsic semiconductors**（本征半导体） are perfect semiconductor crystals without any defects or impurities.



Each Si atom is connected to four neighbors through the formation of covalent bonds. Each bond holds two electrons that are shared by the two Si atoms.

# Silicon crystal and energy band diagram



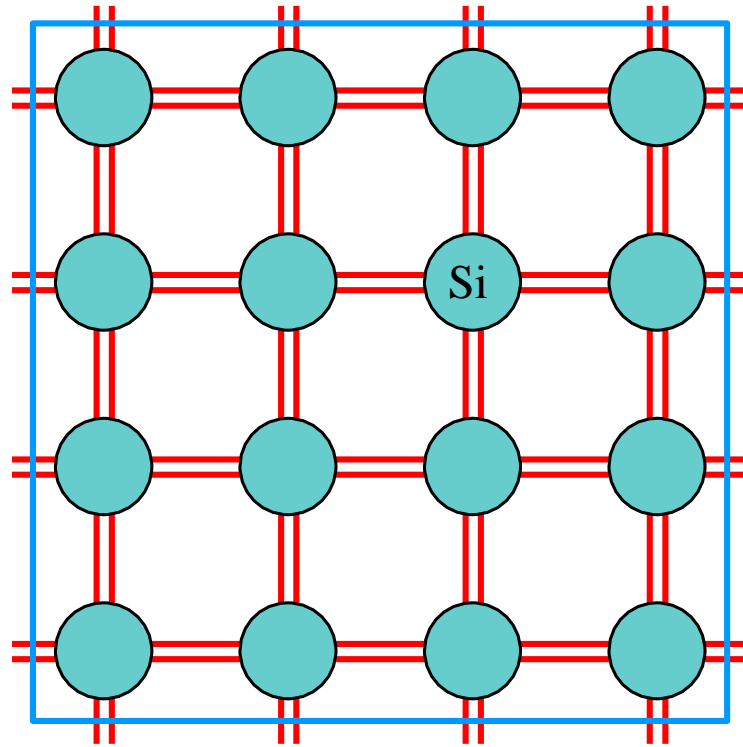
(a) A simplified two dimensional illustration of a Si atom with four hybrid orbitals,  $\psi_{hyb}$ . Each orbital has one electron. (b) A simplified two dimensional view of a region of the Si crystal showing covalent bonds. (c) The energy band diagram at absolute zero of temperature.

$E_g$  = energy gap (bandgap);  $E_v$  = top of the VB;  $E_c$  = bottom of the CB

$\chi$  = electron affinity;

$E_g$ : 能带间隙 (带隙);  $E_v$ : 价带顶;  $E_c$ : 导带底;  $\chi$ : 电子亲和能

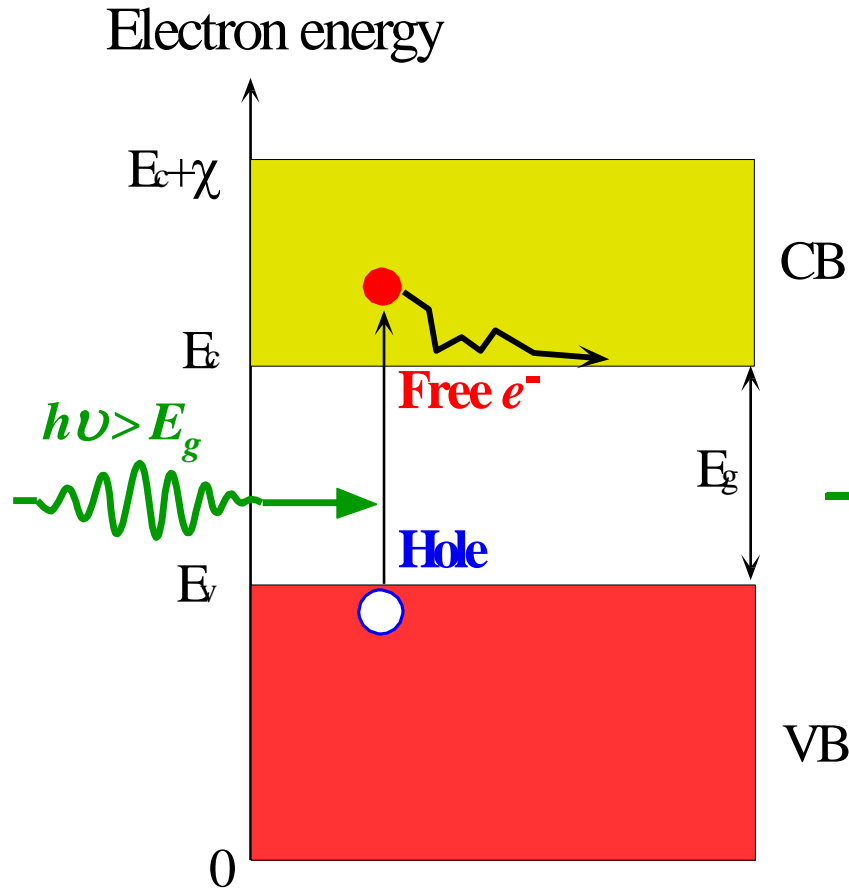
Insulator, Conductor, Semiconductor



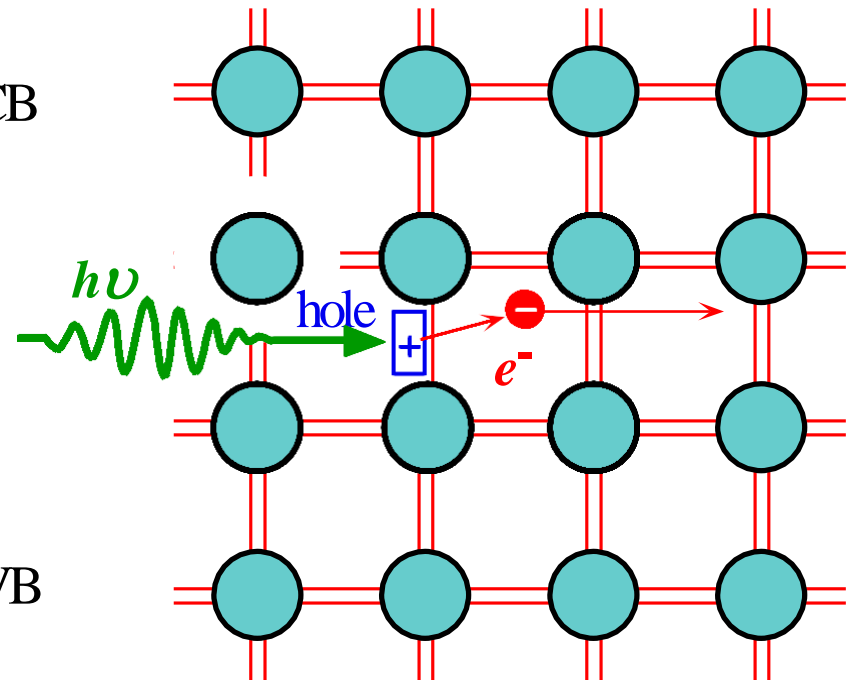
A two dimensional pictorial view of the Si crystal showing covalent bonds as two lines where each line is a valence electron.



