
Chapter

3

SEMICONDUCTOR BANDSTRUCTURE

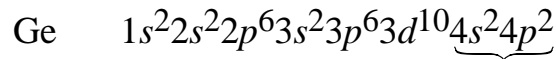
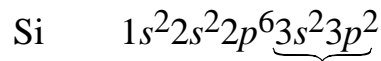
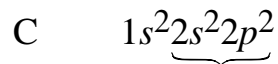


In this chapter we present figures discussing bandstructures of important semiconductors and the concept of doping and mobile carriers.

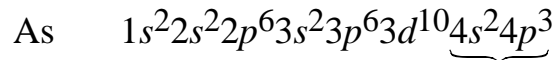
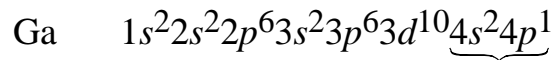
SEMICONDUCTOR BANDSTRUCTURE

In semiconductors we are primarily interested in the valence band and conduction band. Moreover, for most applications we are interested in what happens near the top of the valence band and the bottom of the conduction band. These states originate from the atomic levels of the valence shell in the elements making up the semiconductor.

IV Semiconductors



III-V Semiconductors



Outermost atomic levels are either *s*-type or *p*-type.

BANDSTRUCTURE OF SEMICONDUCTORS

The k -vector for the electrons in a crystal is limited to a space called the Brillouin zone. The figure shows the Brillouin zone for the fcc lattice relevant for most semiconductors. The values and notations of certain important k -points are also shown. Most semiconductors have bandedges of allowed bands at one of these points.

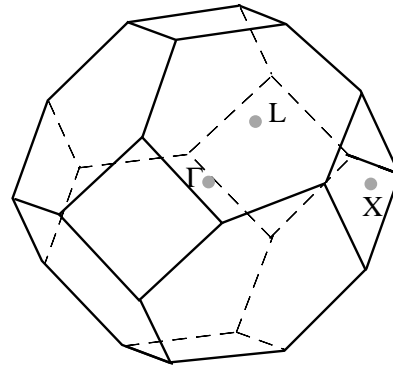
IMPORTANT HIGH SYMMETRY POINTS

Γ point: $k_x = 0 = k_y = k_z$

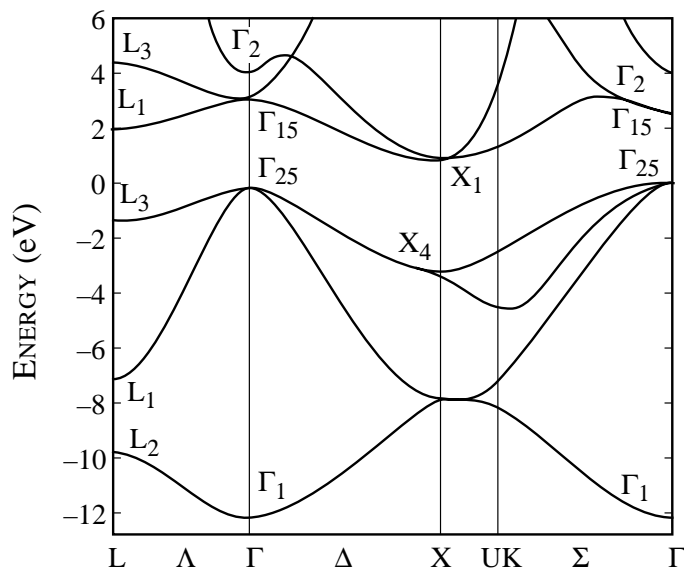
X point: $k_x = \frac{2\pi}{a}; k_y = k_z = 0$

L point: $k_x = k_y = k_z = \frac{\pi}{a}$

a = lattice constant (cube edge)

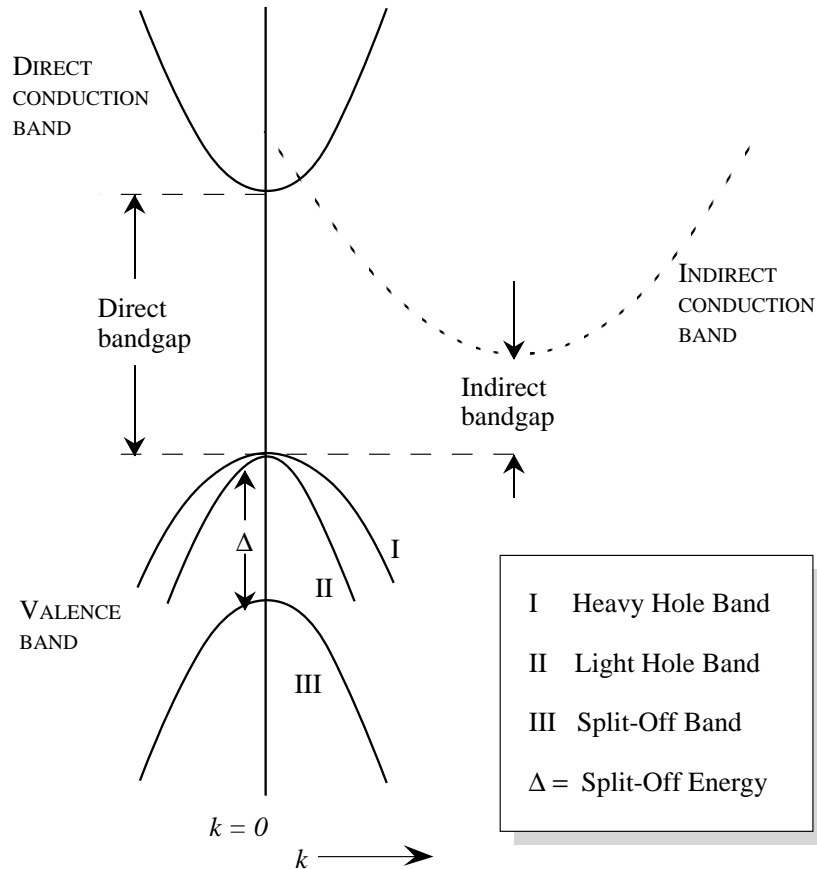


A TYPICAL BANDSTRUCTURE: Si



BANDSTRUCTURE NEAR BANDEDGES

Behavior of electrons near the bandedges determines most device properties. Near the bandedges the electrons can be described by simple effective mass pictures, i.e., the electrons behave as if they are in free space except their masses are m^* .



