Lecture 2

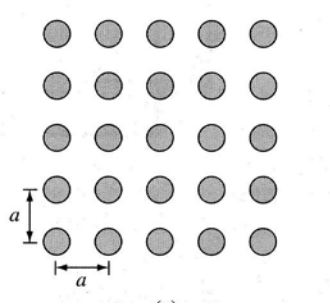
Unit Cells and Miller Indexes

Reading:

(Cont'd) Anderson[2] 1.8, 2.1-2.7

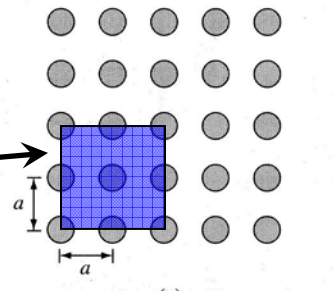
Unit Cell Concept

The crystal lattice consists of a periodic array of atoms.



Unit Cell Concept

A "building block" that can be periodically duplicated to result in the crystal lattice is known as the "unit cell".



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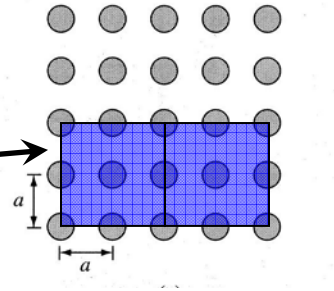

Unit Cell Concept

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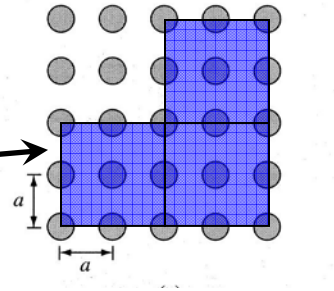

Unit Cell Concept

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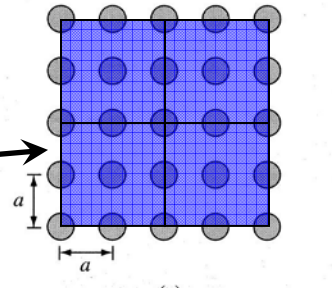


Unit Cell Concept

The crystal lattice consists of a periodic array of atoms.

The smallest "building block" that can be periodically duplicated to result in the crystal lattice is known as the "primative unit cell".

A "building block" that can be periodically duplicated to result in the crystal lattice is known as the "unit cell".

The unit cell may not be unique.

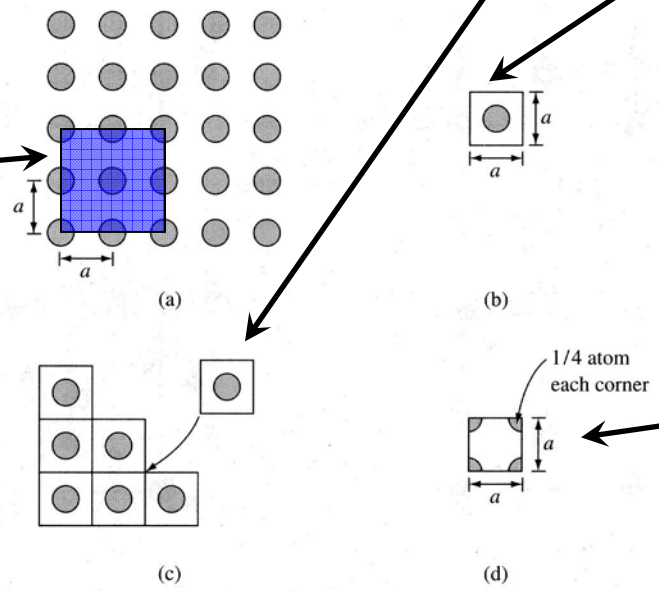


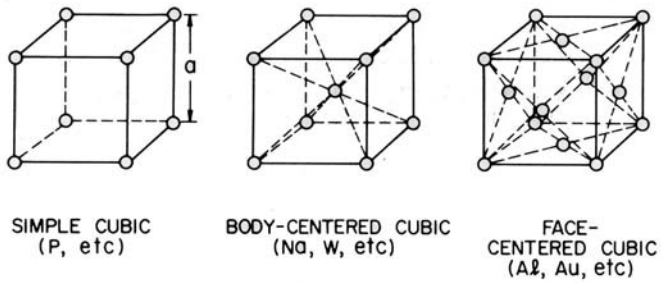
Figure 1.2 Introduction to the unit cell method of describing atomic arrangements within crystals. (a) Sample two-dimensional lattice. (b) Unit cell corresponding to the part (a) lattice. (c) Reproduction of the original lattice. (d) An alternative unit cell.

Unit Cell Concept

Lattice Constant: A length that describes the unit cell. It is normally given in Å, angstroms = 1e-10 meters.

QuickTime Movie QuickTime Movie QuickTime Movie

Diamond Structure: Constructed by 2 "inter-penetrating" FCC Lattices



QuickTime Movie

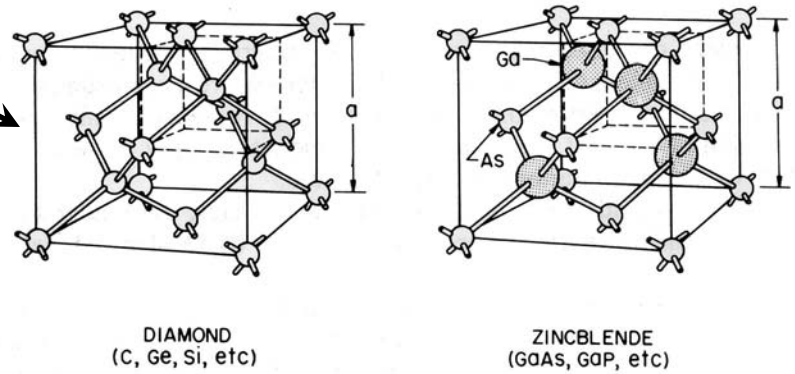
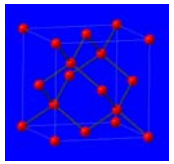
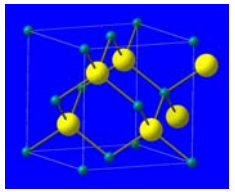


Fig. 1 Some important unit cells (direct lattices) and their representative elements or compounds; a is the lattice constant.

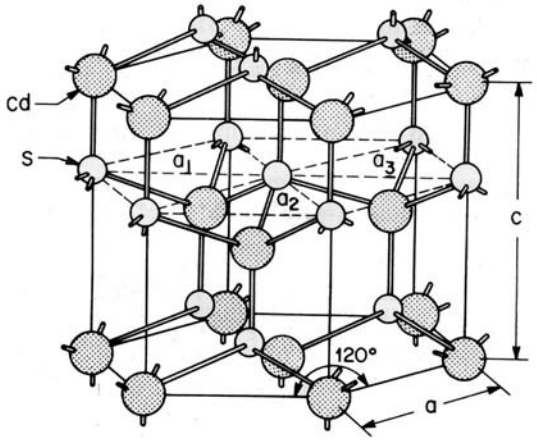
Zincblende is a diamond structure with every other atom a different element. Example: Ga only bonds to As and As only bonds to Ga.



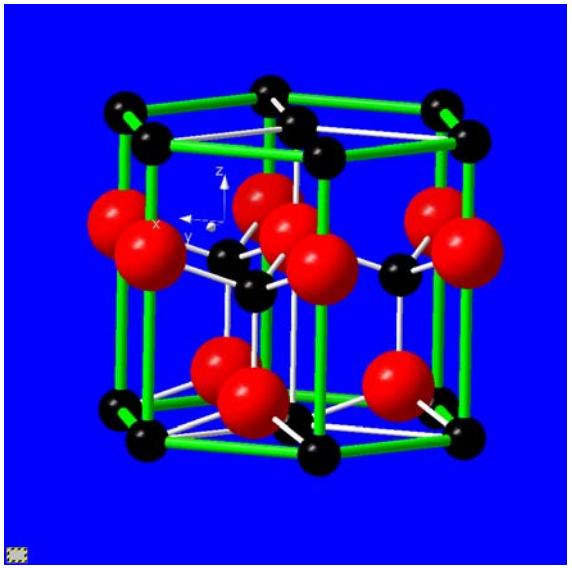


Unit Cell Concept

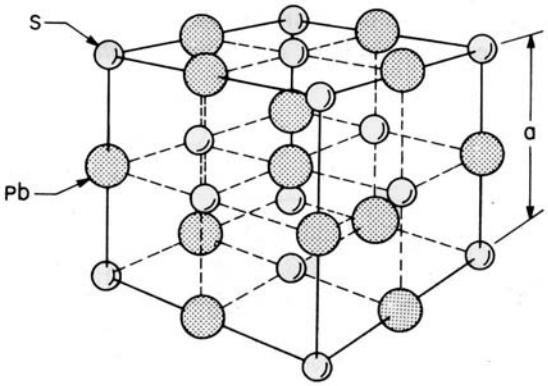
Some unit cells have hexagonal symmetry.



(a)



Rocksalt unit cells are one of the simplest practical unit cells.

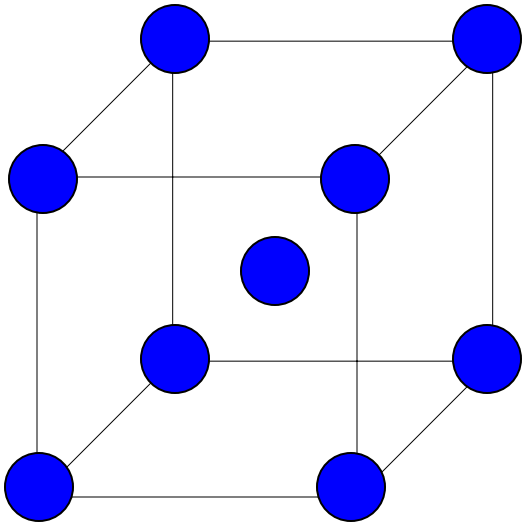


(b)

Fig. 2 Two unit cells of compound semiconductors. (*a*) Wurtzite lattice (CdS, ZnS, etc.). (*b*) Rock-salt lattice (PbS, PbTe, etc.).

Atomic Density

What is the atomic density of a BCC material with lattice constant 5.2 angstroms?