# Conduction electron due to optical excitation



(a)

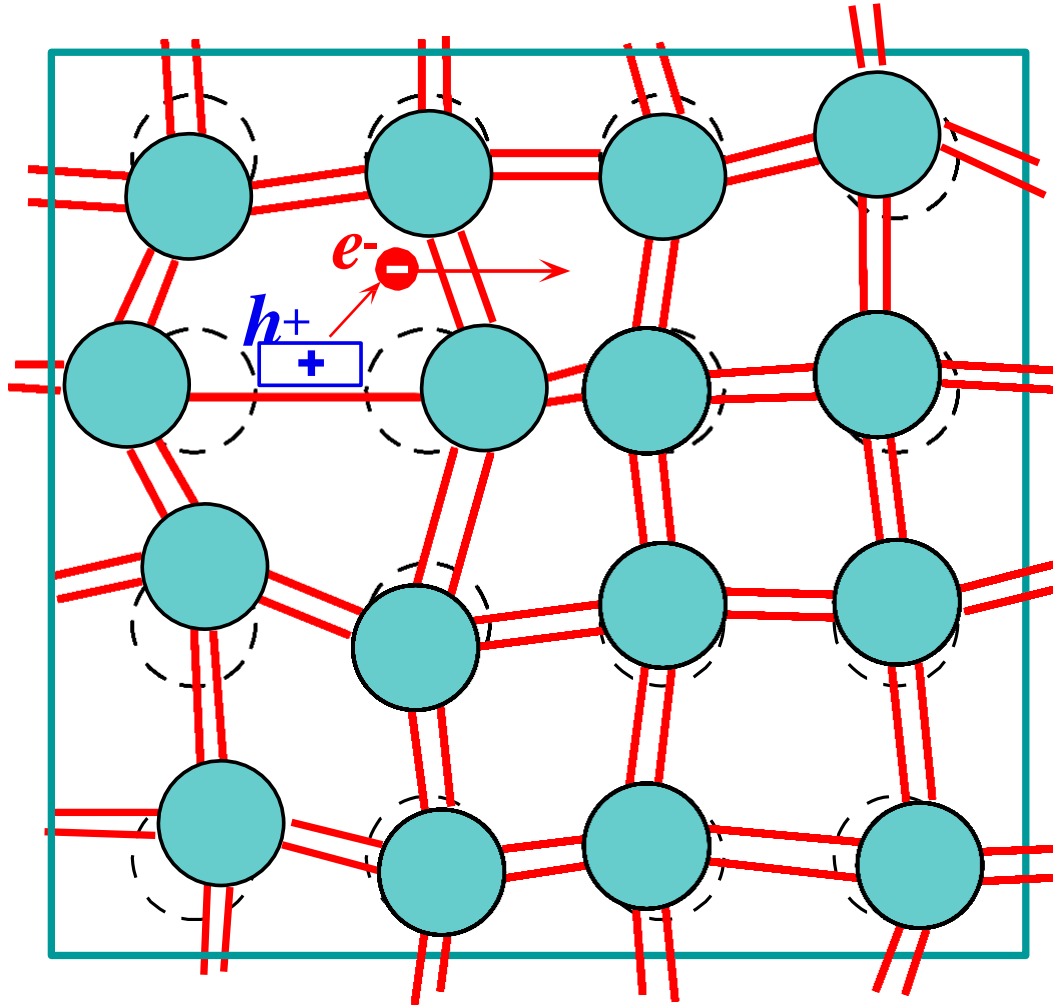


(b)

(a) A photon with an energy greater than  $E_g$  can excite an electron from the VB to the CB. 4

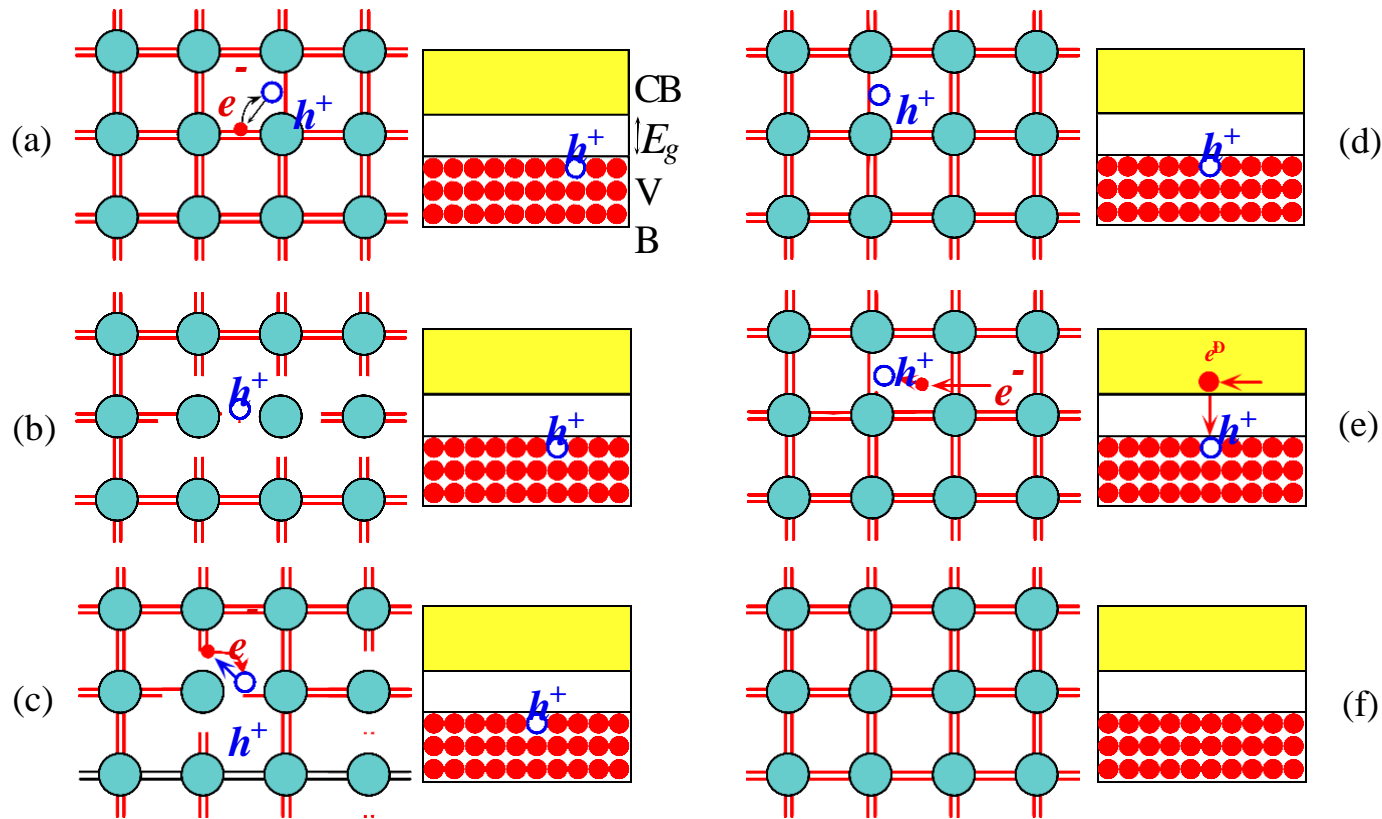
(b) When a photon breaks a Si-Si bond, a free **electron** and a **hole** in the Si-Si bond is created.

