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Electronic Devices

Lecture 4

11-08-2018

Energy Bands and Charge carriers in Semiconductors

- Specific mechanisms by which current flows in a solid
- Dependence of the conductivity of a semiconductor on the temperature and impurity concentration
- Discrete energy levels within atoms
- Large gaps in the energy scale where no energy states are available
- Basic difference between <u>electron in an isolated atom</u> and <u>one in an atom in a solid</u>

Bonding Forces in Solids

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- ***Ionic bonding***
- ***Metallic bonding***
- ***Covalent bonding***

Bonding Forces in Solids

Ionic bonding : NaCl (Alkali halides)

- Each **Na** atom is surrounded by 6 Cl atoms, and vice versa.
- **Na** (Z=11) has [Ne]$3s^1$ and Cl (Z=17) has [Ne]$3s^2 3p^5$ electronic structure.
- Each **Na** atom gives up its outer **3s** electron to a Cl atom so that the crystal is made of ions with the electronic structures of the inert atoms **Ne** or **Ar :**
- **Thus, NaCl is called "a good insulator".**

Ionic Bonding (NaCl) & Covalent Bonding (Si)

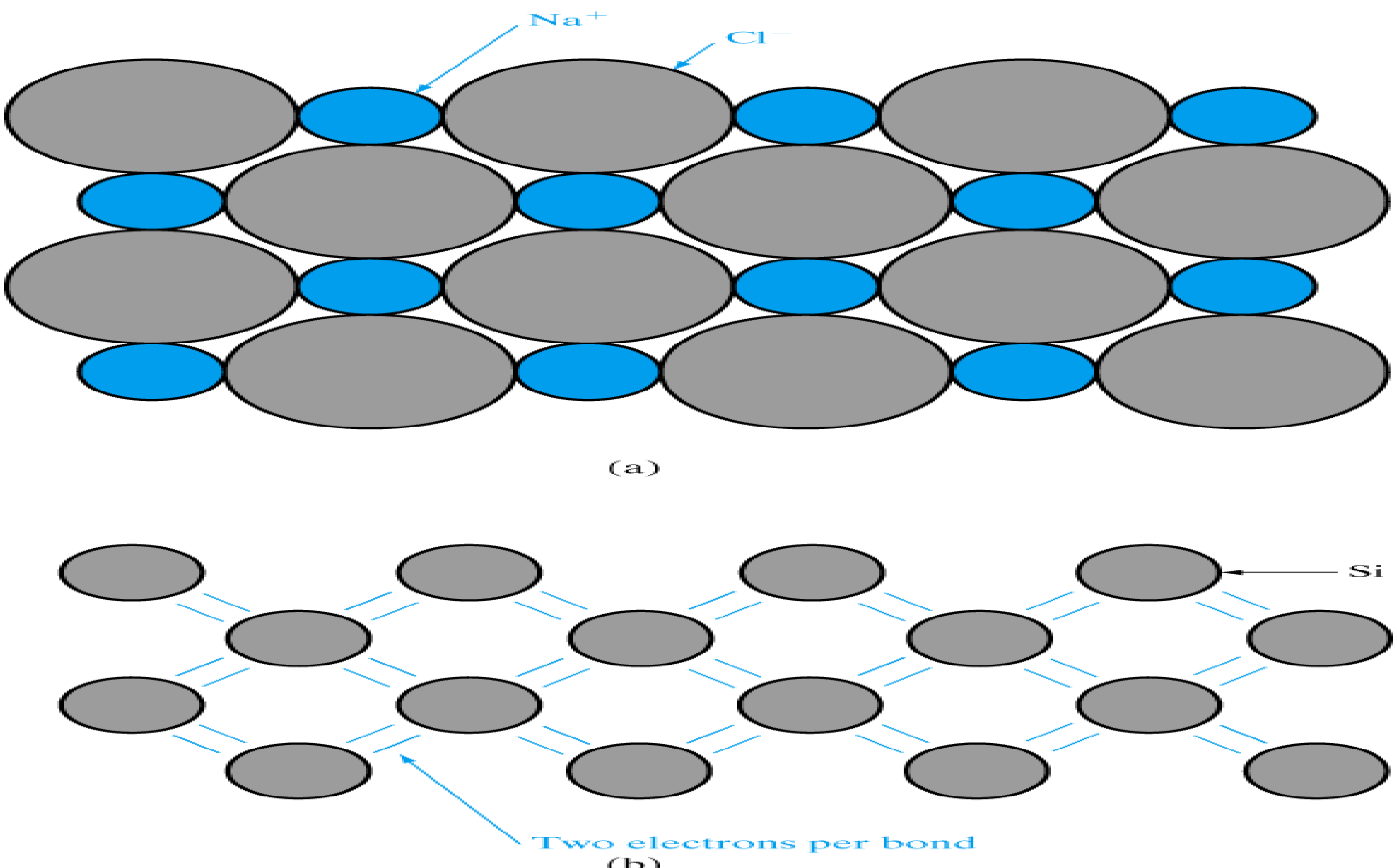

Figure 3—1

Different types of chemical bonding in solids: (a) an example of ionic bonding in NaCl; (b) covalent bonding in the Si crystal, veiwed along a <100> direction (see also Figs. 1–8 and 1–9).

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Metallic bonding

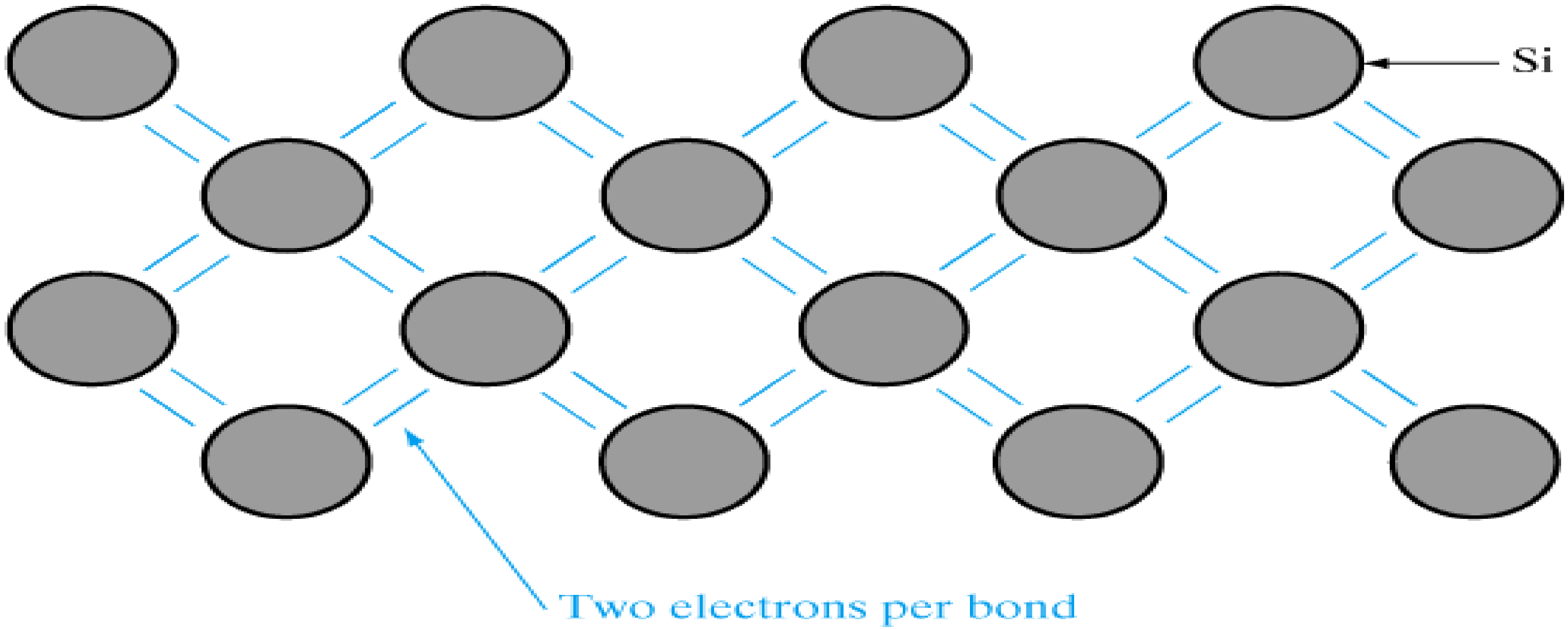
- **A metal atom has the outer electronic shell which is partially filled, usually no more than 3 electrons**.
- The alkali metals such as **Na** have only one electron in the outer orbit that is loosely bound and easily given up in ion formation.
- This fact accounts for not only **the great chemical activity of the alkali metals** but also **their high electrical conductivity**.