Schematic of the valence band, direct bandgap, and indirect bandgap conduction bands. The conduction band of the direct gap semiconductor is shown in the solid line, while the conduction band of the indirect semiconductor is shown in the dashed line. The curves I, II, and III in the valence band are called *heavy hole*, *light hole*, and *split-off hole states*, respectively.

EFFECTIVE MASS DESCRIPTION

CONDUCTION BAND: Direct bandgap material

$$E_c(\mathbf{k}) = E_c(0) + \frac{\hbar^2 k^2}{2m_c^*}$$

with

$$\frac{1}{m_c^*} = \frac{1}{m} + \frac{2p_{cv}^2}{m^2} \frac{1}{3} \left(\frac{2}{E_{g\Gamma}} + \frac{1}{E_{g\Gamma} + \Delta} \right)$$

The smaller the bandgap, the smaller the effective mass.

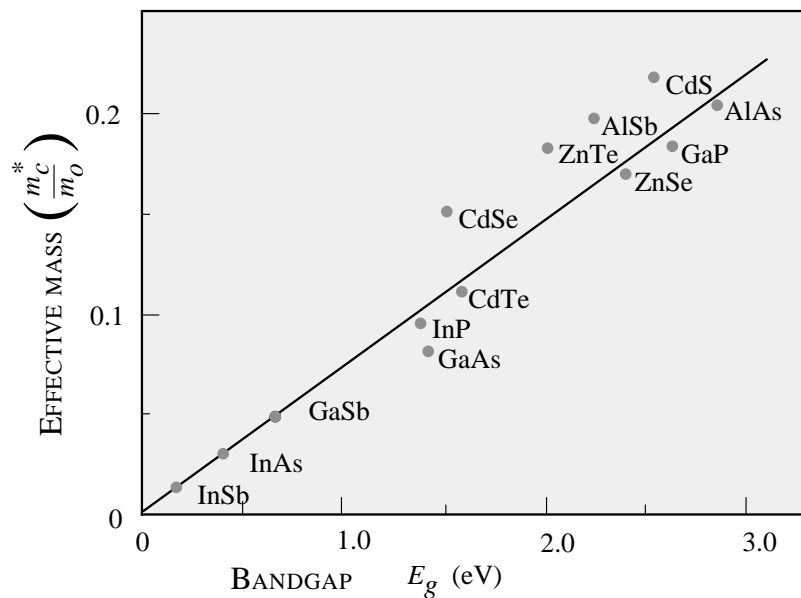
SPLIT-OFF BAND:

$$E_{so} = -\Delta - \frac{\hbar^2 k^2}{2m_{so}^*}$$

$$\frac{1}{m_{so}^*} = \frac{-1}{m} + \frac{2p_{cv}^2}{(3m^2 E_{g\Gamma} + \Delta)}$$

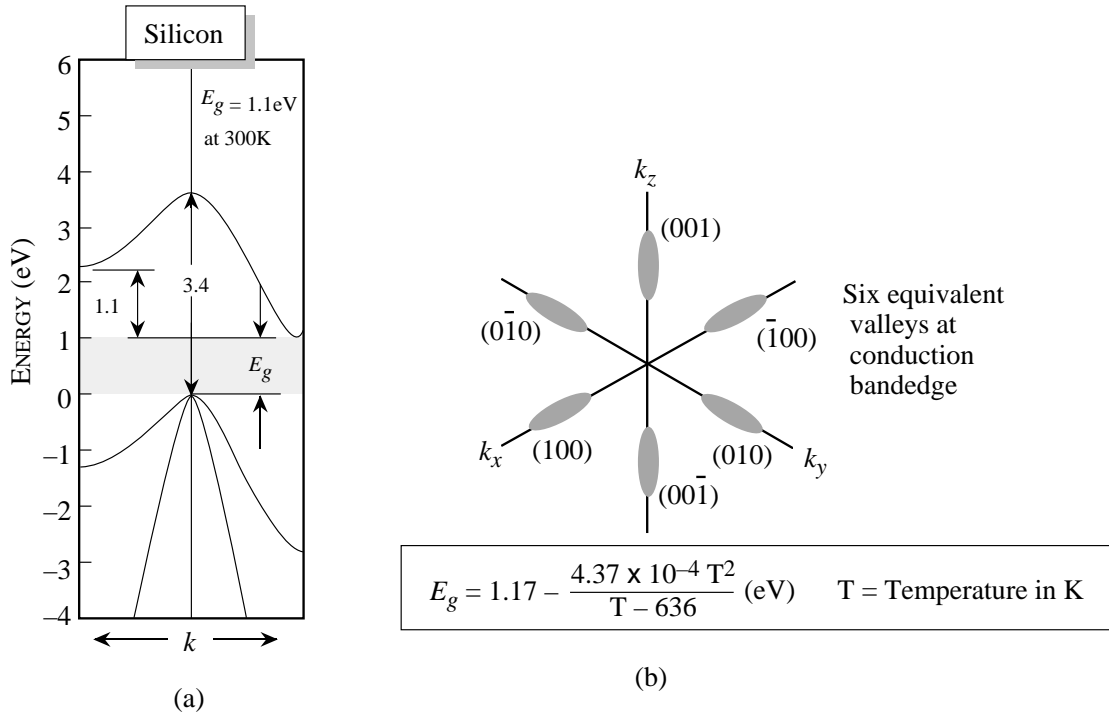
HEAVY HOLE; LIGHT HOLE:

In a simple approximation the heavy hole and light hole bands can also be represented by masses m_{hh}^* and m_{lh}^* . However, the real picture is more complex.