## Conduction electron due to thermal excitation



Due to thermal energy, in a certain region, the atoms, at some instant, may be moving in such a way that a bond becomes overstretched.

Thermal vibrations of atoms can break bonds and thereby create electron-hole pairs.



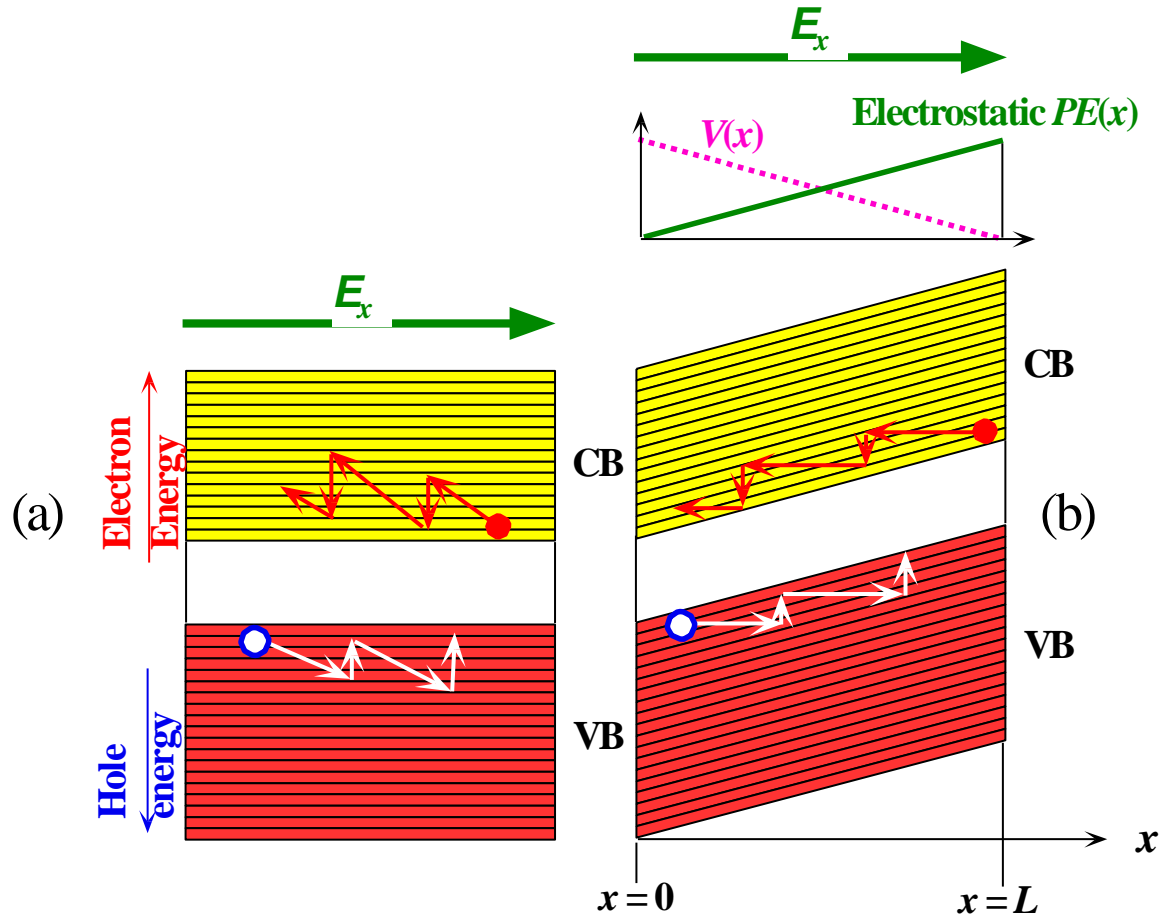
A pictorial illustration of a hole in the valence band wandering around the crystal due to the tunneling of electrons from neighboring bonds.

**Recombination:** When a wandering electron in the CB meets a hole in the VB, the electron has found an empty state of lower energy and therefore occupies the hole.

The excess energy of the electron falling from CB to VB is emitted as a photon, in GaAs and ZnO.

In Si and Ge, the excess energy is lost as lattice vibration (heat).

# Conductivity (电导率) in semiconductors



When an electric field is applied, electrons in the CB and holes in the VB can drift (漂移运动) and contribute to the conductivity.

(a) A simplified illustration of drift in  $E_x$ .

(b) Applied field bends the energy bands, since the electrostatic  $PE$  of the electron is  $-eV(x)$  and  $V(x)$  decreases in the direction of  $E_x$  whereas  $PE$  increases.

The current density  $J$  (漂移电流浓度):

$$J = env_{de} + epv_{dh}$$

Where  $n$  is the concentration of electrons in the CB,  $p$  is the hole concentration in the VB.  
 $n$  = 导带中的电子浓度,  $p$  = 价带中的空穴浓度.

漂移速度:

$$v_{de} = \mu_e E_x \cdots and \cdots v_{dh} = \mu_h E_x$$

迁移率:

$$\mu_e = \frac{e\tau_e}{m_e^*} \cdots and \cdots \mu_h = \frac{e\tau_e}{m_h^*}$$