Covalent bonding

- In diamond lattice semiconductors (Si, Ge, and C),   each atom is surrounded by 4 nearest neighbors, each with four electrons in the outer orbit.
- Each atom shares its valence electrons with its four neighbors.
- The bonding forces arises from a quantum mechanical interaction between the shared electrons. Each electron pair constitutes a covalent bond.
- In the sharing process it is no longer relevant to ask which electron belongs to a particular atom, in other words, both electrons belong to the bond.

Covalent Bonding (Si)

(a)



(b)

Energy Band

- **What will happen when several isolated atoms are brought together to form a solid ?** → The forces of attraction and repulsion between atoms will find a balance at the proper interatomic spacing for the crystal. In this process, important changes occur in electron energy level configurations, thus resulting in the varied electrical properties of solids.**[(ex) For Si atoms, the <u>outermost</u> shell (or valence shell), n = 3, where two 3s and 3p electrons interact each other to form the four "<u>hybridized</u>" sp^3 electrons when the atoms are brought close together].**

$$Si - 1S^2\ 2S^2\ 2P^6\ 3S^2\ 3P^2$$

Energy Band in a Silicon Solid

As many atoms are brought together, the split energy levels form continuous bands of energies.

- An isolated Si atom has an electronic structure in ground state : $1s^2 2s^2 2p^6 3s^2 3p^2$

- Noted that each atom has available ***two 1s states***, ***two 2s states, six 2p states, two 3s states, six 3p states, and higher states*** .

- For *N* atoms, there will be available ***2N 1s states, 2N 2s states, 6N 2p states, 2N 3s states, 6N 3p states.***

Energy Band in a Silicon Solid

As the interatomic spacing decreases, these energy levels split into bands, beginning with the outer shell (***n* = *3***). As the "**3s**" and "**3p**" bands grow, they merge into a single band **composed of a mixture of energy levels**. This band of "***3s-3p***" levels contains ***8N available states***.

As the distance between atoms approaches the equilibrium interatomic spacing of Si, this band splits into two bands separated by an energy gap, $\mathbf{E_g}$. The upper band (**conduction band**) contains ***4N states*** and the lower band (**valence band**) contains ***4N states***.