BANDSTRUCTURE: SILICON

Although the bandstructure of Si is far from ideal, having an indirect bandgap, high hole masses, and small spin-orbit splitting, processing related advantages make Si the premier semiconductor for consumer electronics. On the right we show constant energy ellipsoids for Si conduction band. There are six equivalent valleys in Si at the bandedge.



• Indirect gap material \Rightarrow weak optical transitions, cannot be used to produce lasers.

• Valleys along the x -axis and $-x$ -axis: $k_{0x} = \frac{2\pi}{a} (0.85, 0, 0)$ and $k_{0x} = \frac{2\pi}{a} (-0.85, 0, 0)$:

$$E(k) = E_c + \frac{\hbar^2}{2} \left[\frac{(k_x - k_{0x})^2}{m_l^*} + \frac{k_x^2 + k_z^2}{m_t^*} \right]; m_l = 0.98 m_0; m_t = 0.19 m_0$$

similar E - k relations for other 4 valleys.

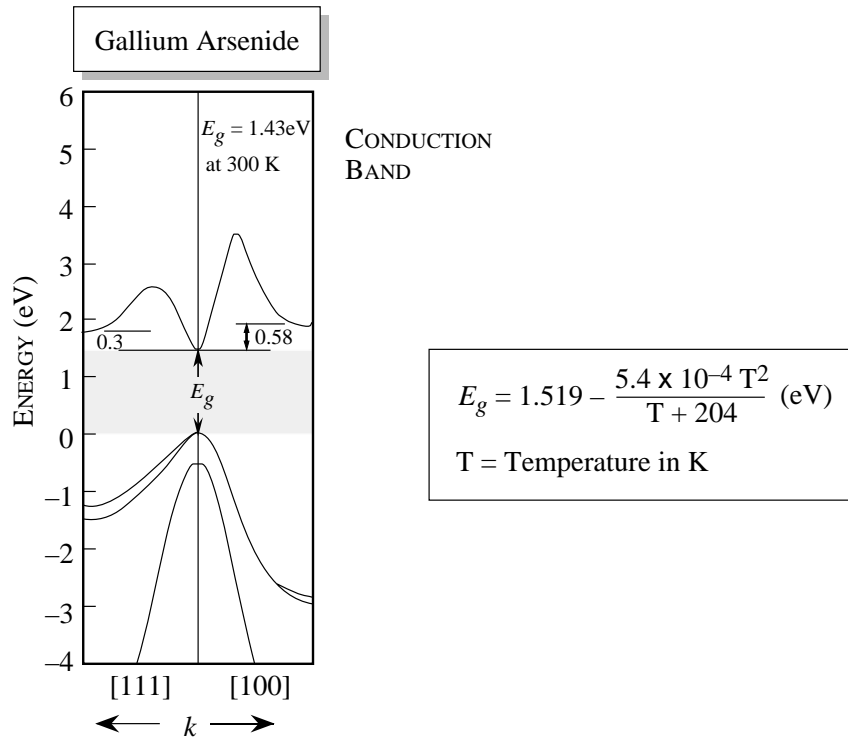
• Density of states mass = $1.08 m_0$ (6 valleys included).

• Heavy hole mass: $0.49 m_0$; light hole mass: $0.16 m_0$.

• Intrinsic carrier concentration at 300 K: $1.5 \times 10^{10} \text{ cm}^{-3}$.

BANDSTRUCTURE: GaAs

The bandgap at 0 K is 1.51 eV and at 300 K it is 1.43 eV. The bottom of the conductionband is at $k = (0,0,0)$, i.e., the G-point. The upper conduction band valleys are at the L -point.



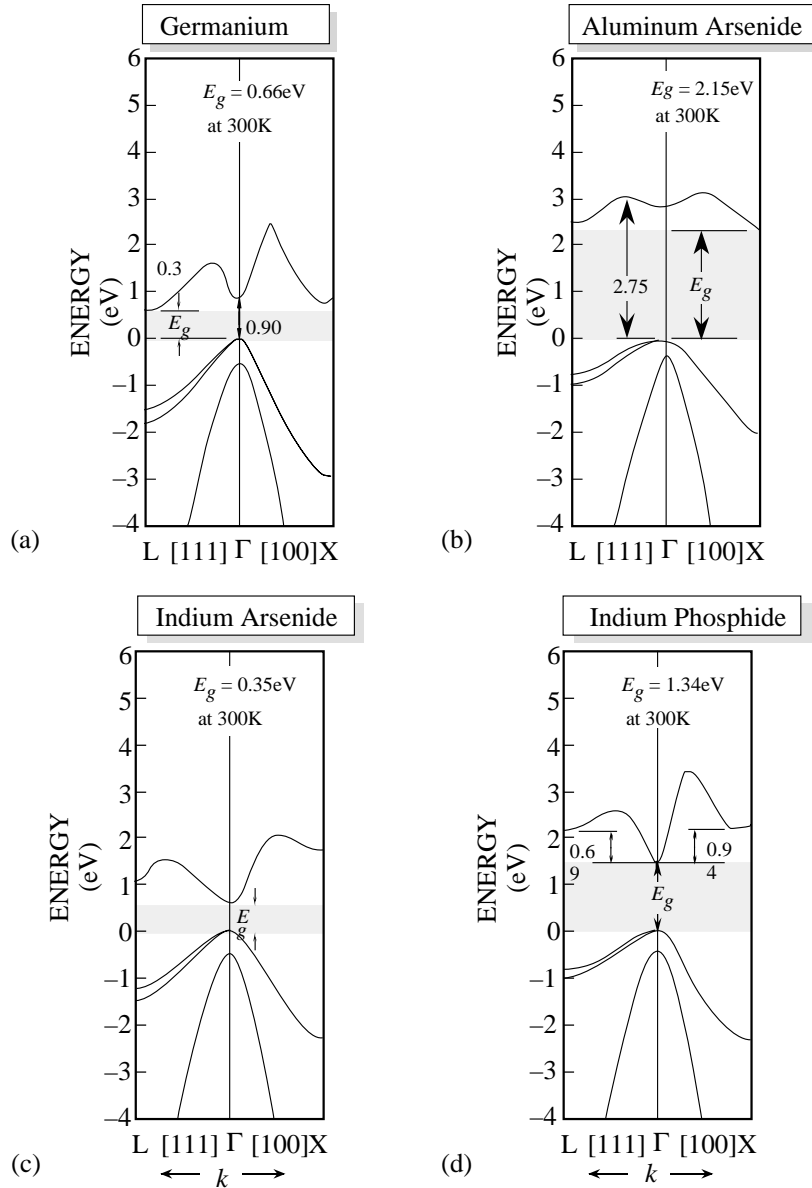
CONDUCTION BAND:

- Electron mass is light. $m^* = 0.067 m_0$
- Upper valley mass is large. $m^* = 0.25 m_0$ results in negative differential resistance at higher fields.
- Material is direct bandgap and has strong optical transitions \Rightarrow can be used for light emission.

VALENCE BAND:

- Heavy hole mass: $0.45 m_0$; light hole mass = $0.08 m_0$.
- Intrinsic carrier concentration at 300 = $1.84 \times 10^6 \text{ cm}^{-3}$.

BANDSTRUCTURE: Ge AlAs, InAs, InP



(a) Bandstructure of Ge. (b) Bandstructure of AlAs. (c) Bandstructure of InAs. Since no adequate substitute matches InAs directly, it is often used as an alloy (InGaAs, InAlAs, etc.,) for devices. (d) Bandstructure of InP. InP is a very important material for high speed devices as well as a substrate and barrier layer material for semiconductor lasers.

ELECTRONIC PROPERTIES OF SOME SEMICONDUCTORS

Material	Bandgap (eV)	Relative Dielectric Constant	Material	Electron Mass (m_0)	Hole Mass (m_0)
C	5.5, I	5.57	AlAs	0.1	
Si	1.124, I	11.9	AlSb	0.12	$m_{dos}^* = 0.98$
Ge	0.664, I	16.2	GaN	0.19	$m_{dos}^* = 0.60$
SiC	2.416, I	9.72	GaP	0.82	$m_{dos}^* = 0.60$
GaAs	1.424, D	13.18	GaAs	0.067	$m_{lh}^* = 0.082$ $m_{hh}^* = 0.45$
AlAs	2.153, I	10.06	GaSb	0.042	$m_{dos}^* = 0.40$
InAs	0.354, D	15.15	Ge	$m_l = 1.64$ $m_t = 0.082$ $m_{dos} = 0.56$	$m_{lh}^* = 0.044$ $m_{hh}^* = 0.28$
GaP	2.272, I	11.11	InP	0.073	$m_{dos}^* = 0.64$
InP	1.344, D	12.56	InAs	0.027	$m_{dos}^* = 0.4$
InSb	0.230, D	16.8	InSb	0.13	$m_{dos}^* = 0.4$
CdTe	1.475, D	10.2	Si	$m_l = 0.98$ $m_t = 0.19$ $m_{dos} = 1.08$	$m_{lh}^* = 0.16$ $m_{hh}^* = 0.49$
AlN	6.2, D	9.14			
GaN	3.44, D	10.0			
ZnSe	2.822, D	9.1			
ZnTe	2.394, D	8.7			

Properties of some semiconductors. D and I stand for direct and indirect gap, respectively. The data are at 300 K. Note that Si has six conduction band valleys, while Ge has four.

SOME IMPORTANT PROPERTIES OF Si AND GaAs

PROPERTY	Si	GaAs
Electron effective mass (m_0)	$m^*_l = 0.98$ $m^*_t = 0.19$ $m^*_{dos} = 1.08$ $m^*_\sigma = 0.26$	$m^* = 0.067$
Hole effective mass (m_0)	$m^*_{hh} = 0.49$ $m^*_{lh} = 0.16$ $m^*_{dos} = 0.55$	$m^*_{hh} = 0.45$ $m^*_{lh} = 0.08$ $m^*_{dos} = 0.47$
Bandgap (eV)	$1.17 - \frac{4.37 \times 10^{-4} T^2}{T + 636}$	$1.519 - \frac{5.4 \times 10^{-4} T^2}{T + 204}$
Electron affinity (eV)	4.01	4.07

For Si: m^*_{dos} : To be used in calculating density of states, position of Fermi level
 m^*_σ : To be used in calculating response to electric field, e.g., in mobility

HOLES IN SEMICONDUCTORS: WHAT ARE HOLES?

In a filled band (valence band) no current can flow, since electrons are normally Fermi particles and obey the Pauli exclusion principle. The electrons can “move” if there is an empty state available. The empty states in the valence band are called holes.