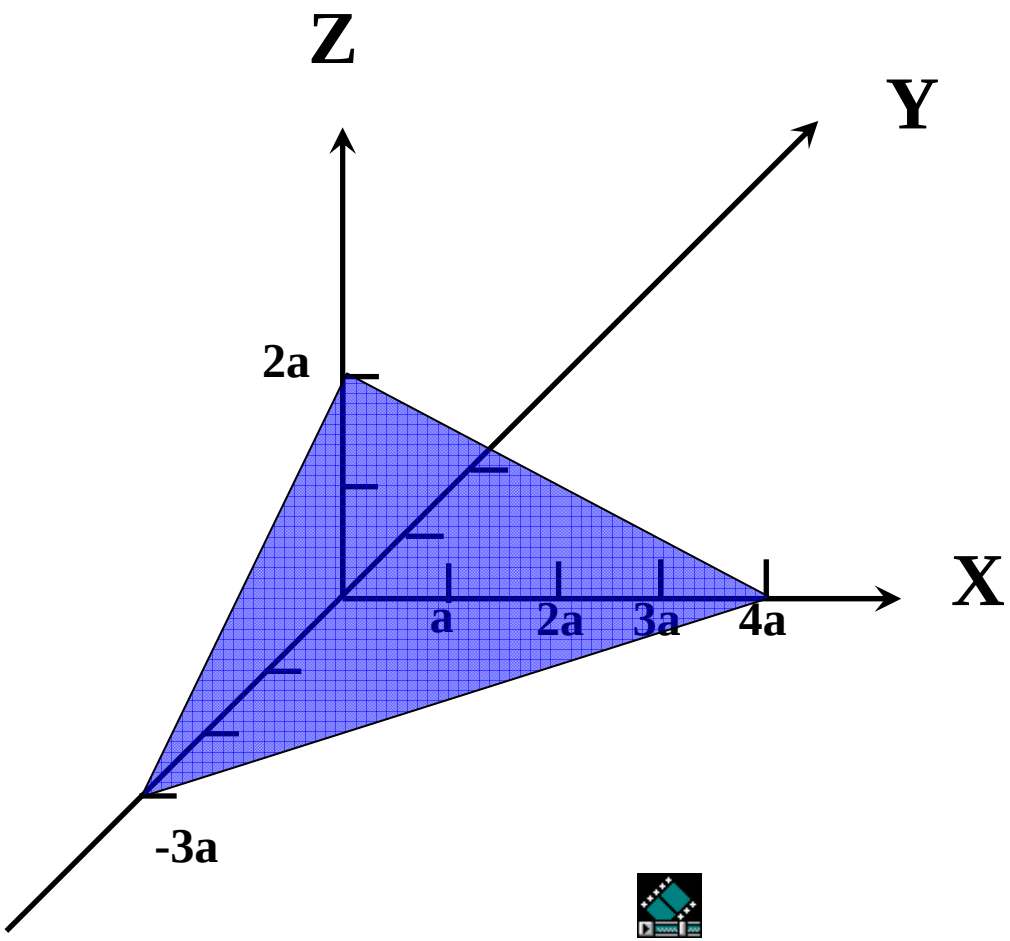


$$Number\ of\ \ Atoms\ \ per\ unit\ cell = 2$$

$$Volume\ of\ \ unit\ cell = a^3 = (5.2e-8\ cm)^3 = 1.41e-22\ cm^3$$

$$Density = \frac{Number\ of\ \ Atoms\ \ per\ unit\ cell}{Volume\ of\ \ unit\ cell} = 1.4e22\ \frac{atoms}{cm^3}$$

Crystalline Planes and Miller Indices



QuickTime Movie

Identify Intercepts in x,y,z order = 4a, -3a, 2a

Divide by unit cell length in each direction x,y,z order = 4, -3, 2

Invert the values = 1/4, -1/3, 1/2

Multiply by a number (12 in this example) to give smallest whole number set = 3, -4, 6

Place any minus signs over their index and place set in parenthesis = (3$\bar{4}$6)

Crystalline Planes and Miller Indices: Planes and directions

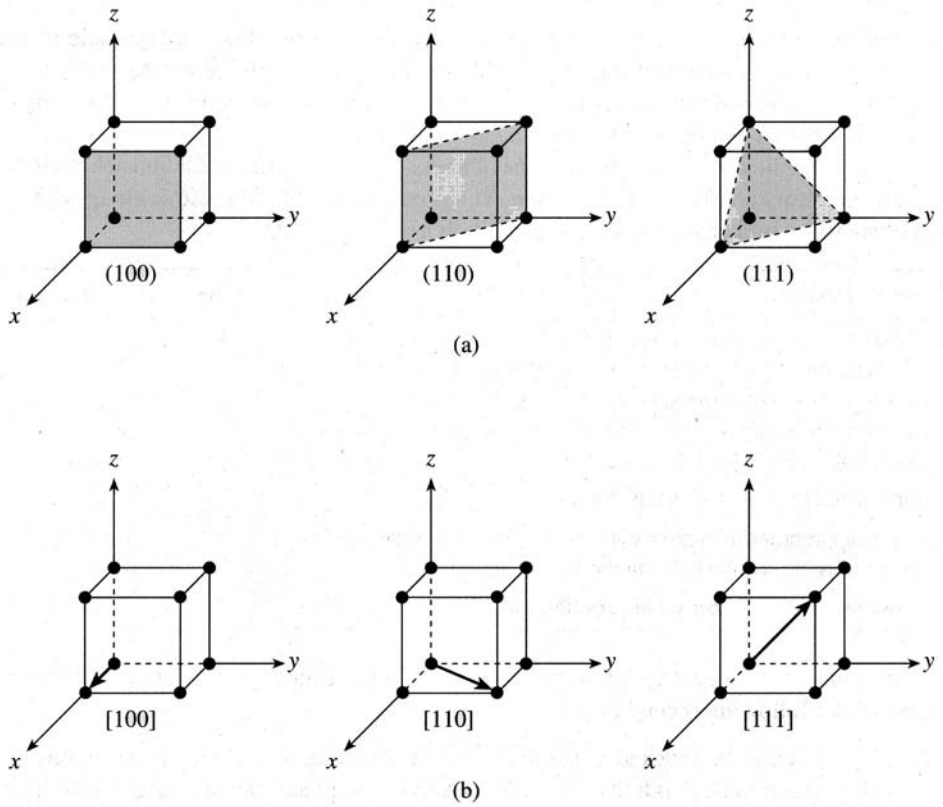
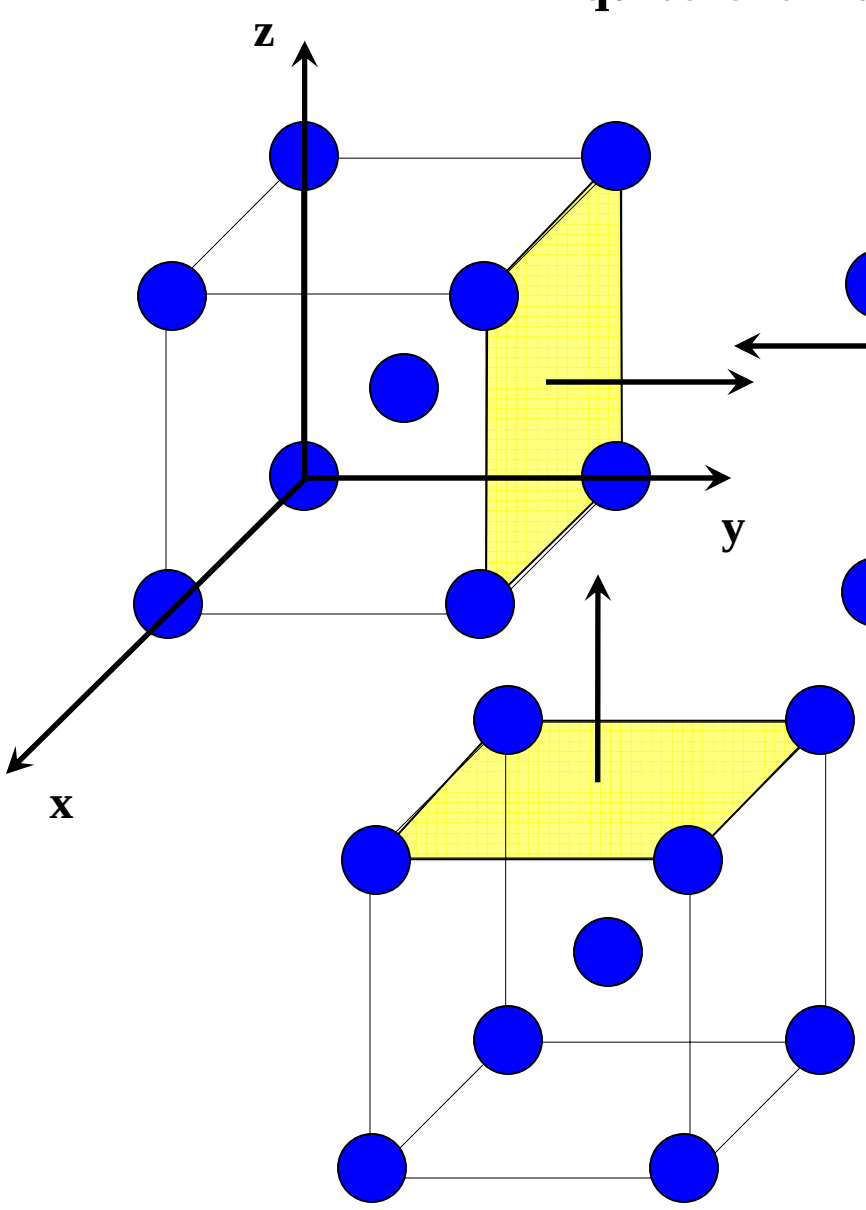
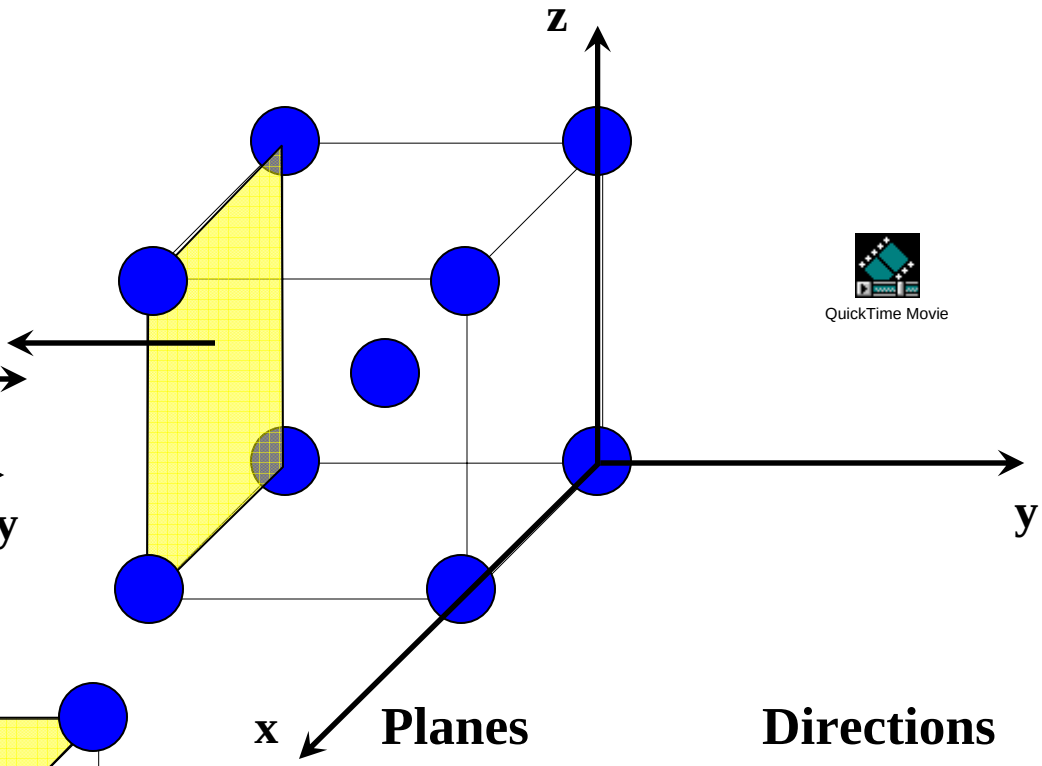