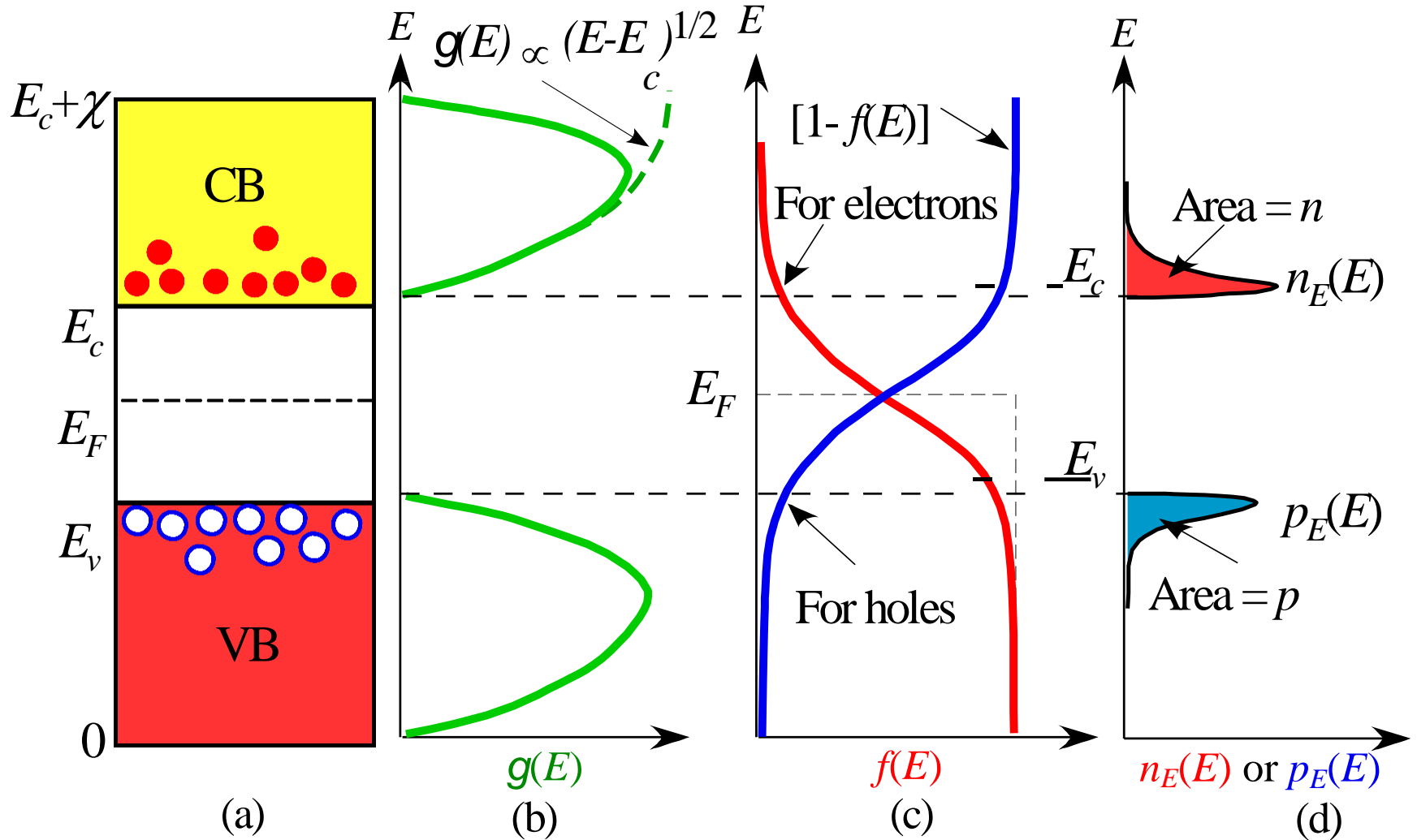
$\tau$  is the mean free time between scattering events,  $m^*$  effective mass

The conductivity of a semiconductor:

$$\sigma = en\mu_e + ep\mu_h$$



# Calculate carrier (载流子) concentration



(a) Energy band diagram.

(b) **Density of states  $g(E)$ :** number of states per unit energy per unit volume.

(c) **Fermi-Dirac probability function  $f(E)$ :** probability of occupancy of a state.

(d) **Carrier distributions  $n_E(E)$ :** the product of  $g(E)$  and  $f(E)$  is the energy density of electrons in the CB (number of electrons per unit energy per unit volume). The area under  $n_E(E)$  vs.  $E$  is the electron concentration in the CB.

## Calculate carrier (载流子) concentration

$g_{cb}(E)$  is the density of states in the CB. The actual number of electrons per unit energy per unit volume  $n_E(E)$  in the CB:

$$n_E dE = g_{cb}(E) f(E) dE$$

The electron concentration (number of electrons per unit volume):

$$n = \int_{E_c}^{E_c + \chi} n_E(E) dE = \int_{E_c}^{E_c + \chi} g_{cb}(E) f(E) dE$$

Assume that  $(E_c - E_F) \gg kT$ :

$$f(E) \approx \exp[-(E - E_F) / kT]$$

Replacing Fermi-Dirac statistics by Boltzmann statistics assuming that the number of electrons in the CB is far less than the number of states in this band.

## Calculate carrier (载流子) concentration

From 
$$g_{cb}(E) = \frac{(8\pi\sqrt{2})m_e^{*3/2}}{h^3} (E - E_c)^{1/2}$$

$$\Rightarrow n \approx \frac{(\pi 8\sqrt{2})m_e^{*3/2}}{h^3} \int_{E_c}^{\infty} (E - E_c)^{1/2} \exp\left[-\frac{E - E_F}{kT}\right] dE$$

The solution is:

$$n \approx N_c \exp\left[-\frac{E_c - E_F}{kT}\right]$$

Where 
$$N_c = 2 \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2}$$

$N_c$  is a temperature-dependent constant, called the effective density of states at the CB edge.

## Calculate carrier (载流子) concentration

We can carry out a similar analysis for the concentration of holes in the VB.

$$p = \int_0^{E_v} p_E dE = \int_0^{E_v} g_{vb}(E)[1 - f(E)]dE$$

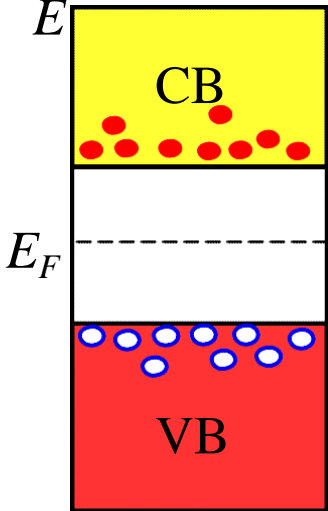
With the assumption that  $E_F$  is a few  $kT$  above  $E_v$ , the integration simplifies to

$$p = N_v \exp\left[-\frac{(E_F - E_v)}{kT}\right]$$

Where  $N_v$  is the effective density of states at the VB edge.

$$N_v = 2 \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2}$$

# Important Equations for Intrinsic Semiconductors

$$n = N_c \exp\left[-\frac{E_c - E_F}{kT}\right]$$

$$p = N_v \exp\left[-\frac{E_F - E_v}{kT}\right]$$

In intrinsic semiconductor, the numbers of electron and hole are the same ( $n=p$ ), as they are generated in pair.

The product is a constant determined by the band gap.

$$np = n_i^2 = N_c N_v \exp\left(-\frac{E_g}{kT}\right)$$

$n_i$ , the intrinsic concentration (本征载流子浓度)



# Fermi levels

We first consider an intrinsic semiconductor,  $n=p=n_i$ .

$$N_v \exp\left[-\frac{E_{Fi} - E_v}{kT}\right] = (N_c N_v)^{1/2} \exp\left(-\frac{E_g}{2kT}\right)$$

If  $m_e^* = m_h^*$ :

$$\Rightarrow E_{Fi} = E_v + \frac{1}{2} E_g$$

$E_{Fi}$  is right in the middle of the energy gap. Normally, the Fermi level will be slightly down from the midgap by an amount of  $\frac{3}{4} kT \ln(m_e^*/m_h^*)$ .

# Fermi levels

In a n-type semiconductor,  $n > p$  (for example through doping), the Fermi level must be closer to  $E_c$  than  $E_v$ .