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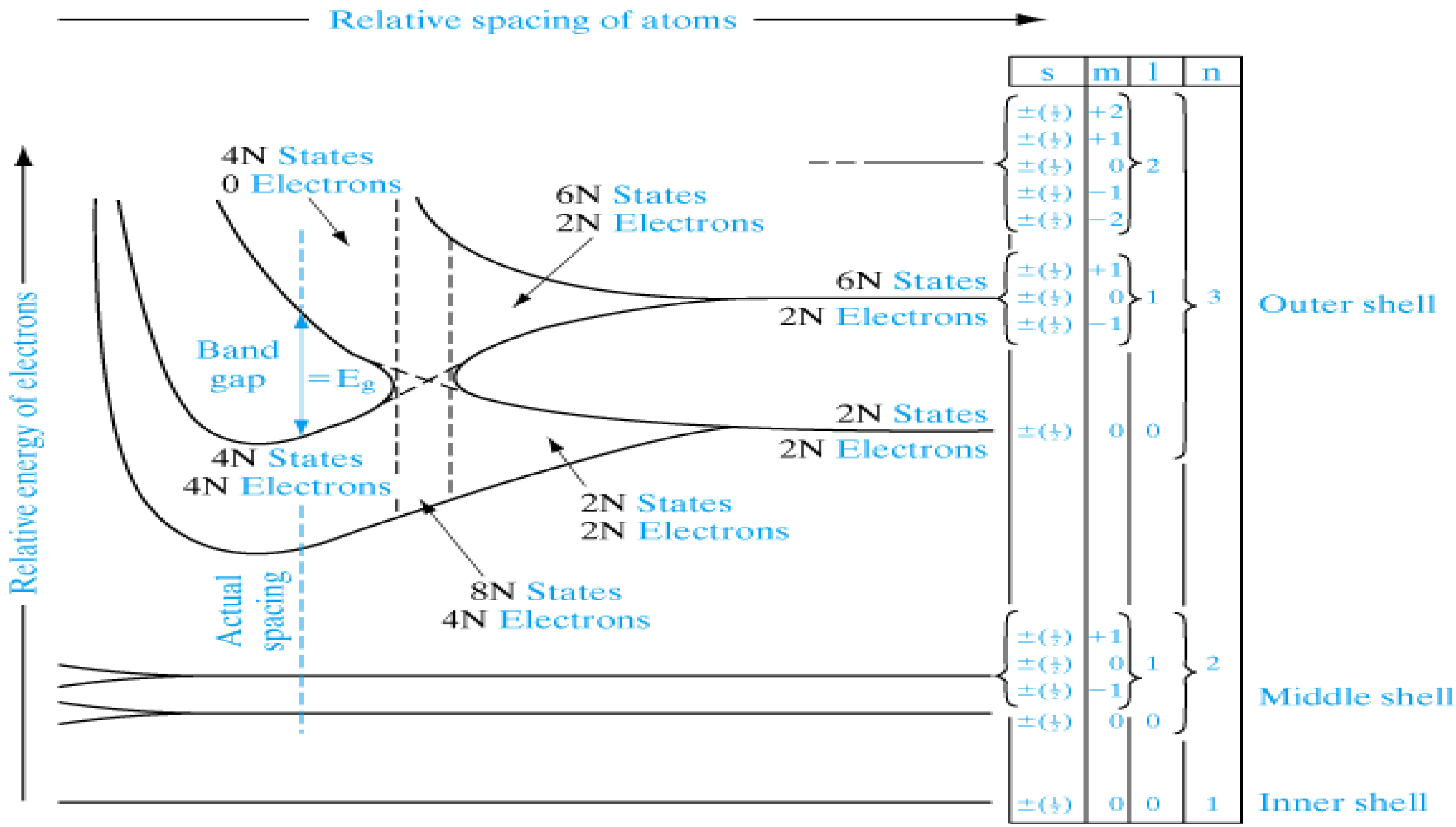
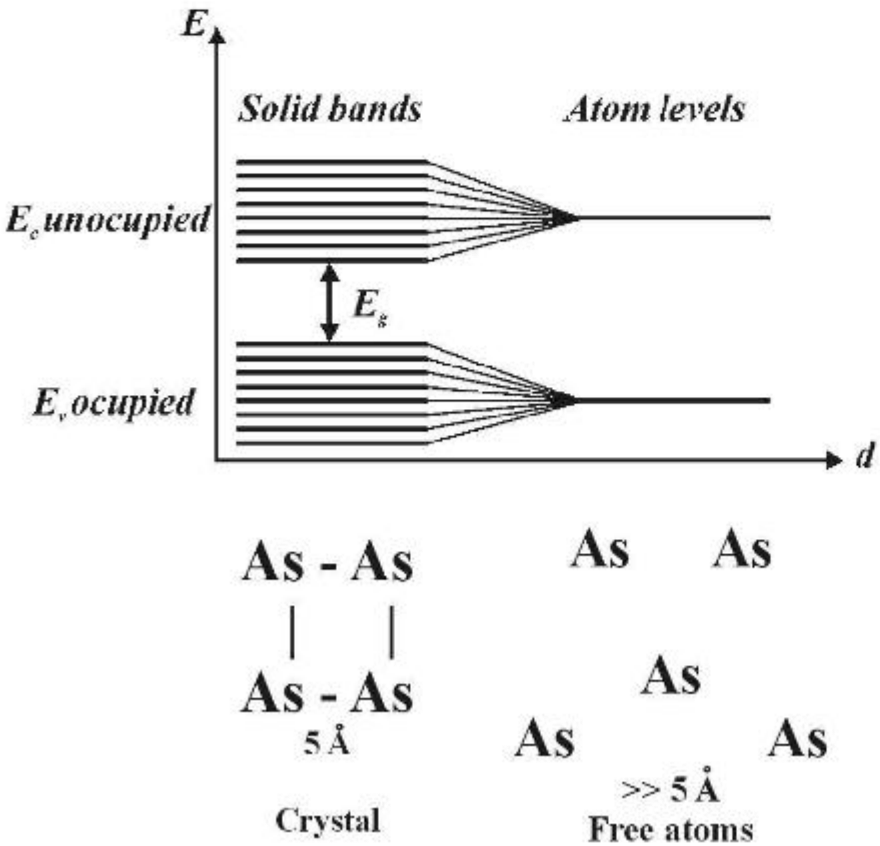