Figure 1.7 Visualization and Miller indices of commonly encountered (a) crystalline planes and (b) direction vectors.

Crystalline Planes and Miller Indices:

Equivalent Planes and directions





QuickTime Movie

Planes	Directions
{100} =	[100] =
(100), $(\bar{1}00)$	<100>, $<\bar{1}00>$
(010), $(0\bar{1}0)$	<010>, $<0\bar{1}0>$
(001), $(00\bar{1})$	<001>, $<00\bar{1}>$

Lecture 3

Bonding Model and Dopants

Reading:

(Cont'd) Pierret 1.1, 1.2, 1.4, 2.1-2.6

Comparison of the Hydrogen Atom and Silicon Atom

$$Energy_{Hydrogen\ electron} = -\frac{m_o q^4}{2(4\pi\varepsilon_0 \hbar n)^2} = -\frac{13.6\ eV}{n^2}$$

$$where\ m_o = electron\ mass,\ \hbar = planks\ constant/2\pi = h/2\pi$$

$$q = electron\ charge,\ and\ n = 1,2,3...$$

Hydrogen

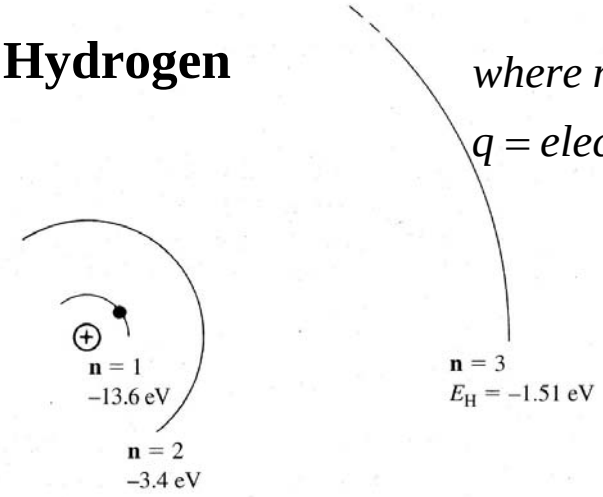
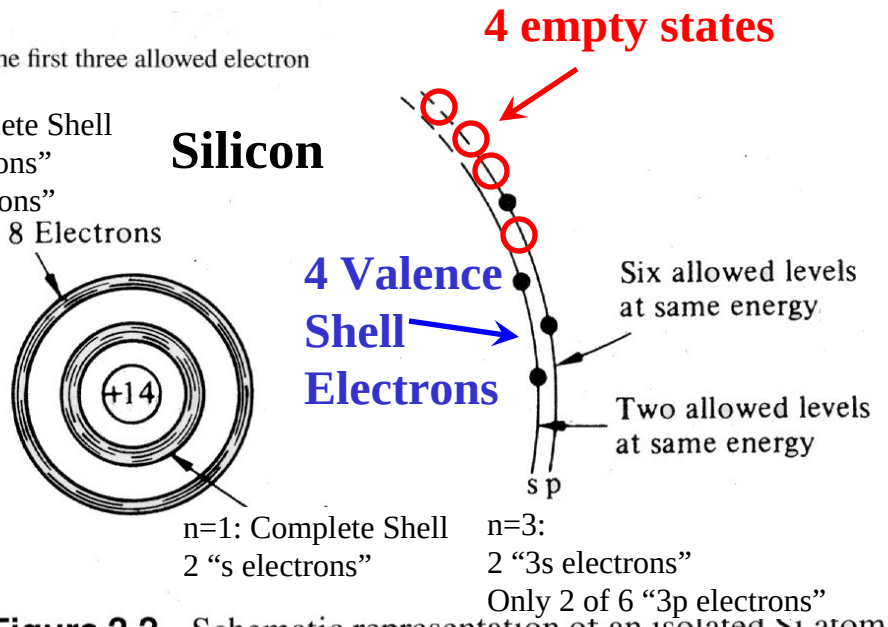


Figure 2.1 The hydrogen atom—idealized representation showing the first three allowed electron orbits and the associated energy quantization.

Silicon

n=2: Complete Shell
2 "2s electrons"
6 "2p electrons"



n=1: Complete Shell
2 "s electrons"

n=3:
2 "3s electrons"
Only 2 of 6 "3p electrons"

Figure 2.2 Schematic representation of an isolated Si atom.

Pauli Exclusion Principle

Only 2 electrons, of spin+/-1/2, can occupy the same energy state at the same point in space.

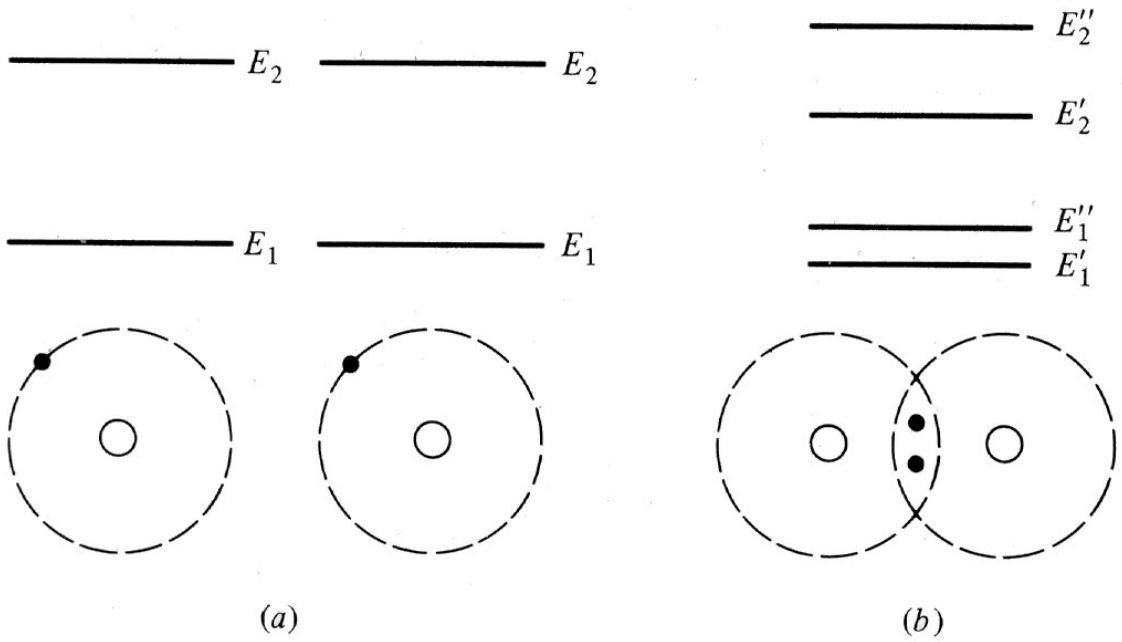


FIGURE 1-9
Two hydrogen atoms: (*a*) noninteracting and (*b*) interacting. Splitting of energy levels is illustrated for (*b*).