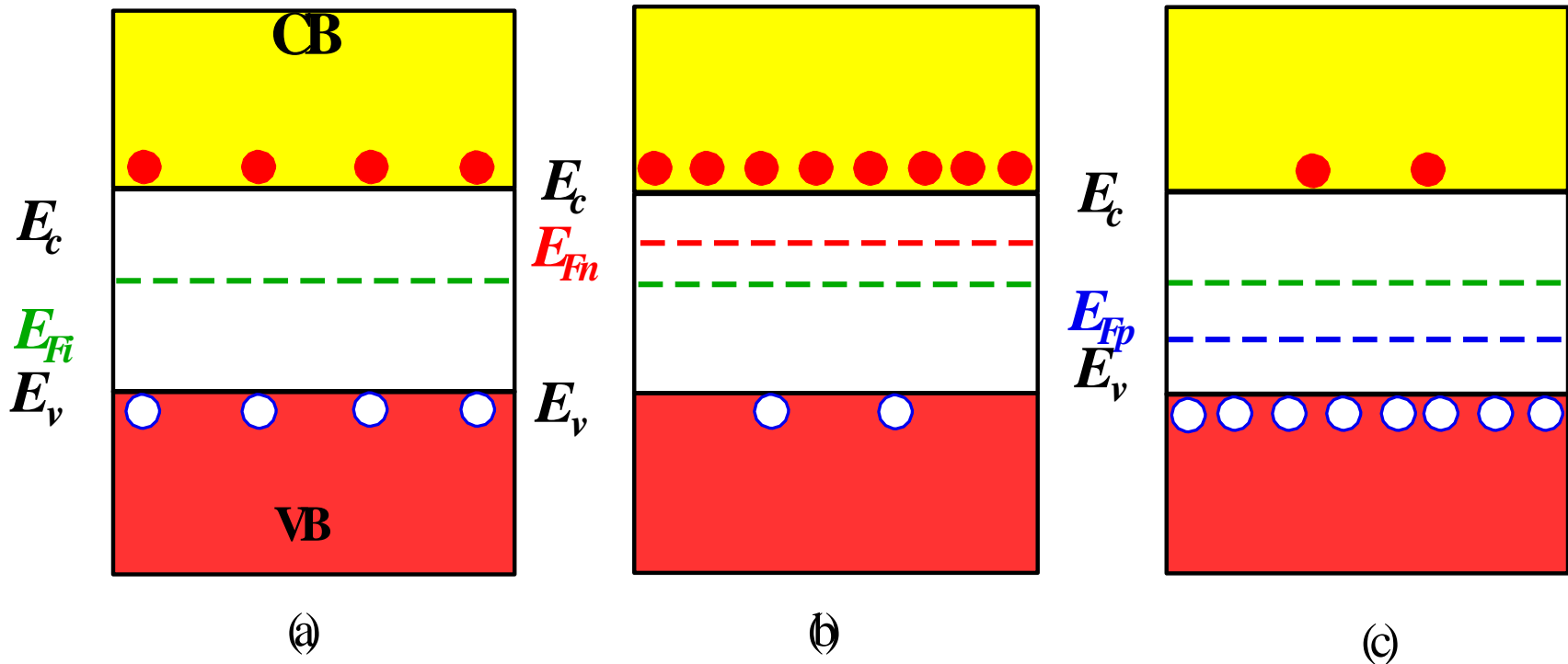
$$E_c - E_F < E_F - E_v$$

In a p-type semiconductor ( $p > n$ ), the Fermi level must be closer to  $E_v$  than to  $E_c$ .

$$E_c - E_F > E_F - E_v$$

$E_F$  is a material property.

The general band diagrams with the appropriate Fermi levels for intrinsic, n-type and p-type semiconductors.



Energy band diagrams for (a) intrinsic (b) *n*-type and (c) *p*-type semiconductors. In all cases,  $np = n_i^2$

$$n = N_c \exp\left[-\frac{E_c - E_F}{kT}\right] \quad p = N_v \exp\left[-\frac{(E_F - E_v)}{kT}\right]$$

**Table 5.1** Selected typical properties of Ge, Si, and GaAs at 300 K

	$E_g$ (eV)	$\chi$ (eV)	$N_c$ (cm <sup>-3</sup> )	$N_v$ (cm <sup>-3</sup> )	$n_i$ (cm <sup>-3</sup> )	$\mu_e$ (cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> )	$\mu_h$ (cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> )	$m_e^*/m_e$	$m_h^*/m_e$	$\epsilon_r$
Ge	0.66	4.13	$1.04 \times 10^{19}$	$6.0 \times 10^{18}$	$2.3 \times 10^{13}$	3900	1900	0.12 <i>a</i> 0.56 <i>b</i>	0.23 <i>a</i> 0.40 <i>b</i>	16
Si	1.10	4.01	$2.8 \times 10^{19}$	$1.2 \times 10^{19}$	$1.0 \times 10^{10}$	1350	450	0.26 <i>a</i> 1.08 <i>b</i>	0.38 <i>a</i> 0.60 <i>b</i>	11.9
GaAs	1.42	4.07	$4.7 \times 10^{17}$	$7 \times 10^{18}$	$2.1 \times 10^6$	8500	400	0.067 <i>a,b</i>	0.40 <i>a</i> 0.50 <i>b</i>	13.1

NOTE: Effective mass related to conductivity (labeled *a*) is different than that for density of states (labeled *b*). In numerous textbooks,  $n_i$  is taken as  $1.45 \times 10^{10}$  cm<sup>-3</sup> and is therefore the most widely used value of  $n_i$  for Si, though the correct value is actually  $1.0 \times 10^{10}$  cm<sup>-3</sup>. (M. A. Green, *J. Appl. Phys.*, **67**, 2944, 1990.)

$$g_{cb}(E) = \frac{(\pi 8 \sqrt{2}) m_e^{*3/2}}{h^3} (E - E_c)^{1/2}$$

思考：宽禁带半导体/第三代半导体

**Example (intrinsic concentration and conductivity of Si):** Given that the density of states related effective masses of electrons and holes in Si are approximately  $1.08m_e$  and  $0.60m_e$ , respectively, and the electron and hole drift mobilities at room temperature are  $1350$  and  $450 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ , respectively, calculate the intrinsic concentration and intrinsic resistivity of Si.

$$N_c = 2 \left( \frac{2\pi m_e^* kT}{h^2} \right)^{3/2} = 2 \left[ \frac{2\pi (1.08 \times 9.1 \times 10^{-31}) \times (1.38 \times 10^{-23}) \times 300}{(6.63 \times 10^{-34})^2} \right]^{3/2} = 2.81 \times 10^{25} \text{ m}^{-3} = 2.81 \times 10^{19} \text{ cm}^{-3}$$

$$N_v = 2 \left( \frac{2\pi m_h^* kT}{h^2} \right)^{3/2} = 1.16 \times 10^{25} \text{ m}^{-3} = 1.16 \times 10^{19} \text{ cm}^{-3}$$