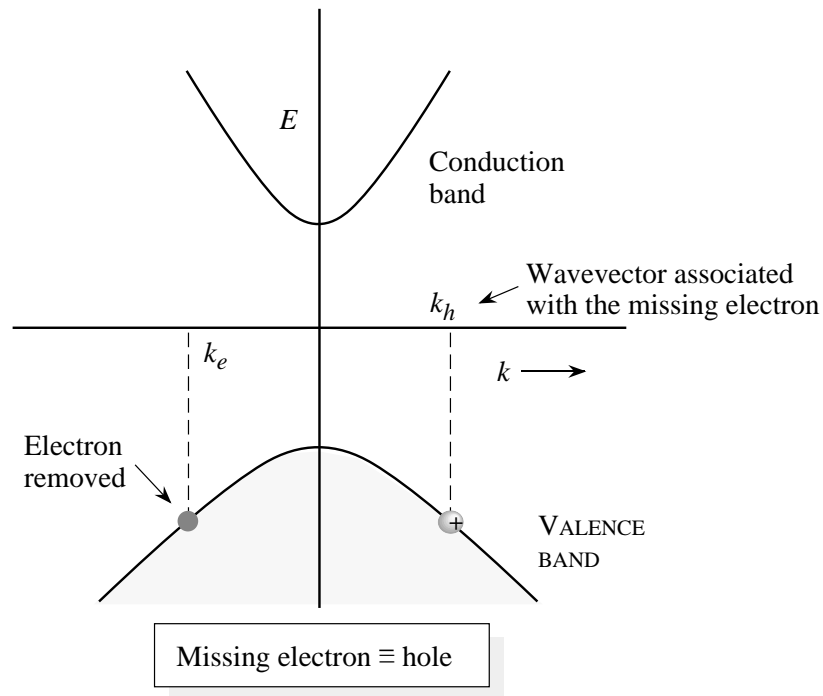
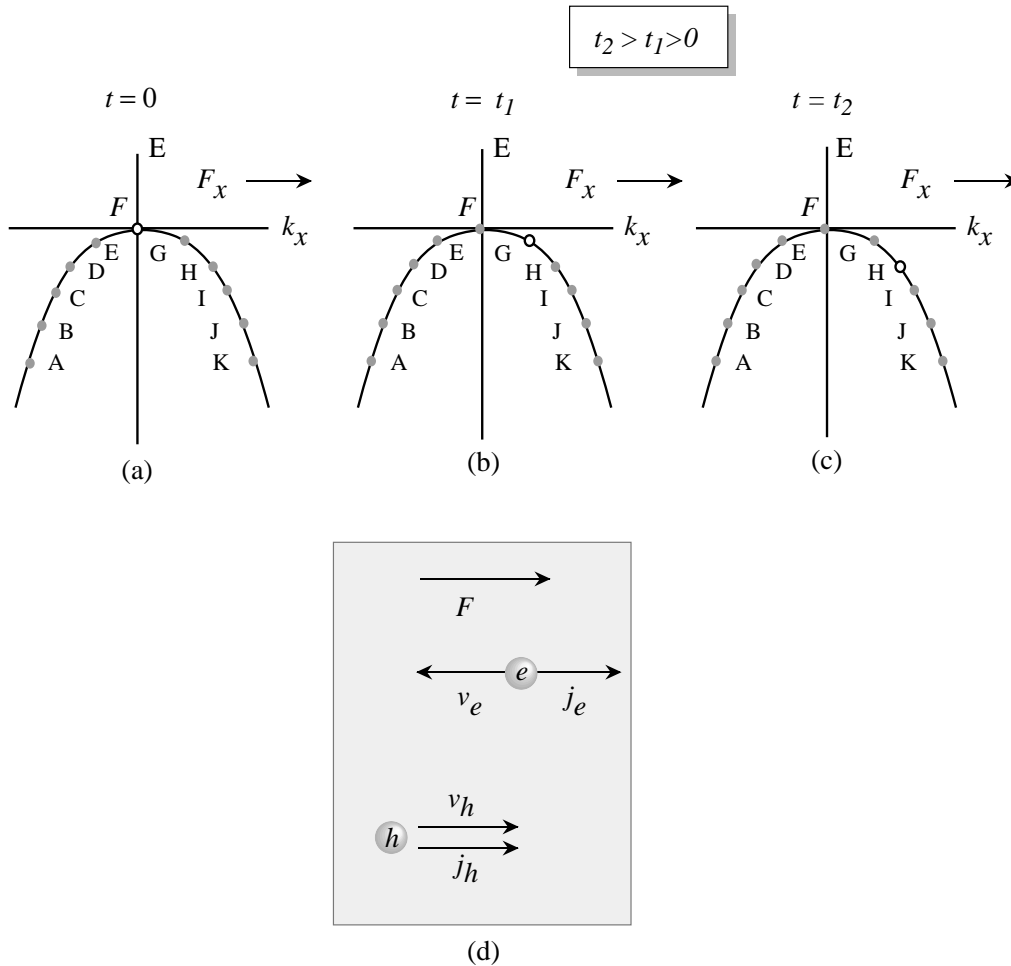


Diagram illustrating the wavevector of the missing electron k_e . The wavevector of the system with the missing electron is $-k_e$, which is associated with the hole.

HOLES IN SEMICONDUCTORS: HOW DO HOLES MOVE?

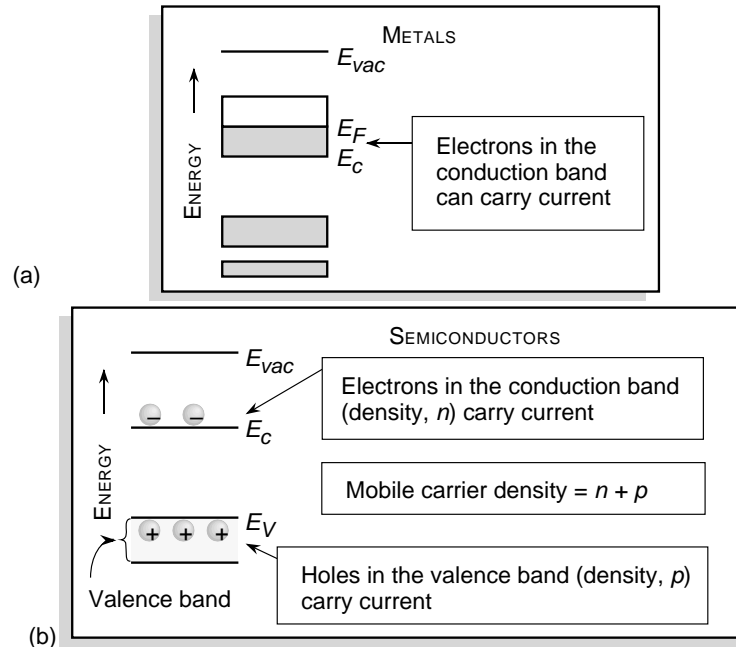
Holes behave *as if* they carry a positive charge.