Banding of Discrete states and the Simplified Model

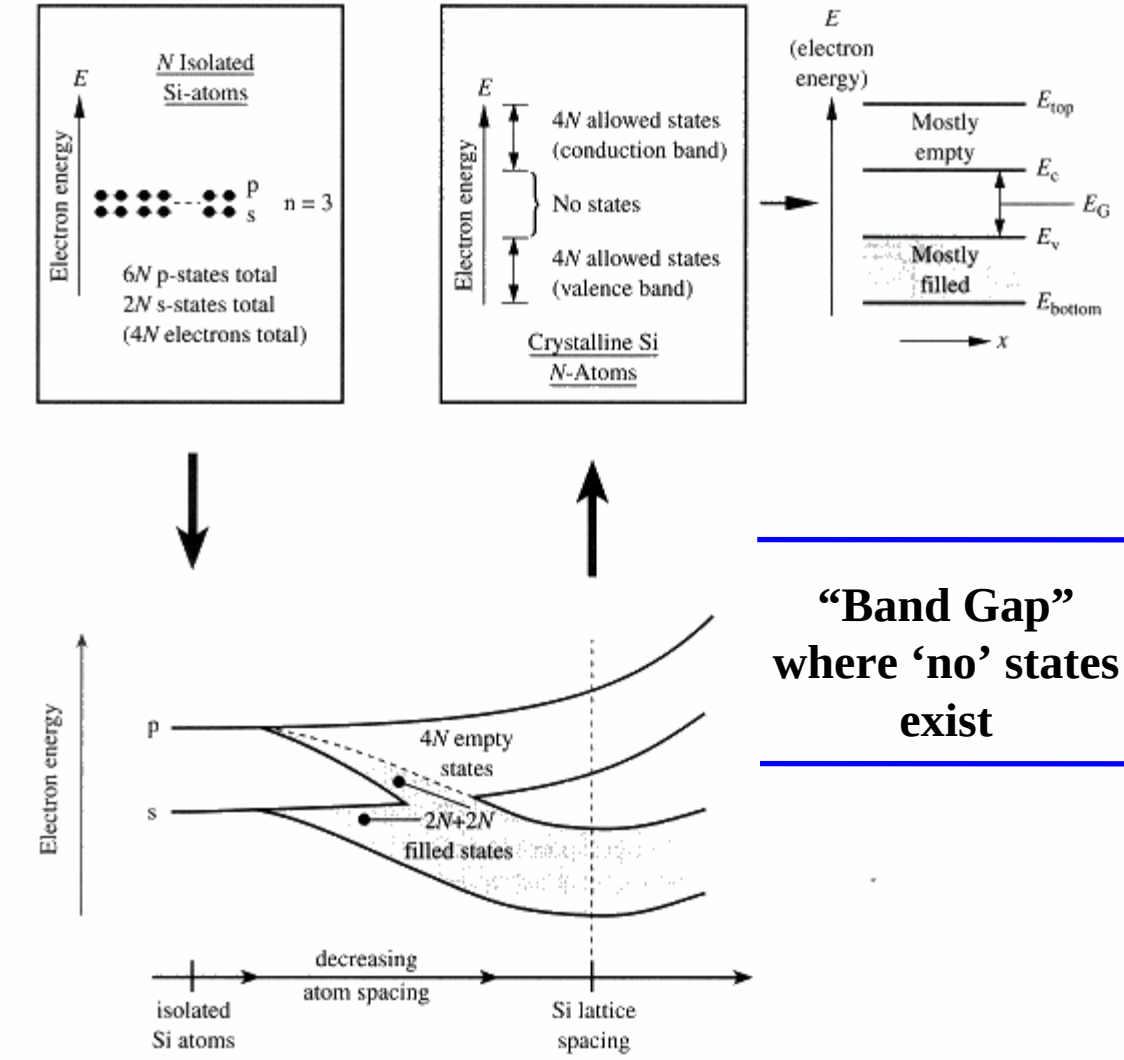


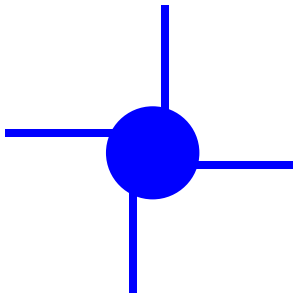
Figure 2.5 Conceptual development of the energy band model starting with N isolated Si atoms on the top left and concluding with a "dressed-up" version of the energy band model on the top right.

T=0K

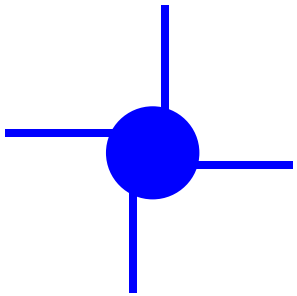
E_C or conduction band

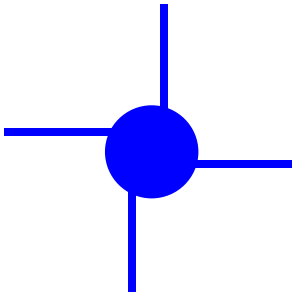
"Band Gap" where 'no' states exist

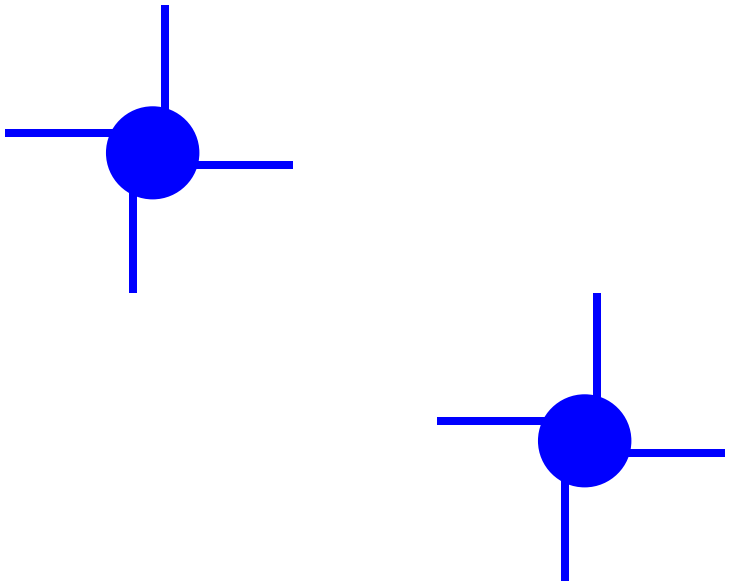
E_V or valence band

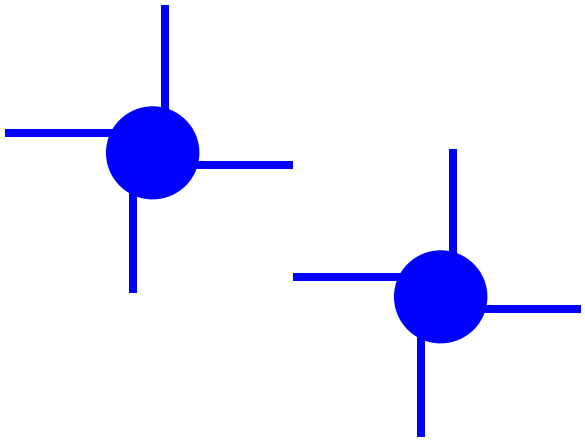


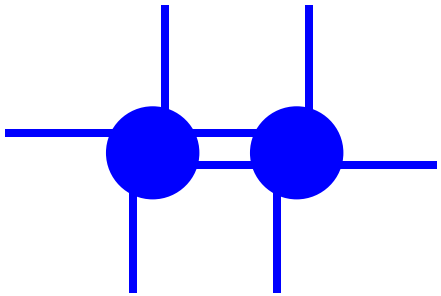
4 electrons available for sharing (covalent bonding) in outer shell of atoms