E
Solid bands
Atom levels
E_c unocupied
E_g
E_v ocupied
d
As - As
As - As
5 Å
Crystal
As As
As
As As
>> 5 Å
Free atoms

Metals, Semiconductors, and Insulators in Energy Band Structure

- For electrons to experience an acceleration in an applied electric field, they must be able to move into new energy states.

- This implies that there must be ***empty states*** (***allowed energy states which are not already occupied by electrons***) available to the electrons.

- For example, if relatively few electrons reside in an otherwise empty band, ample unoccupied states are available **into which the electrons can move**.

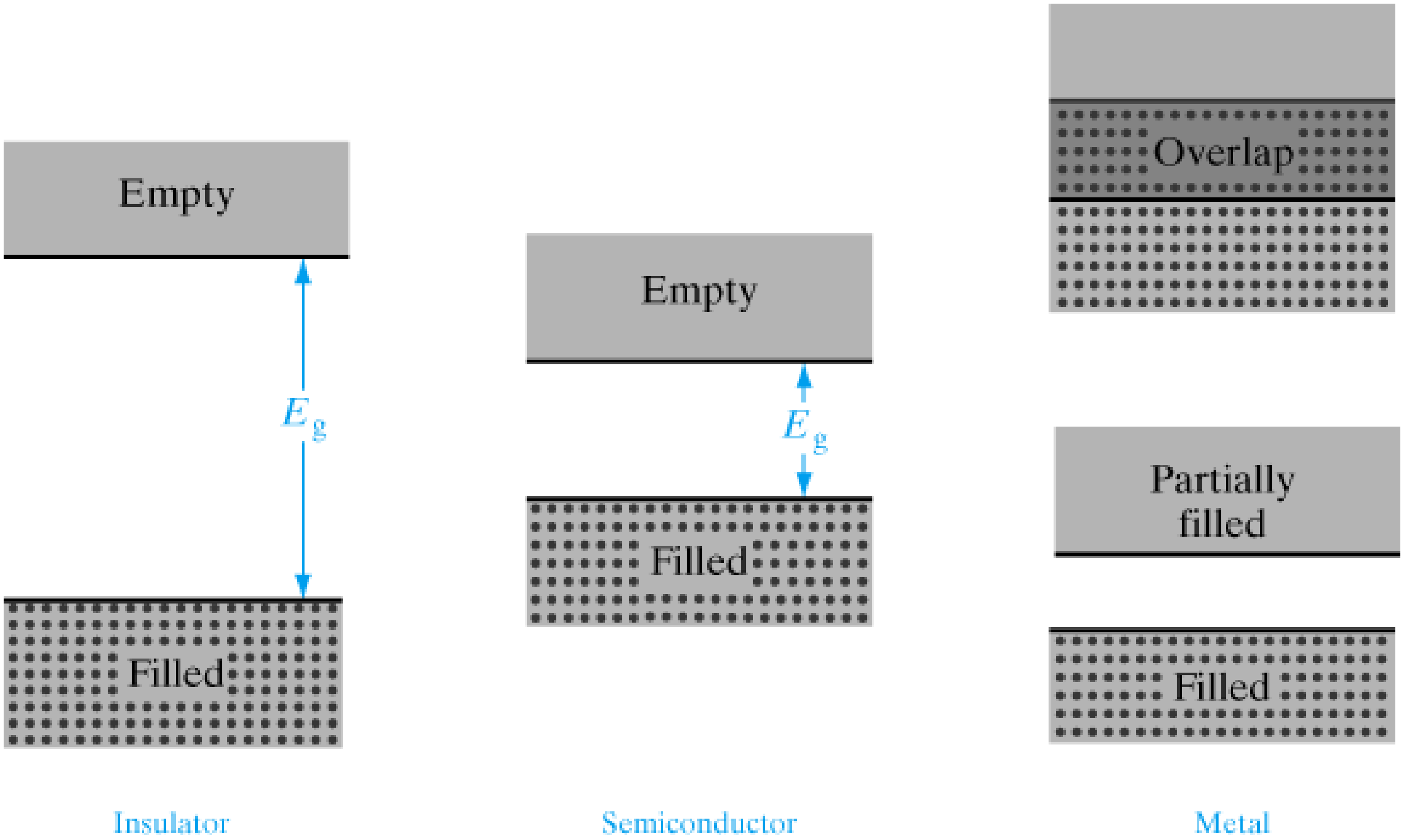
Metals, Semiconductors, and Insulators in Energy Band Structure