The movement of an empty electron state, i.e., a hole under an electric field. The electrons move in the direction opposite to the electric field so that the hole moves in the direction of the electric field thus behaving as if it were positively charged, as shown in (a), (b), and (c). (d) The velocities and currents due to electrons and holes. The current flow is in the same direction, even though the electron and holes have opposite velocities. The electron effective mass in the valence band is negative, but the hole behaves as if it has a positive mass.

FREE CARRIERS IN SEMICONDUCTORS: INTRINSIC CARRIERS

In semiconductors, at finite temperatures, there are electrons in the conduction band and holes in the valence band.



(a) A schematic showing allowed energy bands in electrons in a metal. The electrons occupying the highest partially occupied band are capable of carrying current. (b) A schematic showing the valence band and conduction band in a typical semiconductor. In semiconductors only electrons in the conduction band holes in the valence band can carry current.

For small electron (n), hole (p) densities we can use Boltzmann approximation:

$$n = N_c \exp [(E_F - E_c)/k_B T]$$

where

$$N_c = 2 \left(\frac{m_e^* k_B T}{2\pi\hbar^2} \right)^{3/2}$$

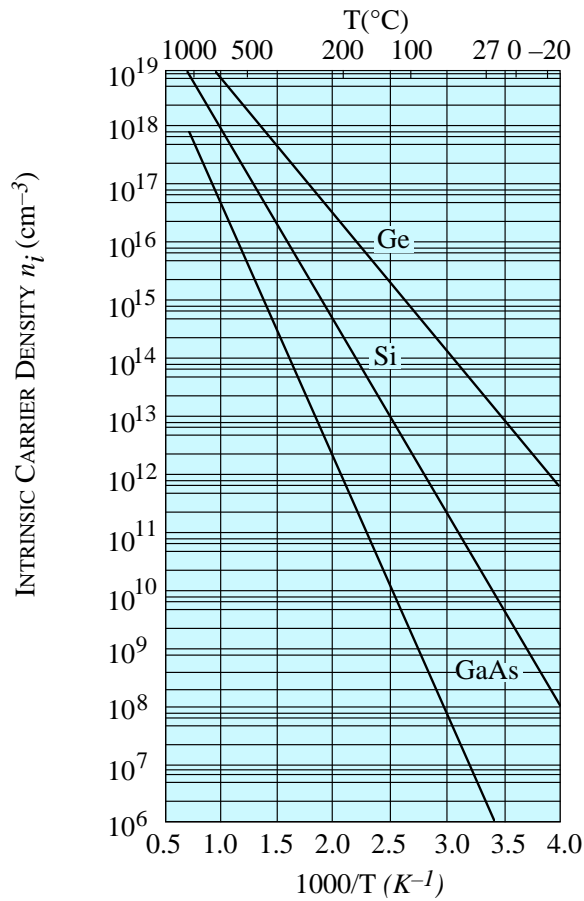
$$p = 2 \left(\frac{m_h^* k_B T}{2\pi\hbar^2} \right)^{3/2} \exp [(E_v - E_F)/k_B T]$$

$$= N_v \exp [(E_v - E_F)/k_B T]$$

Intrinsic case:

$$n_i = p_i = 2 \left(\frac{k_B T}{2\pi\hbar^2} \right)^{3/2} (m_e^* m_h^*)^{3/4} \exp (-E_g/2k_B T)$$

INTRINSIC CARRIER DENSITIES FOR SOME SEMICONDUCTORS



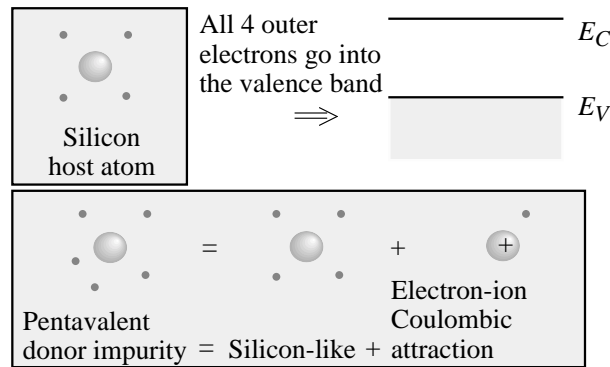
Temperature dependence of n_i, p_i in Si, Ge, GaAs

MATERIAL	CONDUCTION BAND EFFECTIVE DENSITY (N_C)	VALENCE BAND EFFECTIVE DENSITY (N_V)	INTRINSIC CARRIER CONCENTRATION ($n_i = p_i$)
Si (300 K)	$2.78 \times 10^{19} \text{ cm}^{-3}$	$9.84 \times 10^{18} \text{ cm}^{-3}$	$1.5 \times 10^{10} \text{ cm}^{-3}$
Ge (300 K)	$1.04 \times 10^{19} \text{ cm}^{-3}$	$6.0 \times 10^{18} \text{ cm}^{-3}$	$2.33 \times 10^{13} \text{ cm}^{-3}$
GaAs (300 K)	$4.45 \times 10^{17} \text{ cm}^{-3}$	$7.72 \times 10^{18} \text{ cm}^{-3}$	$1.84 \times 10^6 \text{ cm}^{-3}$