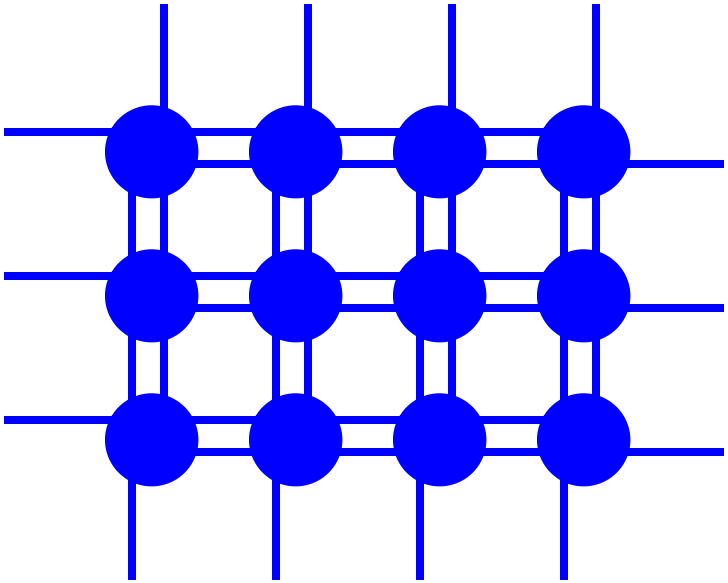


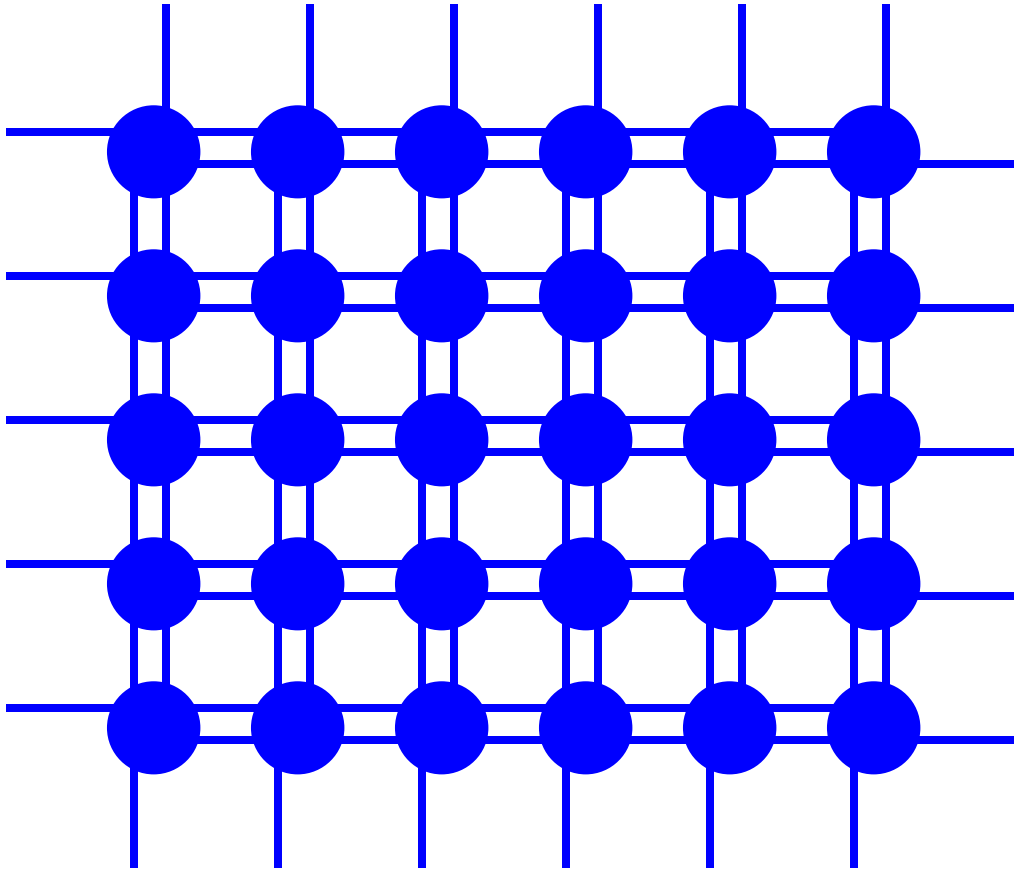


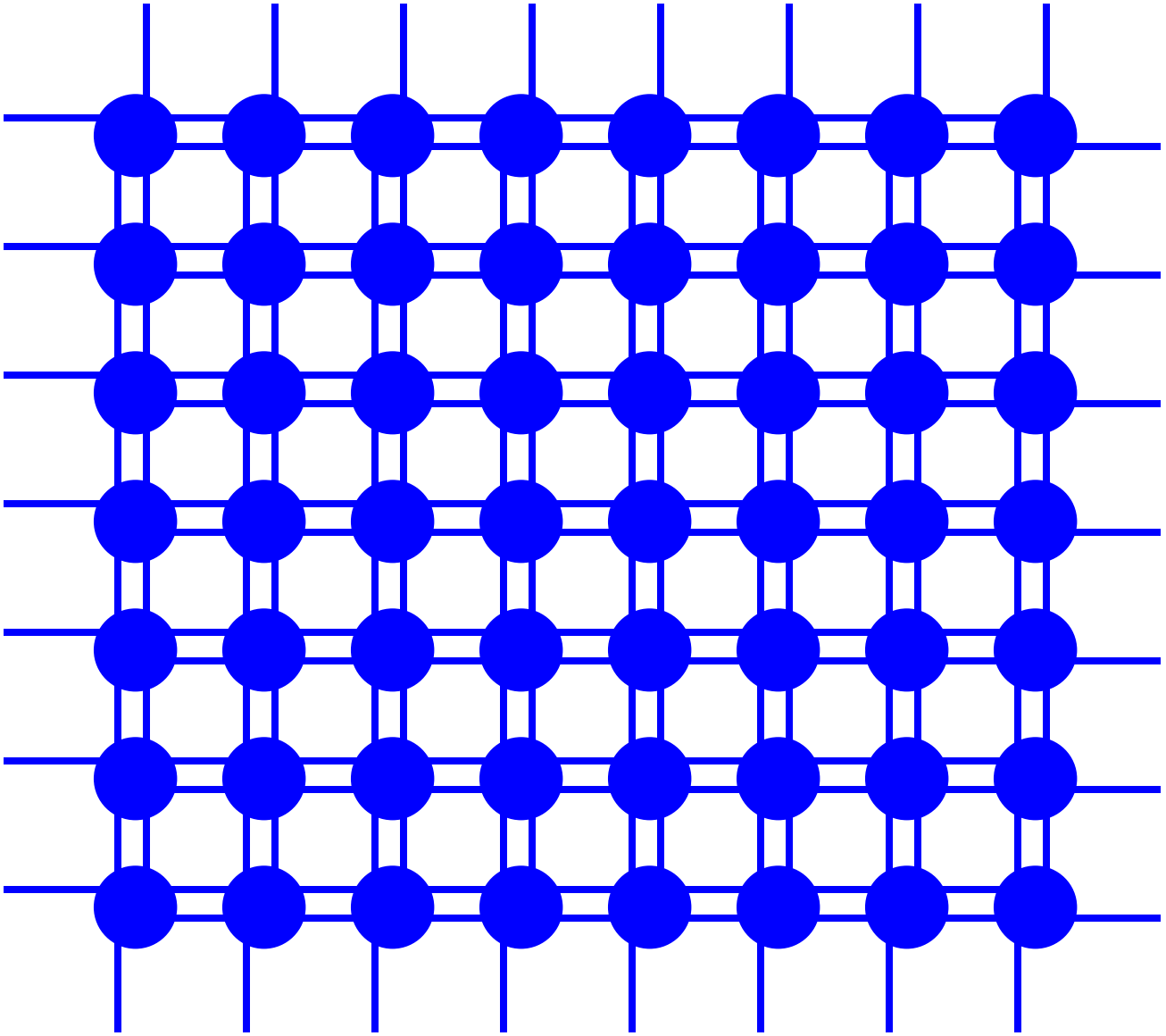






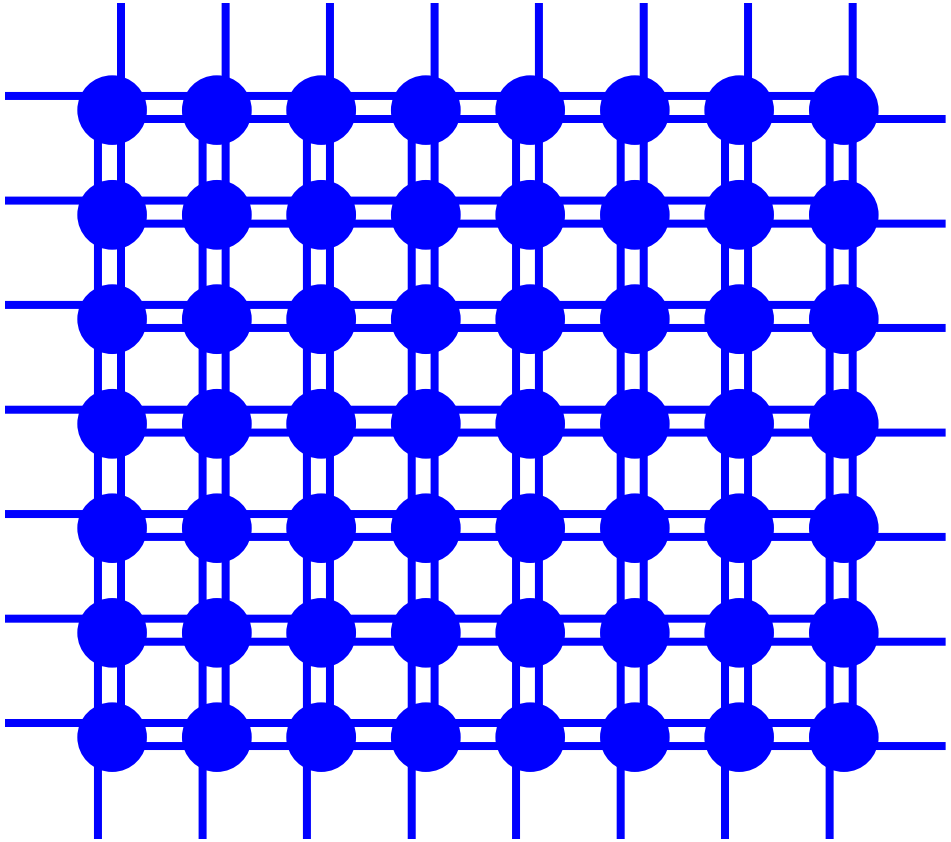




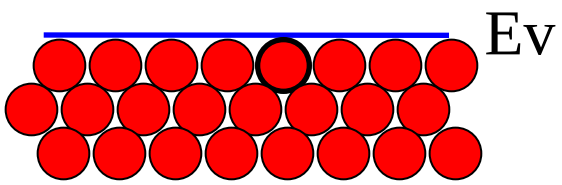


Band Occupation at Low Temperature (0 Kelvin)

For ($E_{thermal}$=kT)=0



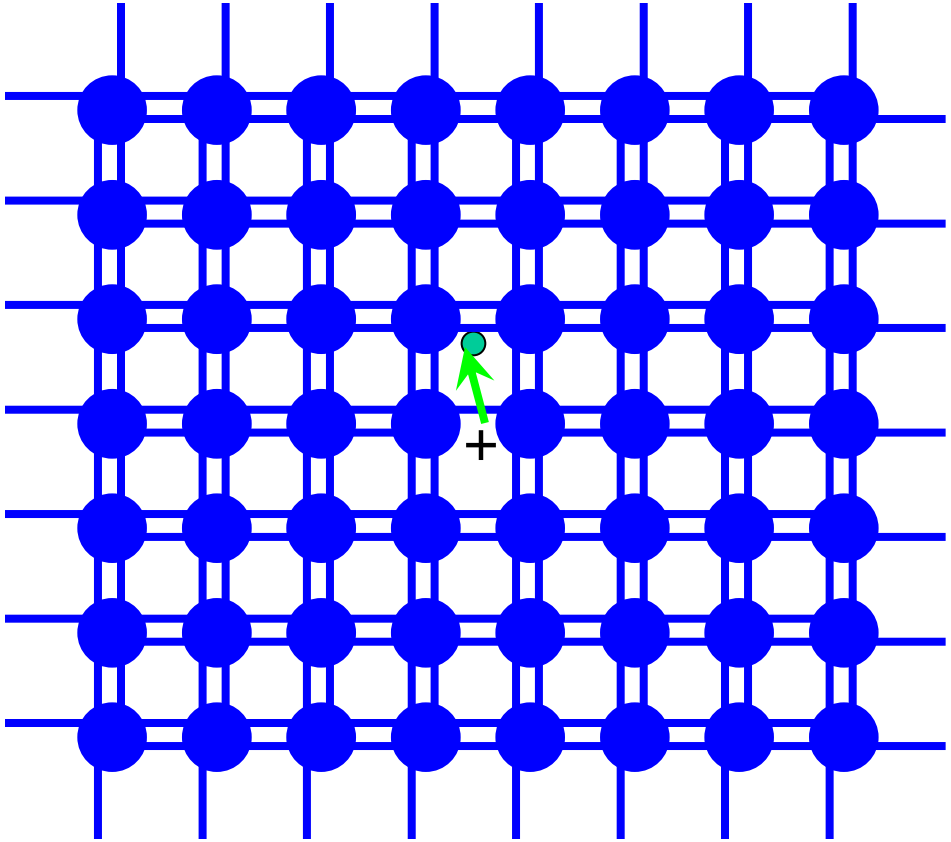
No electrons in conduction band means no electron conduction is possible



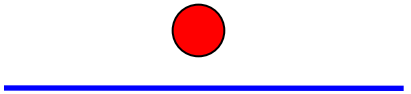
No “Holes” valence band means no “hole” conduction is possible

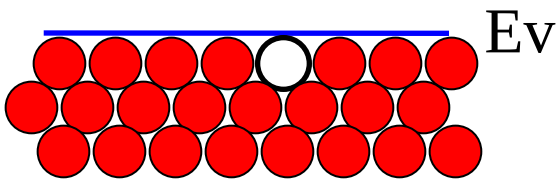
Band Occupation at Higher Temperature (T>0 Kelvin)