- On the other hand, the Si band structure is such that at 0K, the valence band is completely filled with electrons and the conduction band is empty.

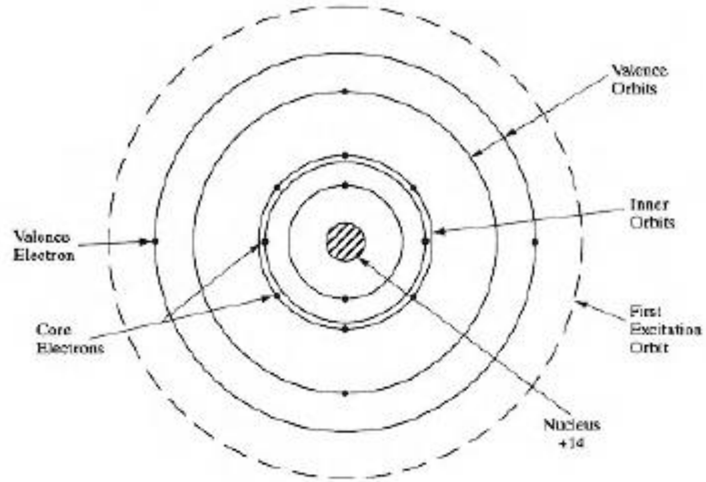
- Thus, there can be no charge transport within the valence band because no empty states are available **into which electrons can move**.

- Also, there are no electrons in the conduction band so that no charge transport can take place there either. **This is why a pure Si has a high resistivity typical of insulators**.

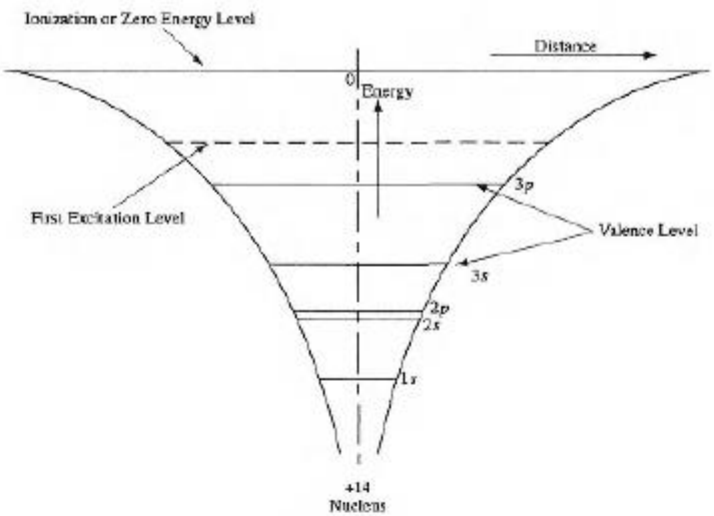
Typical Energy Bands (Insulator, Semiconductor, Metal)