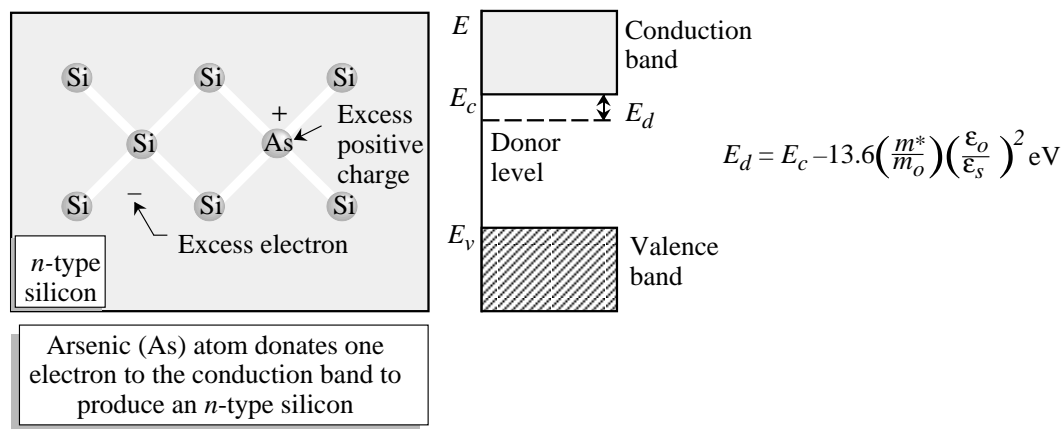
Effective densities and intrinsic carrier concentrations of Si, Ge and GaAs. The numbers for intrinsic carrier densities are the accepted values even though they are smaller than the values obtained by using the equations derived in the text.

DOPING OF SEMICONDUCTORS: DONORS AND ACCEPTORS

If an impurity atom replaces a host semiconductor atom in a crystal it could donate (donor) an extra electron to the conduction band or it could accept (acceptor) an electron from the valence band producing a hole.



A schematic showing the approach one takes to understand donors in semiconductors. The donor problem is treated as the host atom problem together with a Coulombic interaction term. The silicon atom has four “free” electrons per atom. All four electrons are contributed to the valence band at 0 K. The dopant has five electrons out of which four are contributed to the valence band, while the fifth one can be used for increasing electrons in the conduction band.



Charges associated with an arsenic impurity atom in silicon. Arsenic has five valence electrons, but silicon has only four valence electrons. Thus four electrons on arsenic form tetrahedral covalent bonds similar to silicon, and the fifth electron is available for conduction. The arsenic atom is called a donor because when ionized it donates an electron to the conduction band.

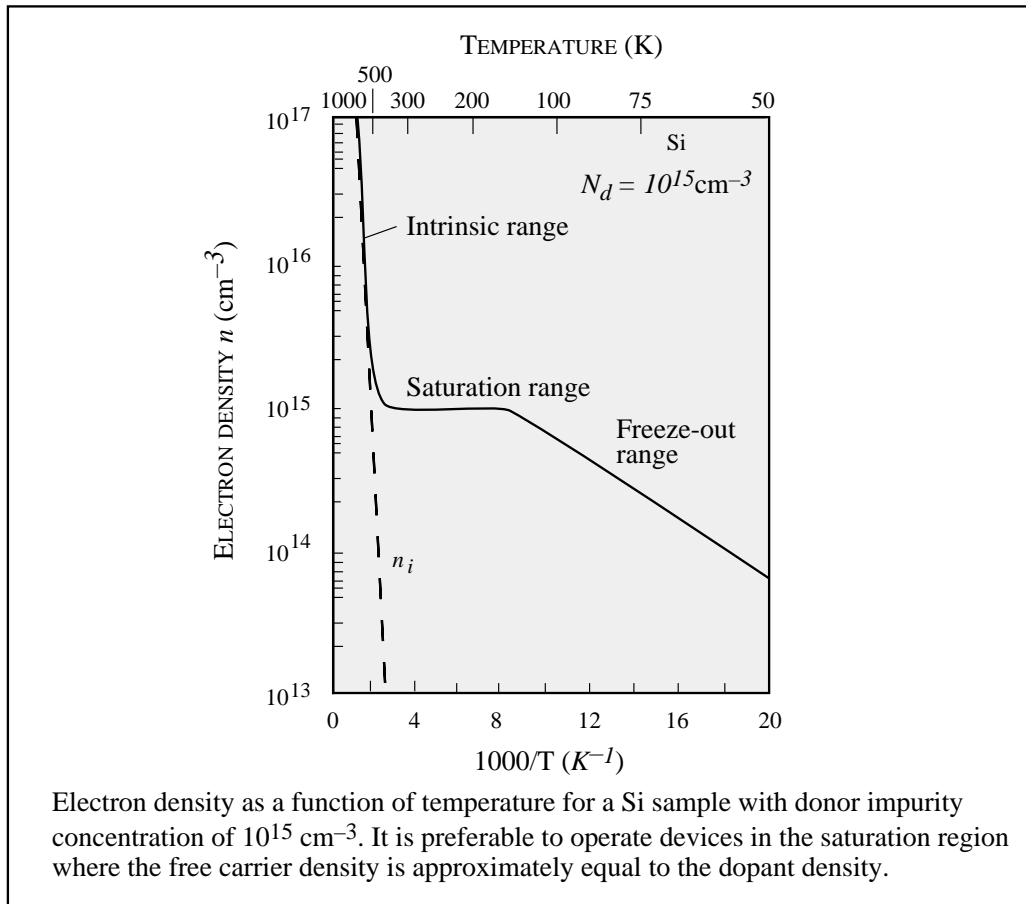
FREE CARRIERS IN DOPED SEMICONDUCTORS

If electron (hole) density is measured as a function of temperature in a doped semiconductor, one observes three regimes:

Freezeout: Temperature is too small to ionize the donors (acceptors), i.e., $k_B T < E_C - E_D$ ($k_B T < E_D - E_V$).