For ($E_{thermal}$=kT)>0



Electron free to move in conduction band

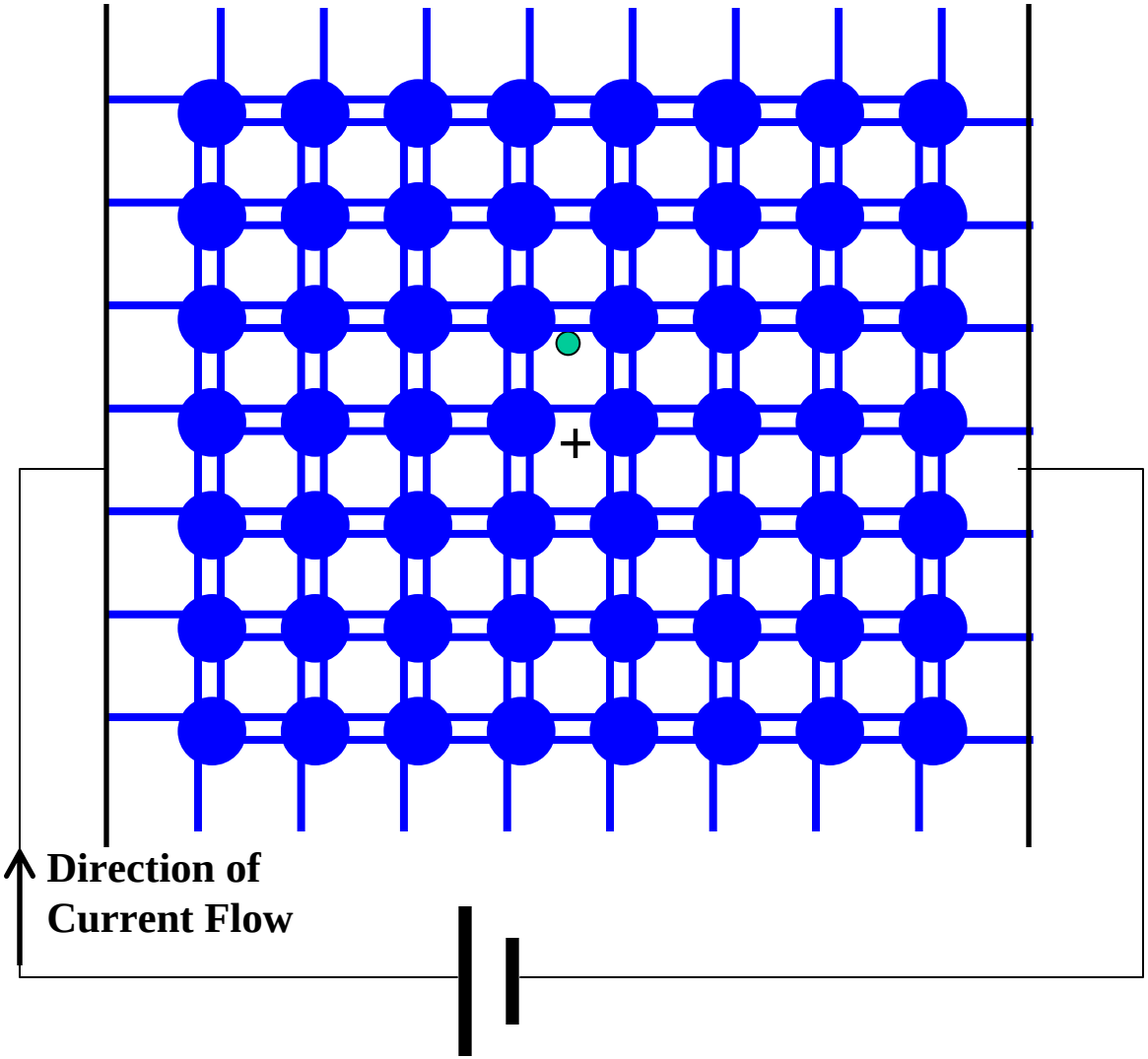




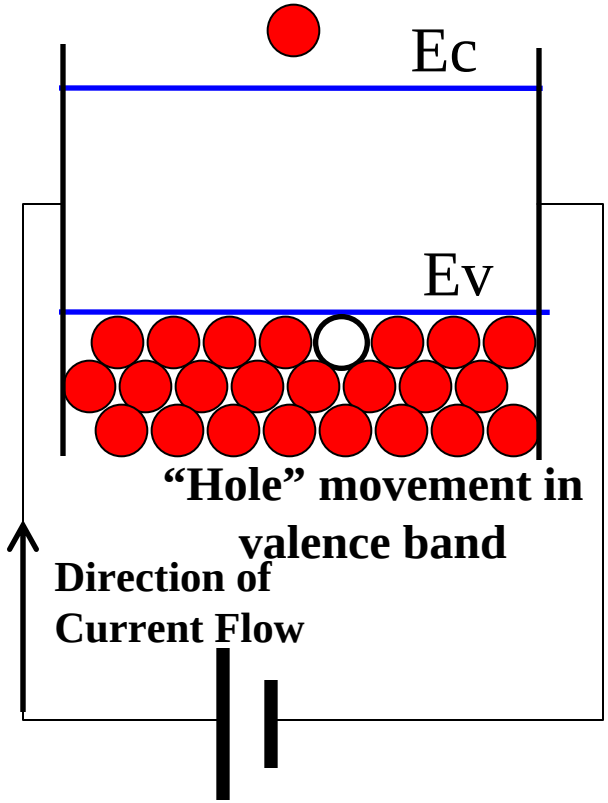
"Hole" free to move in valence band

Carrier Movement Under Bias

For ($E_{thermal}$=kT)>0

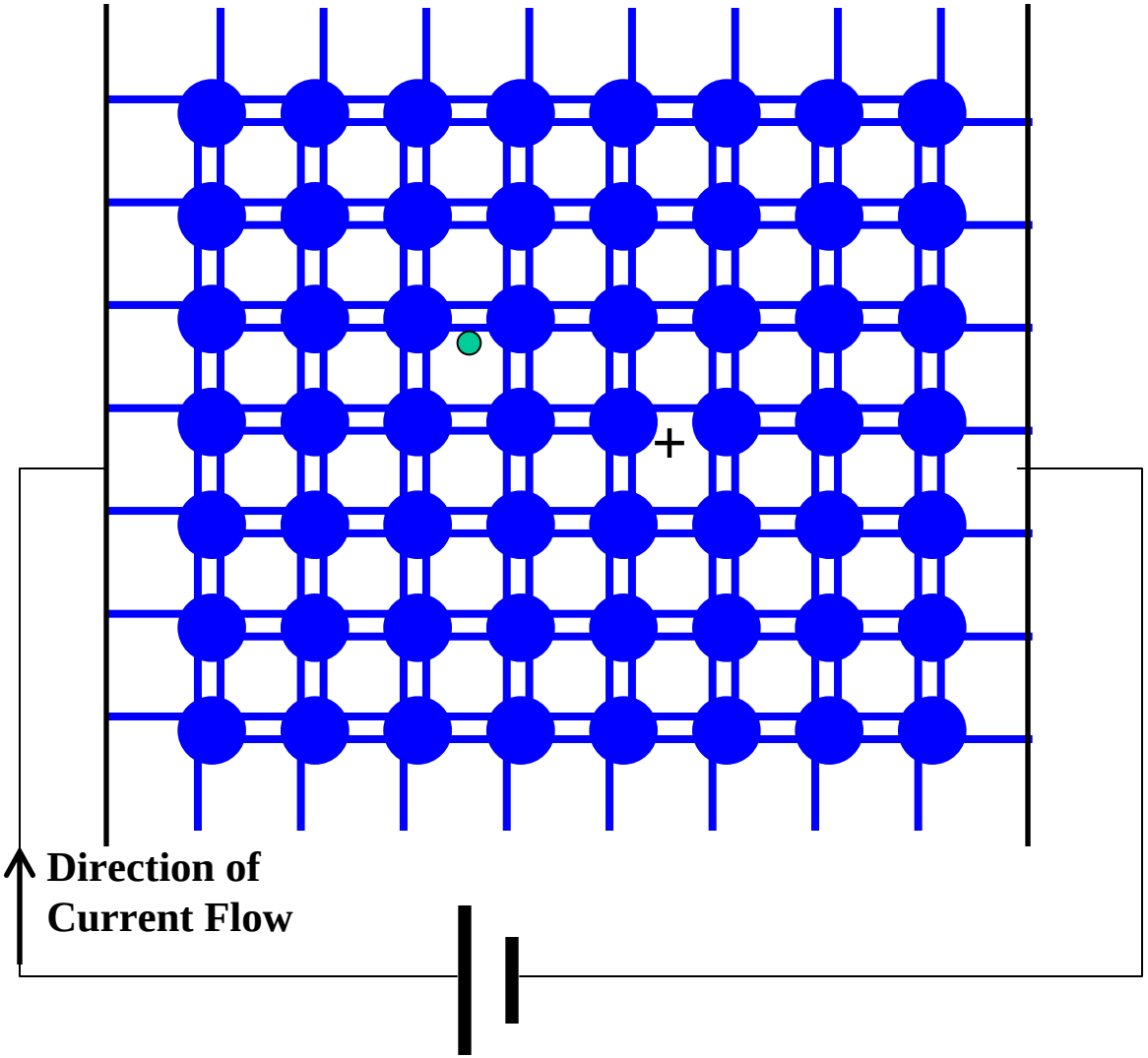


Electron free to move in conduction band