The intrinsic concentration is:

$$n_i = (N_c N_v)^{1/2} \exp\left(-\frac{E_g}{2kT}\right) = (2.81 \times 10^{19} \cdot 1.16 \times 10^{19})^{1/2} \exp\left(-\frac{1.10 \cdot 1.6 \times 10^{-19}}{2 \cdot 1.38 \times 10^{-23} \cdot 300}\right) = 1.0 \times 10^{10} \text{ cm}^{-3}$$

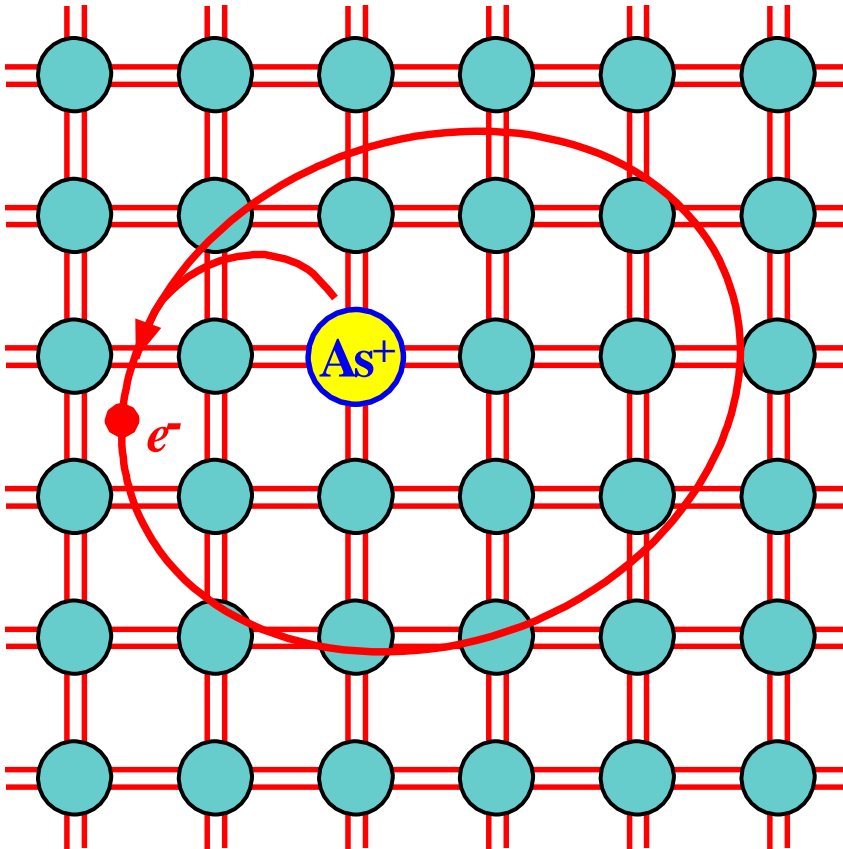
The conductivity is

$$\sigma = en\mu_e + ep\mu_h = en_i (\mu_e + \mu_h) = 1.6 \times 10^{-19} \cdot 1.0 \times 10^{10} (1350 + 450) = 2.9 \times 10^{-6} \Omega^{-1} \text{ cm}^{-1}$$

$$\Rightarrow \rho = 1/\sigma = 3.5 \times 10^5 \Omega \text{ cm}$$



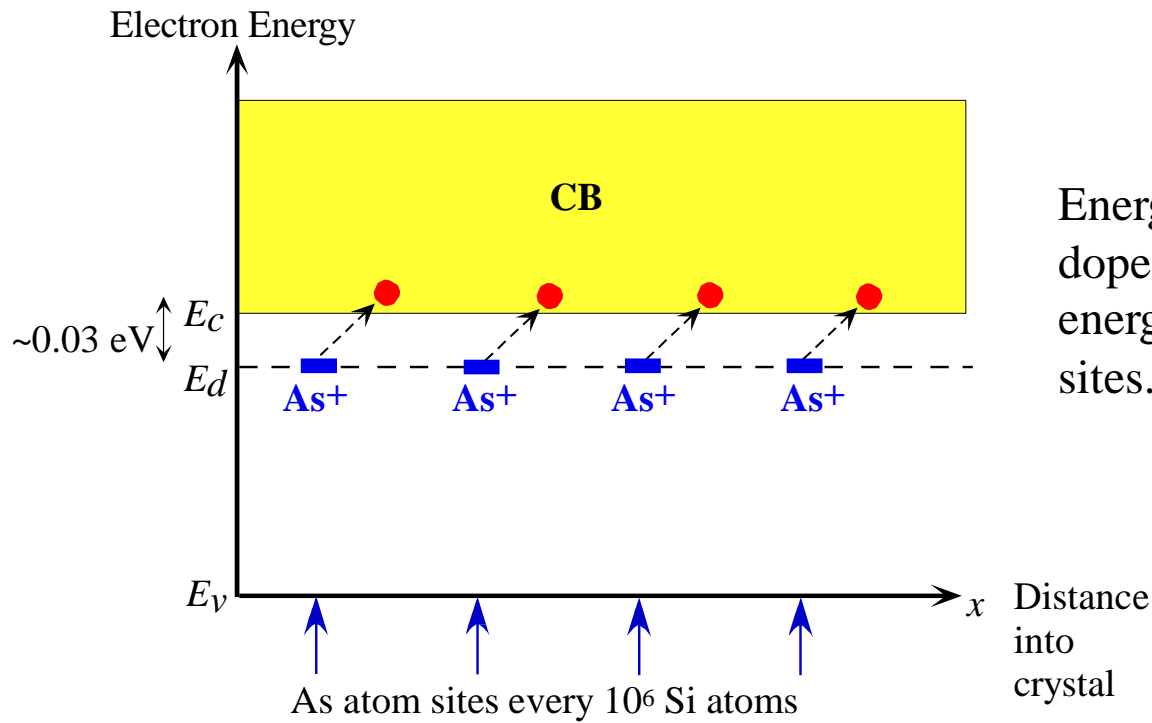
## Extrinsic semiconductors, n-type



Consider what happens when small amount of a pentavalent (valence of 5) element from Group V, such as As or P, are introduced into a pure Si crystal (donor atoms).

Donor impurity

Arsenic doped Si crystal. The four valence electrons of As allow it to bond just like Si but the fifth electron is left orbiting the As site. The energy required to release to free fifth-electron into the CB is very small.



Energy band diagram for an n-type Si doped with 1 ppm As. There are donor energy levels just below  $E_c$  around  $\text{As}^+$  sites.