Saturation: Most of the donors (acceptors) are ionized.

Intrinsic: Temperature is so high that $n_i >$ doping density.



It is not possible to operate devices in the intrinsic regime, since the devices always have a high carrier density that cannot be controlled by electric fields.

→ every semiconductor has an upper temperature beyond which it cannot be used in devices. The larger the bandgap, the higher the upper limit.

Zinc Blende and Wurtzite

MATERIAL	CRYSTAL STRUCTURE	BANDGAP (eV)	STATIC DIELECTRIC CONSTANT	LATTICE CONSTANT (Å)	DENSITY (gm-cm ⁻³)
C	DI	5.50, I	5.570	3.56683	3.51525
Si	DI	1.1242, I	11.9	5.431073	2.329002
SiC	ZB	2.416, I	9.72	4.3596	3.166
Ge	DI	0.664, I	16.2	5.6579060	5.3234
BN	HEX	5.2, I	$\epsilon_{ } = 5.06$ $\epsilon_{\perp} = 6.85$	$a = 6.6612$ $c = 2.5040$	2.18
BN	ZB	6.4, I	7.1	3.6157	3.4870
BP	ZB	2.4, I	11.	4.5383	2.97
BAs	ZB	—	—	4.777	5.22
AlN	W	6.2, D	$\bar{\epsilon} = 9.14$	$a = 3.111$ $c = 4.981$	3.255
AlP	ZB	2.45, I	9.8	5.4635	2.401
AlAs	ZB	2.153, I	10.06	5.660	3.760
AlSb	ZB	1.615, I	12.04	6.1355	4.26
GaN	W	3.44, D	$\epsilon_{ } = 10.4$ $\epsilon_{\perp} = 9.5$	$a = 3.175$ $c = 5.158$	6.095
GaP	ZB	2.272, I	11.11	5.4505	4.138
GaAs	ZB	1.4241, D	13.18	5.65325	5.3176
GaSb	ZB	0.75, D	15.69	6.09593	5.6137
InN	W	1.89, D	—	$a = 3.5446$ $c = 8.7034$	6.81
InP	ZB	1.344, D	12.56	5.8687	4.81
InAs	ZB	0.354, D	15.15	6.0583	5.667
InSb	ZB	0.230, D	16.8	6.47937	5.7747
ZnO	W	3.44, D	$\epsilon_{ } = 8.75$ $\epsilon_{\perp} = 7.8$	$a = 3.253$ $c = 5.213$	5.67526
ZnS	ZB	3.68, D	8.9	5.4102	4.079
ZnS	W	3.9107, D	$\bar{\epsilon} = 9.6$	$a = 3.8226$ $c = 6.2605$	4.084
ZnSe	ZB	2.8215, D	9.1	5.6676	5.266
ZnTe	ZB	2.3941, D	8.7	6.1037	5.636
CdO	R	0.84, I	21.9	4.689	8.15
CdS	W	2.501, D	$\bar{\epsilon} = 9.83$	$a = 4.1362$ $c = 6.714$	4.82
CdS	ZB	2.50, D	—	5.818	—
CdSe	W	1.751, D	$\epsilon_{ } = 10.16$ $\epsilon_{\perp} = 9.29$	$a = 4.2999$ $c = 7.0109$	5.81
CdSe	ZB	—	—	6.052	—
CdTe	ZB	1.475, D	10.2	6.482	5.87
PbS	R	0.41, D*	169.	5.936	7.597
PbSe	R	0.278, D*	210.	6.117	8.26
PbTe	R	0.310, D*	414.	6.462	8.219

Data are given at room temperature values (300 K).

Key: DI: diamond; HEX: hexagonal; R: rocksalt; W: wurtzite; ZB: zinc blende;

*: gap at L point; D: direct; I: indirect $\epsilon_{||}$: parallel to c -axis; ϵ_{\perp} : perpendicular to c -axis

Bandgaps (in eV) of some semiconductors

TETRAHEDRALLY BONDED MATERIALS				
V	C	Si	Ge	α -Sn
C	5.5i,D			
Si	2.6i,Z/W	1.1i,D	0.7-1.1i	
Ge		0.7-1.1	0.74i,D	
α -Sn				0.09,D
III-V	N	P	As	Sb
B	3.8,W	2.0i,Z	1.5i,Z	
Al	5.9,W	2.5,Z	2.2,Z	1.7,Z
Ga	3.5,W	2.4i,Z	1.5,Z	0.81,Z
In	2.4,W	1.4,Z	0.41,Z	0.24,Z
II-VI	O	S	Se	Te
Zn	3.4,W	3.6,Z/W	2.8,Z/W	2.4,Z
Cd	1.3i,R	2.5,Z/W	1.8,Z/W	1.6,Z
Hg	2.2,O/Rh	2.3,T	-.06,Z	-.3,Z
I-VII	F	Cl	Br	I
Cu		3.4,Z	3.1,Z	3.1,Z
Ag	2.8i,R	3.2i,R	2.7i,R	3.0,W

i: Indirect gap
D: Diamond
Z: Zinc Blende
W: Wurtzite
R: Rocksalt
O: Orthorhombic
Rh: Rhombohedral
T: Trigonal
OR: Orthorhombic distorted rocksalt
M: Monoclinic

NON-TETRAHEDRAL BONDED MATERIALS

IV-VI compounds

IV-VI	O	S	Se	Te
Ge		1.7,OR	1.1,OR	0.15,R
Sn		1.1,OR	0.9,OR	2.1,R
Pb	2.0,i	0.29,R	0.15,R	0.19,R

Group VI elements

VI	S	Se	Te
	3.6,O	1.9i,T 2.5,M	0.33,T

Group V elements

V	P	As	Sb	Bi
	.33,O	.17,Rh	.10	.015