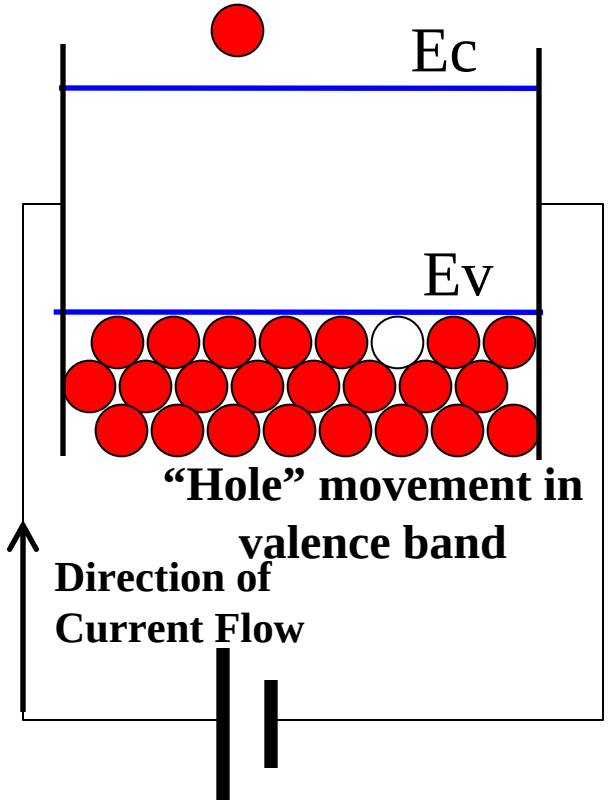


Carrier Movement Under Bias

For ($E_{thermal}$=kT)>0

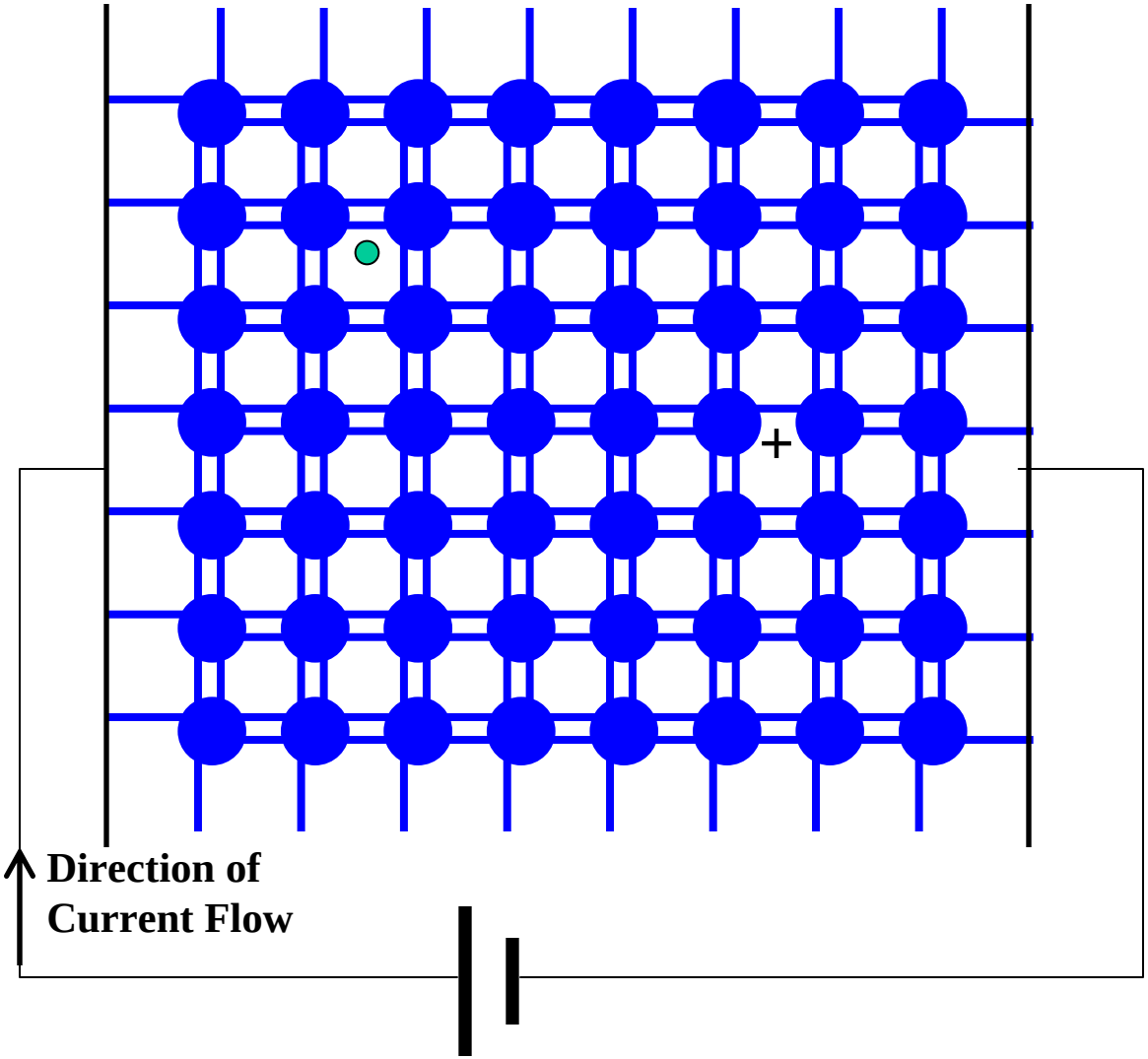


Electron free to move in conduction band

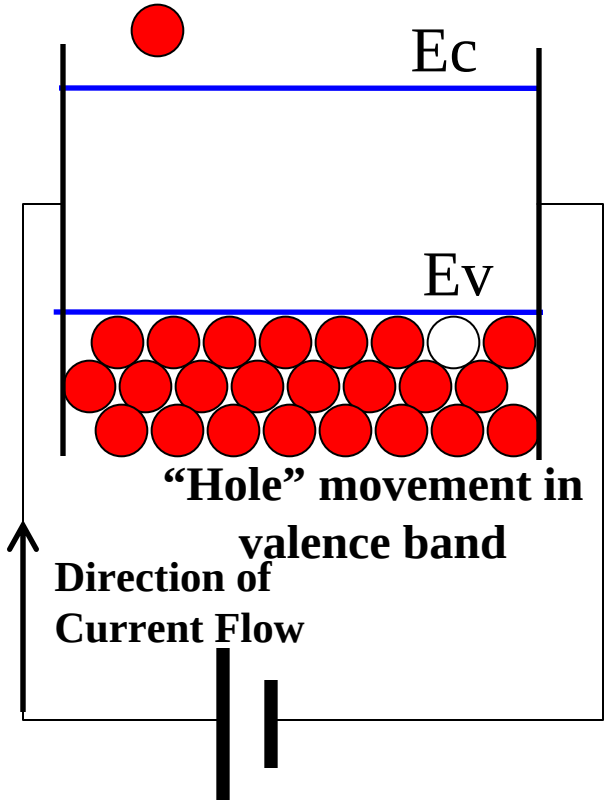


Carrier Movement Under Bias

For ($E_{thermal}$=kT)>0



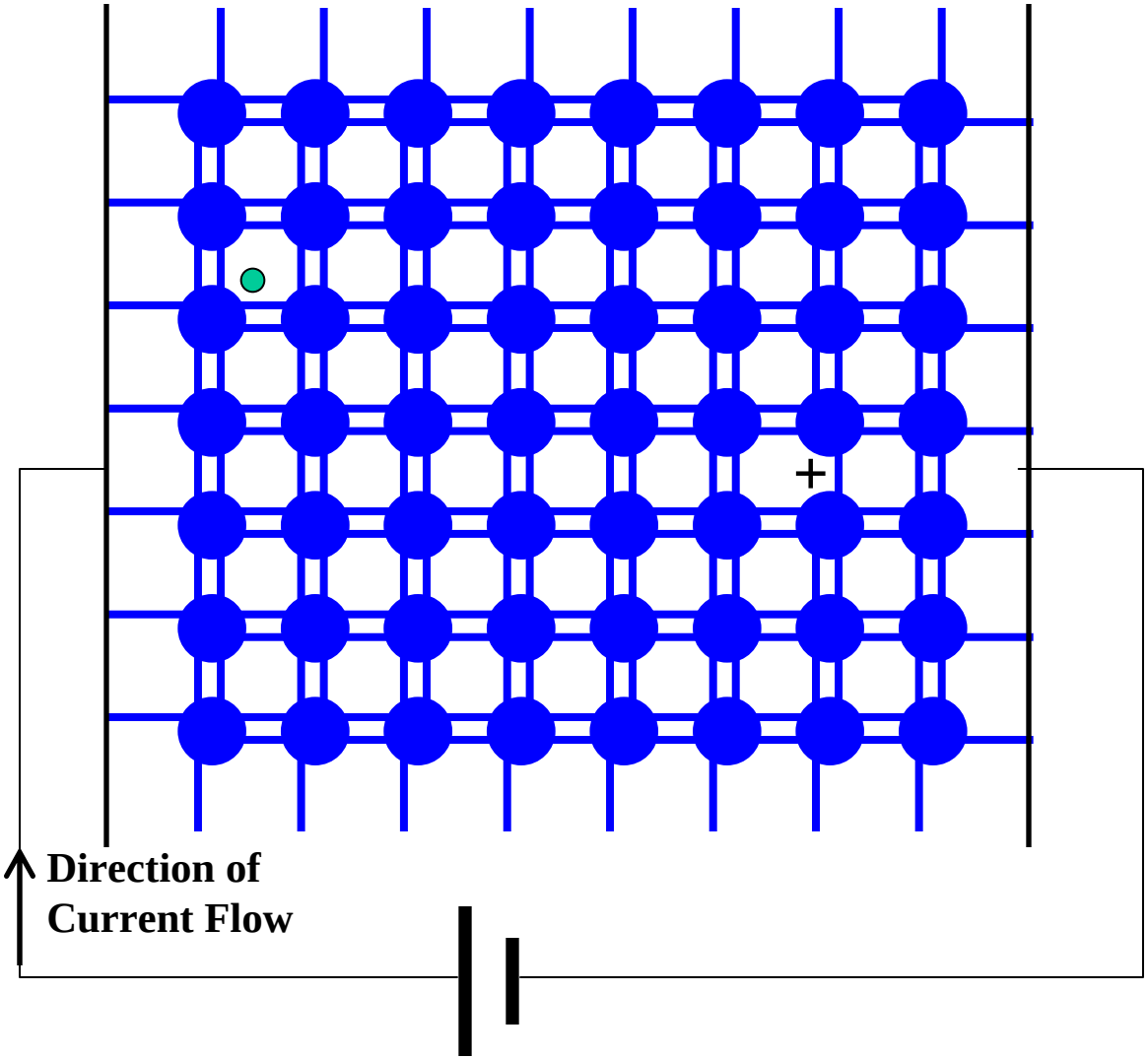
Electron free to move in conduction band