Electronic Structure and energy levels in a Si atom



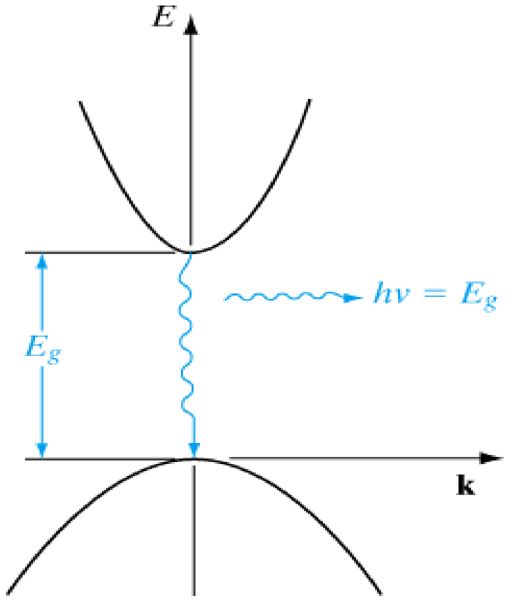
(a)



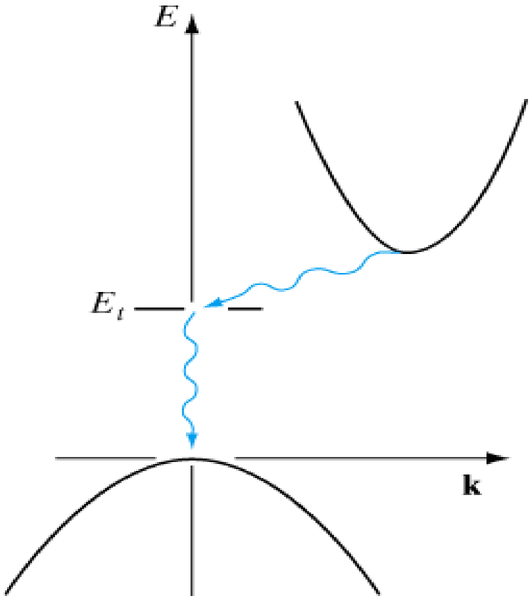
(b)

Direct and Indirect Semiconductors

When a single electron is assumed to travel through a perfectly periodic lattice, the wave function of the electron is assumed to be in the form of a plane wave moving in the ***x***-direction with **propagation constant** (or wave vector) ***k***.



(a) Direct



(b) Indirect

(a) Direct Semiconductor (GaAs) : an electron in the conduction band can fall to an empty state in the valence band, giving off the energy difference (E_g) as a photon of light. Thus, this semiconductor material is used for light emitters and lasers.

(b) Indirect Semiconductor (Si) : an electron in the conduction band minimum in Si can not fall directly to the valence band maximum. Instead, it **must undergo a momentum change as well as changing its energy**. **The indirect transition involves a change in *k*, and the energy is generally given up as heat to the lattice rather than as an emitted photon**.

Energy Bands Variation vs. Composition (x)