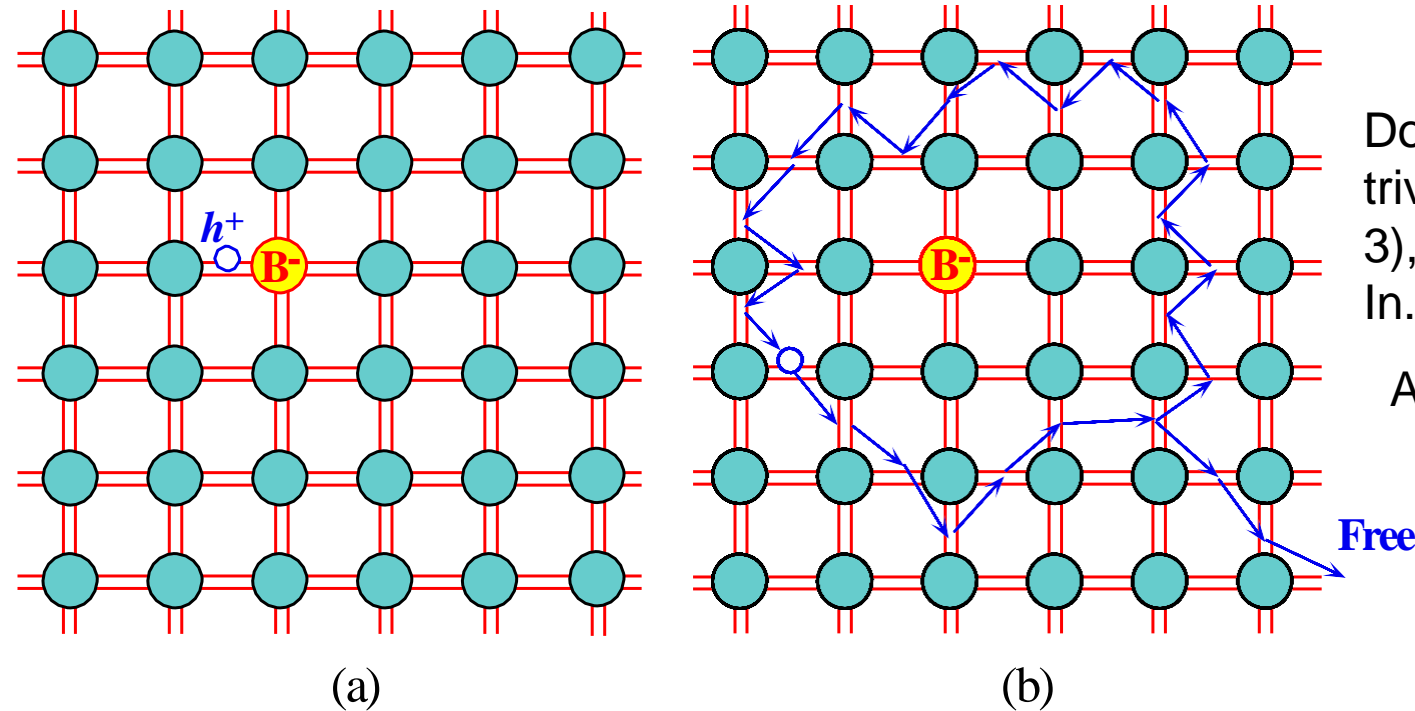
If the  $N_d$  is the donor atom concentration in the crystal, then provided that  $N_d \gg n_i$ , at room temperature the electron concentration in the CB will be nearly equal to  $N_d$ , that is  $n \approx N_d$ .

$$p = \frac{n_i^2}{N_d}$$

The conductivity  $\sigma$  :

$$= eN_d\mu_e + e\left(\frac{n_i^2}{N_d}\right)\mu_h \approx eN_d\mu_e$$

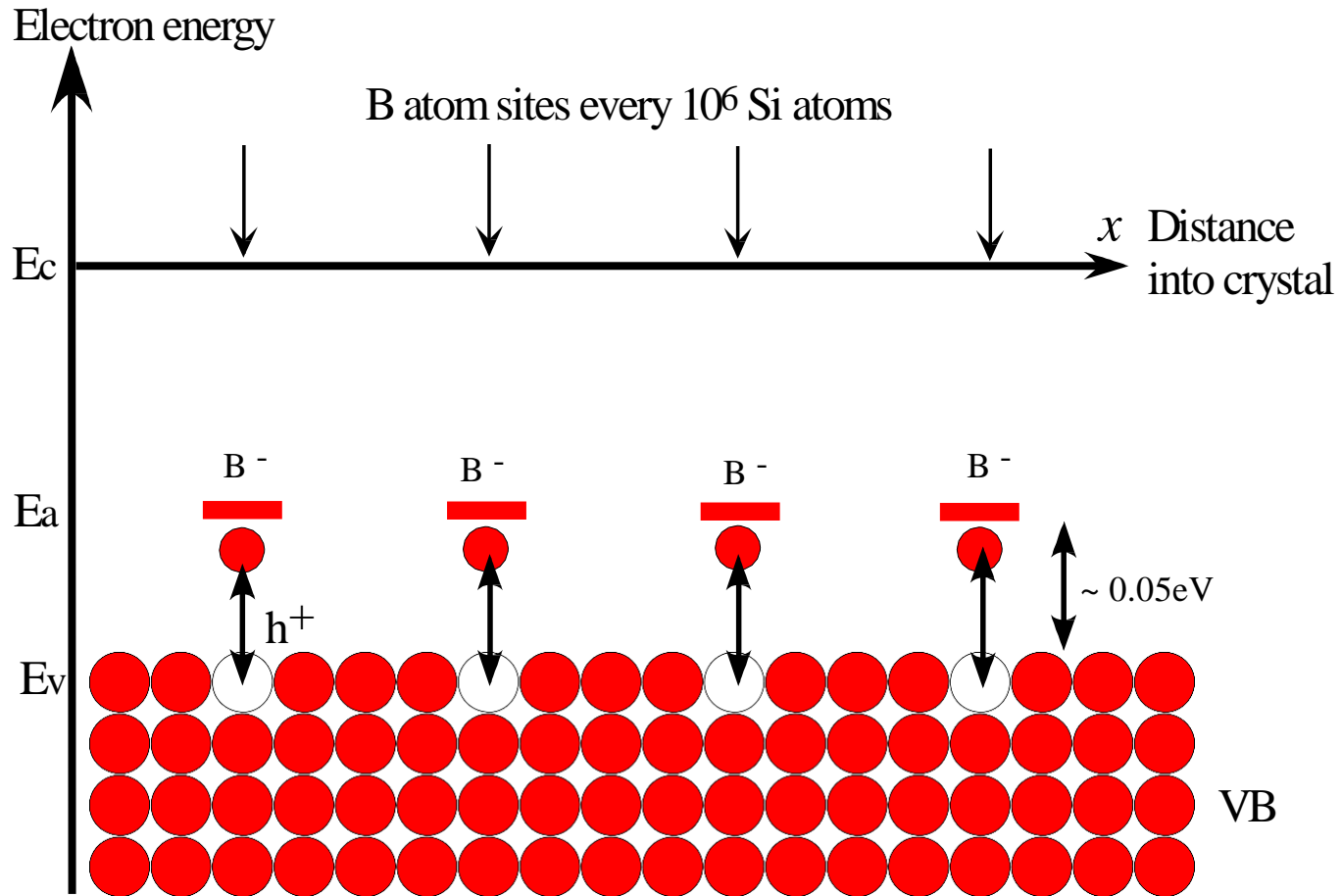
# Extrinsic semiconductors, p-type



Doping a Si crystal with a trivalent atom (valence of 3), such as B, Al, Ga or In.