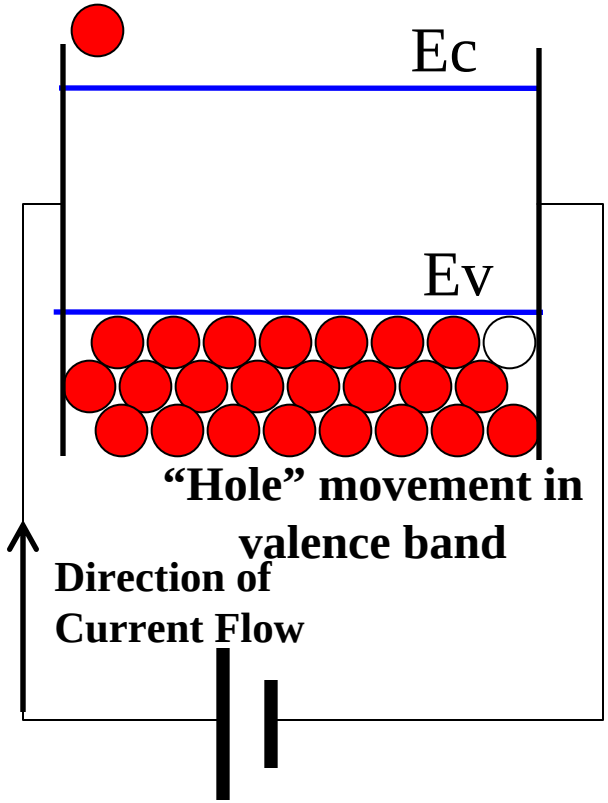
Carrier Movement Under Bias

QuickTime Movie

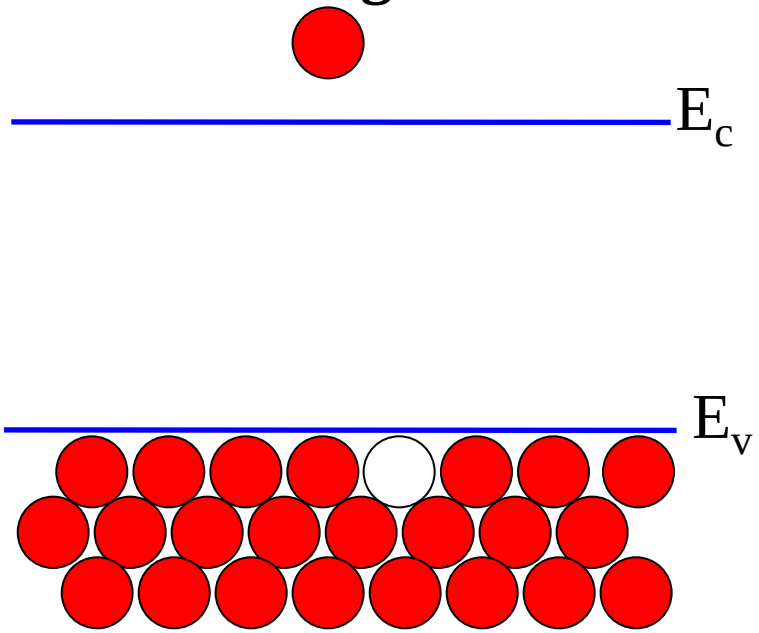
For ($E_{thermal}$=kT)>0



Electron free to move in conduction band



Clarification of confusing issues:“Holes” and Electrons



The valance band may have ~4e22 cm^{-3} valence electrons “participating in the bonding processes holding the crystal together.

The valance band might only have ~1e6 to 1e19 cm^{-3} “holes” in the valence band (missing valence electrons). Thus, it is easier to account for the influence of the holes by counting the holes directly as apposed to counting very small changes in the valence electron concentrations.

Example: If there are 1e 22 cm-3 atoms in a crystal with each atom having 4 valence electrons. What is the difference in valence electron concentration for 1e12 holes verses 1e13 cm-3 holes?

Answer: 4 x 1e22 cm^{-3} -1e12 cm^{-3} = 3.999999999e22cm^{-3} verses

4 x 1e22 cm^{-3} -1e13 cm^{-3} = 3.999999999e22cm^{-3}

For “accounting reasons” keeping track of holes is easier!

Clarification of confusing issues:“Holes” and Electrons

Terminology

Only these “particles” carry electricity. Thus, we call these “carriers”

Electrons: Sometimes referred to as conduction electrons: The electrons in the conduction band that are free to move throughout the crystal.

Holes: Missing electrons normally found in the valence band (or empty states in the valence band that would normally be filled).

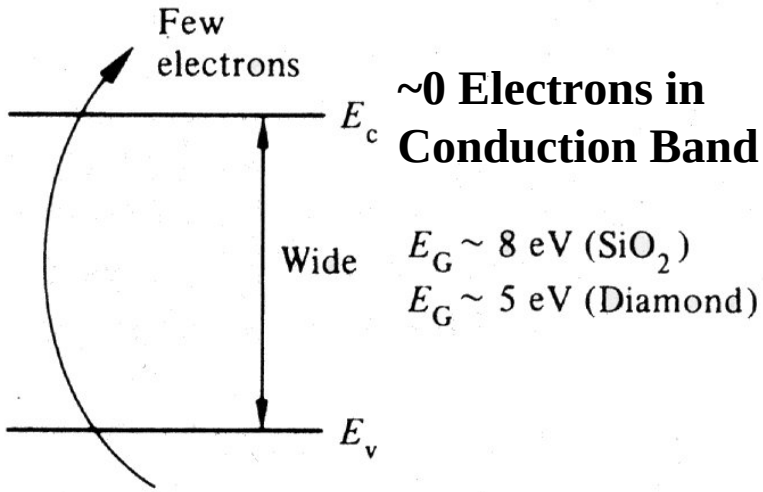
If we talk about empty states in the conduction band, we DO NOT call them holes! This would be confusing. The conduction band has mostly empty states and a few electrons.

If we talk about filled states in the valence band, we DO NOT call them electrons! This would be confusing. We can call them Valence Electrons to indicate they are bond to atoms (in the valence shells of atoms). The valence band has mostly filled states and a few holes.

For the vast majority of this class we only talk about electrons (conduction band electrons) and holes (empty states in the valence band)!

Material Classification based on Size of Bandgap:

Ease of achieving thermal population of conduction band determines whether a material is an insulator, semiconductor, or metal

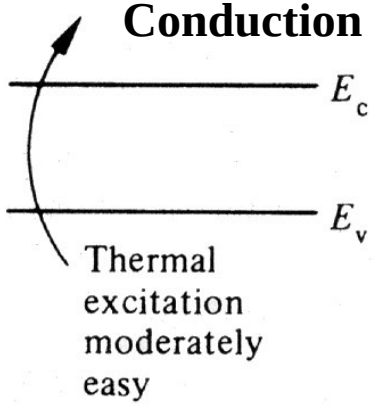


~0 Electrons in Conduction Band

$E_G \sim 8$ eV (SiO_2)
$E_G \sim 5$ eV (Diamond)

(a) Insulator

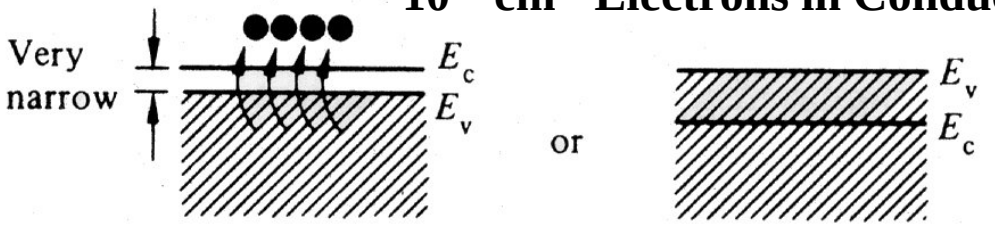
~10^6 - 10^{14} cm^{-3} Electrons in Conduction Band without "help"



$E_G = 1.42$ eV (GaAs)
$E_G = 1.12$ eV (Si)
$E_G = 0.66$ eV (Ge)
(Room temperature)

(b) Semiconductor

~10^{22} cm^{-3} Electrons in Conduction Band



(c) Metal

Figure 2.8 Explanation of the distinction between (a) insulators, (b) semiconductors, and (c) metals using the energy band model.

Intrinsic Carrier Concentration

•For each electron promoted to the conduction band, one hole is left in the valence band. Thus, the number of electrons in the conduction band is equal to the number of holes in the valence band unless there is "help" to change the relative populations in each band.

•Intrinsic carrier concentration is the number of electron (=holes) per cubic centimeter populating the conduction band (or valence band) is called the intrinsic carrier concentration, n_i

•n_i = f(T) that increases with increasing T (more thermal energy)

<u>At Room Temperature (T=300 K)</u>

n_i~2e6 cm^{-3} for GaAs with Eg=1.42 eV,
n_i~1e10 cm^{-3} for Si with Eg=1.1 eV,
n_i~2e13 cm^{-3} for Ge with Eg=0.66 eV,
n_i~1e-14 cm^{-3} for GaN with Eg=3.4 eV

Carrier Movement in Free Space

Newtons second law

$$F = -qE = m_o \frac{dv}{dt}$$

$$F \equiv \ force, v \equiv velocity, t \equiv time,$$

$$q \equiv electronic \ \ charge, m_o \equiv electron \ mass$$

Carrier Movement Within the Crystal

•Electron is a quasi-particle that behaves as a “wave” due to quantum mechanical effects.

•The electron “wavelength” is perturbed by the crystals periodic potential.

QuickTime Movie

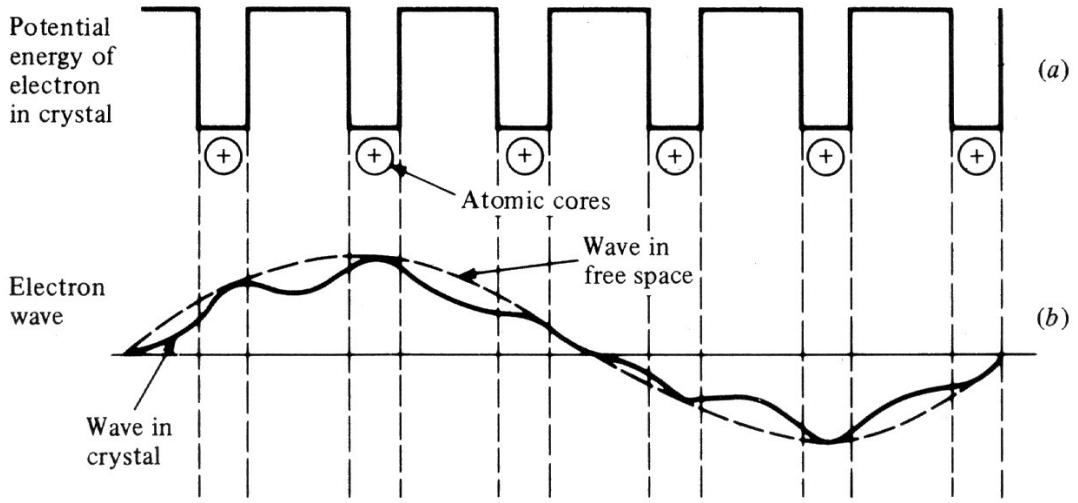


FIGURE 1-11
Representation of motion of electron wave in crystal potential. (*After Wolfendale [3].*)

Carrier Movement Within the Crystal

$$F = -qE = m_n^* \frac{dv}{dt}$$

$F \equiv$ *force*, $v \equiv$ *velocity*, $t \equiv$ *time*,

$q \equiv$ *electronic charge*,

$m_n^* \equiv$ *electron effective mass*

$$F = qE = m_p^* \frac{dv}{dt}$$

$F \equiv$ *force*, $v \equiv$ *velocity*, $t \equiv$ *time*,

$q \equiv$ *electronic charge*,

$m_p^* \equiv$ *hole effective mass*

Table 2.1 Density of States Effective Masses at 300 K.

Material	m_n^*/m_0	m_p^*/m_0
Si	1.18	0.81
Ge	0.55	0.36
GaAs	0.066	0.52

Ge and GaAs have "lighter electrons" than Si which results in faster devices