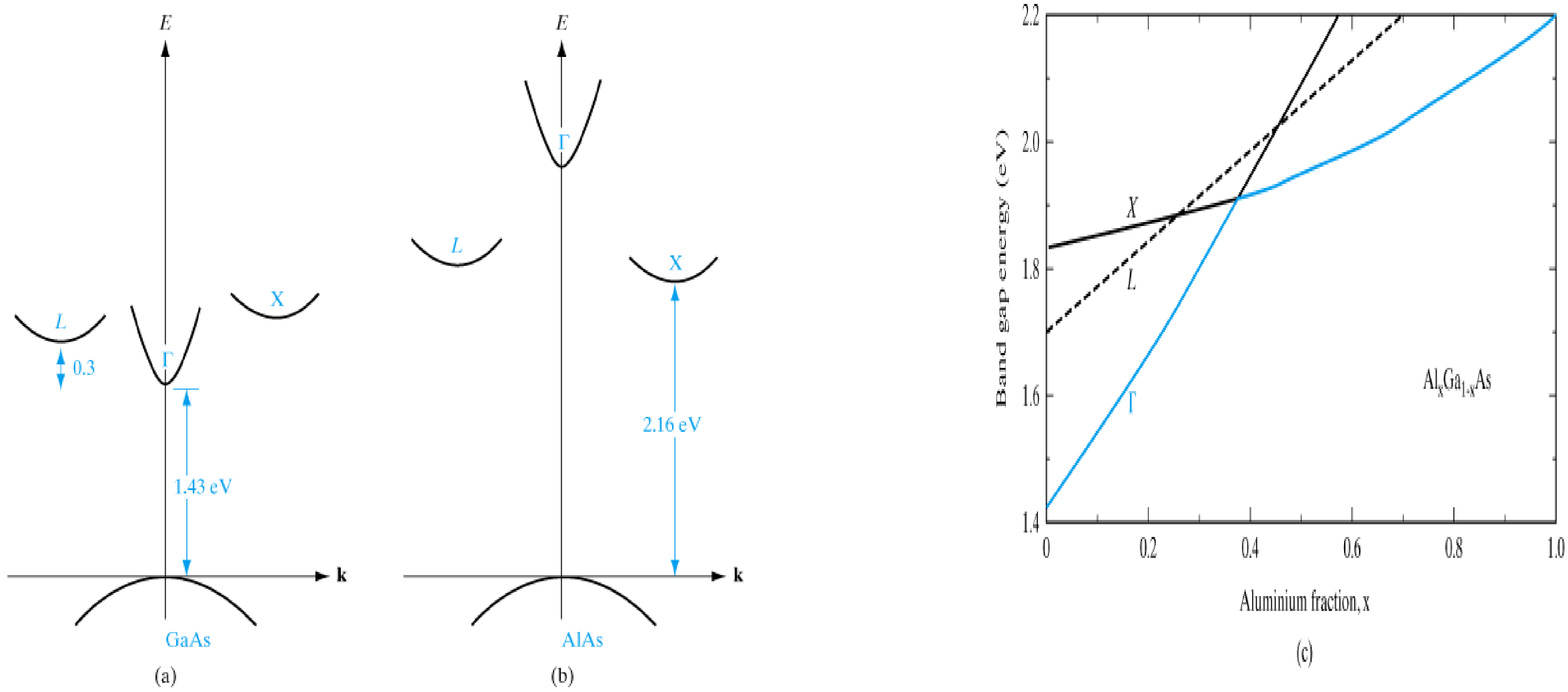


Figure 3—6
Variation of direct and indirect conduction bands in AlGaAs as a function of composition: (a) the (E,k) diagram for GaAs, showing three minima in the conduction band; (b) AlAs band diagram; **(c) positions of the three conduction band minima in Alx Ga1- x As as x varies over the range of compositions from GaAs (x = 0) to AlAs (x = 1). The smallest band gap, Eg (shown in color), follows the direct band to x = 0.38, and then follows the indirect X band**.

Charge Carriers in Semiconductors

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- **Consideration of Current Conductions** :

- **Metals** : Metal atoms are imbedded in a "sea" of free electrons, and these electrons can move as a group under the influence of an electric field.

- **Semiconductors** : Since the semiconductors has a filled valence band and an empty conduction band at **0K**, the increase of electrons in conduction band by thermal excitations across the band gap must be considered as the temp. is raised. In addition, after electrons are excited to the conduction band, the empty states left in the valence band can contribute to the conduction process. Also, the introduction of impurities is considered to have an important effect on the energy band structure and on the availability of charge carriers.

- **Electrons & Holes** : As the temp. is raised from 0K, some electrons in the V.B. receive enough thermal energy to be excited across the band gap to the C.B., and this results in a semiconductor with ***some electrons in an otherwise empty C.B.*** and ***some unoccupied states (called holes) in an otherwise filled V.B.***