Acceptor impurity.

Boron doped Si crystal. B has only three valence electrons. When it substitutes for a Si atom one of its bonds has an electron missing and therefore a hole as shown in (a). The hole orbits around the  $B^-$  site by the tunneling of electrons from neighboring bonds as shown in (b). Eventually, thermally vibrating Si atoms provides enough energy to free the hole from the  $B^-$  site into the VB as shown.



Energy band diagram for a  $p$ -type Si doped with 1 ppm B. There are acceptor energy levels just above  $E_v$  around  $B^-$  sites. These acceptor levels accept electrons from the VB and therefore create holes in the VB.

If the concentration of acceptor impurities  $N_a$  in the crystal is much greater than the intrinsic concentration  $n_i$ , then at room temperature all the acceptors would have been ionized and thus  $p \approx N_a$ . From  $n = n_i^2/N_a$ , which is much smaller than  $p$ :

The conductivity  $\sigma$  :

$$= eN_a\mu_h$$

**Table 5.2** Examples of donor and acceptor ionization energies (eV) in Si

Donors			Acceptors		
P	As	Sb	B	Al	Ga
0.045	0.054	0.039	0.045	0.057	0.072

# Compensation doping

Compensation doping is a term used to describe the doping of a semiconductor with both donors and acceptors to control the properties.

1. More donors:

$$N_d - N_a \gg n_i \quad \Rightarrow \quad n = (N_d - N_a) \quad \text{and} \quad p = \frac{n_i^2}{(N_d - N_a)}$$

2. More acceptors:

$$N_a - N_d \gg n_i \quad \Rightarrow \quad p = (N_a - N_d) \quad \text{and} \quad n = \frac{n_i^2}{(N_a - N_d)}$$

**Example (resistivity of intrinsic and doped Si):** Find the resistance of a  $1\text{ cm}^3$  pure silicon crystal cube. What is the resistance when the crystal is doped with arsenic if the doping is 1 in  $10^9$ , that is, 1 part per billion (ppb) (note that this doping corresponds to one foreigner living in China)? Given data: atomic concentration in silicon is  $5 \times 10^{22}\text{ cm}^{-3}$ ,  $n_i = 1.0 \times 10^{10}\text{ cm}^{-3}$ ,  $\mu_e = 1350\text{ cm}^2\text{ V}^{-1}\text{ s}^{-1}$ , and  $\mu_h = 450\text{ cm}^2\text{ V}^{-1}\text{ s}^{-1}$ .

For the intrinsic case:

$$\sigma = en\mu_e + ep\mu_h = en_i(\mu_e + \mu_h) = 1.6 \times 10^{-19} \cdot 1.0 \times 10^{10} \cdot (1350 + 45) = 2.88 \times 10^{-6}\text{ }\Omega^{-1}\text{ cm}^{-1}$$

Since  $L = 1\text{ cm}$ ,  $A = 1\text{ cm}^2$ :  $R = L/A\sigma = 3.47 \times 10^5\text{ }\Omega = 347\text{ k}\Omega$

When the crystal is doped with 1 in  $10^9$ :

$$N_d = \frac{N_{Si}}{10^9} = \frac{5 \times 10^{22}}{10^9} = 5 \times 10^{13}\text{ cm}^{-3}$$

At room temperature, all the donors are ionized:

$$n = N_d = 5 \times 10^{13}\text{ cm}^{-3}$$

The hole concentration is:

$$p = \frac{n_i^2}{N_d} = \frac{(1.0 \times 10^{10})^2}{5 \times 10^{13}} = 2.0 \times 10^6 \text{ cm}^{-3} \ll n_i$$

$$\Rightarrow \sigma = en\mu = 1.6 \times 10^{-19} \cdot 5 \times 10^{13} \cdot 1350 = 1.08 \times 10^{-2} \Omega^{-1} \text{ cm}^{-1}$$

$$\Rightarrow R = L/A\sigma = 92.6 \Omega$$

If doping with boron instead of arsenic (a p-type semiconductor with the same level of doping):

$$\sigma = ep\mu_h = 1.6 \times 10^{-19} \cdot 5 \times 10^{13} \cdot 450 = 3.6 \times 10^{-3} \Omega^{-1} \text{ cm}^{-1}$$

$$\Rightarrow R = L/A\sigma = 278 \Omega$$



**Example (the Fermi level in n- and p-type Si):** An n-type Si wafer has been doped uniformly with  $10^{16}$  antimony (Sb) atoms  $\text{cm}^{-3}$ . Calculate the position of the Fermi energy with respect to the Fermi energy  $E_{Fi}$  in intrinsic Si. The above n-type Si sample is further doped with  $2 \times 10^{17}$  boron atoms  $\text{cm}^{-3}$ . Calculate the position of the Fermi energy with respect to the Fermi energy  $E_{Fi}$  in intrinsic Si (Assume  $T = 300\text{K}$  and  $kT = 0.0259 \text{ eV}$ ).

Sb gives n-type doping with  $N_d = 10^{16} \text{ cm}^{-3}$ , and  $N_d \gg n_i (=10^{10} \text{ cm}^{-3})$

$$\Rightarrow n = N_d = 10^{16} \text{ cm}^{-3}$$

For intrinsic Si:

$$n_i = N_c \exp\left[-\frac{E_c - E_{Fi}}{kT}\right]$$

For doped Si:

$$n = N_c \exp\left[-\frac{E_c - E_{Fn}}{kT}\right] = N_d$$

$$\Rightarrow \frac{N_d}{n_i} = \exp\left[\frac{E_{Fn} - E_{Fi}}{kT}\right]$$

$$\Rightarrow E_{Fn} - E_{Fi} = kT \ln\left(\frac{N_d}{n_i}\right) = 0.0259 \ln\left(\frac{10^{16}}{1.0 \times 10^{10}}\right) = 0.36 \text{ eV}$$

The semiconductor is compensation doped and compensation converts the semiconductor to p-type Si.

$$p = N_a - N_d = (2 \times 10^{17} - 10^{16}) = 1.9 \times 10^{17} \text{ cm}^{-3}$$

For intrinsic Si:

$$n_i = N_v \exp\left[-\frac{E_{Fi} - E_v}{kT}\right]$$

For doped p-type Si:

$$p = N_v \exp\left[-\frac{E_{Fp} - E_v}{kT}\right] = N_a - N_d$$

$$\Rightarrow \frac{p}{n_i} = \exp\left[-\frac{E_{Fp} - E_{Fi}}{kT}\right]$$

$$\Rightarrow E_{Fp} - E_{Fi} = -kT \ln\left(\frac{p}{n_i}\right) = -0.0259 \ln\left(\frac{1.9 \times 10^{17}}{1.0 \times 10^{10}}\right) = -0.43 \text{ eV}$$