Band Theory in Solids

The energy band structure of a solid determines whether it is a conductor, an insulator, or a semiconductor

References

1. *Solid State Electronic Devices* by Ben Streetman and Sanjay Banerjee **(Chapter 3)**

2. *Solid State Physics,* by RK Puri and VK Babbar **(Chapters 5&6)**

3. *Modern Physics* by R. Murugeshan **(Chapter 46)**

4. *Concepts of Modern. Physics* by Arthur Beiser **(Chapter 10)**

Classification of Solids based on Structures

Crystalline

A regular geometric arrangement or periodicity of atoms or molecules.

Noncrystalline (or Amorphous)

Completely random arrangement of atoms or molecules

Single crystal

Polycrystalline

Grain

Grain boundary
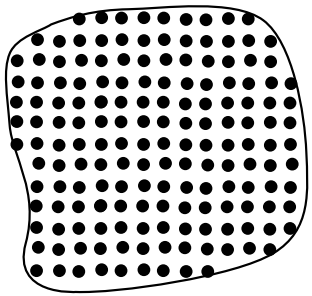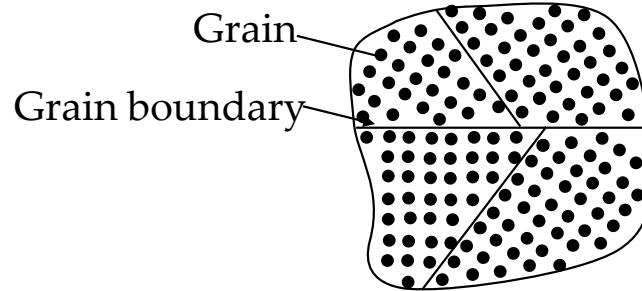
Periodicity of atoms extends throughout the material
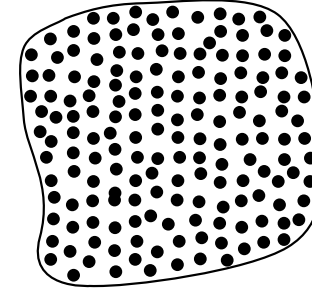or
long-range order

Polycrystalline is an aggregate of a number of small crystallites with random orientation separated by well-defined boundaries .
or
Short -range order

❖ **Most of the solids are crystalline in nature. This is due to the reason that the energy released during the formation of an ordered structure is more than that released during the formation of a disordered structure.**

❖ **The crystalline state is a low energy state and is therefore preferred by most of the solids.**

Classification of Solids based on Conductivity

Metals **Semi-metals** **Semi-conductors** **Insulators**

Conduct current at all temperatures and, generally, the resistivity of such solids increases with temperature

Stop conducting at low temperatures and their resistivity falls with increasing temperature. Semiconductors tend to become insulators at low temperature

Resistivity (Ω-cm)

Metallic materials			Semi-conductors			
10^{-9}	10^{-7}	10^{-5}	10^{-3}	10^{-1}	10^{-1}	10^{3}
Ag, Cu, Al, Au, W, Zn, Ni	Fe, Pt, Pb, Hg, Ti	Carbon (Graphite)	Doped	Ge		Si

Insulators

10^{5}	10^{7}	10^{9}	10^{11}	10^{13}	10^{15}	10^{17}	10^{21}	10^{23}
DI water		Bakelite	Porcelain Diamond Rubber	Lucite Mica	PVC, Air	SiO_2 (pure)	PET	Teflon
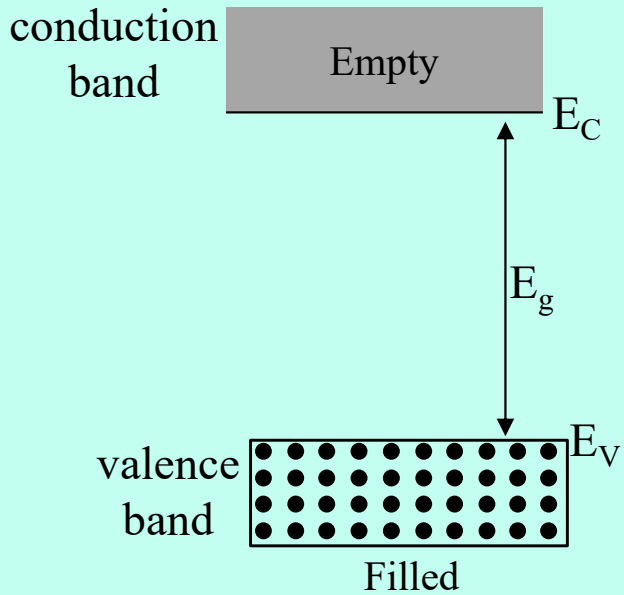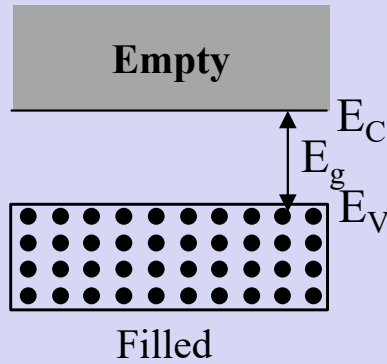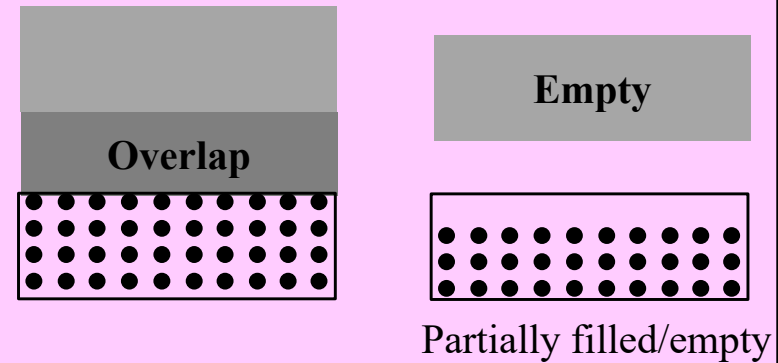
Bonding Forces in Solids

❖ A solid is formed by the chemical bonding of a large number of atoms.

❖ In this process, the total energy of the system is reduced.

❖ The **energy of bonding** is measured by the energy required to separate 1 mole of a solid into individual atoms (or molecules) and is known as cohesive energy.

❖ **Binding energy** denotes the strength of a bond and is the negative of the energy required to break the bond.

❖ When two atoms are brought together to form a molecule, two kinds of forces, namely attractive and repulsive, become important.

❖ As the separation decreases, attractive force come into play first.

Potential Energy *vs* Interatomic spacing
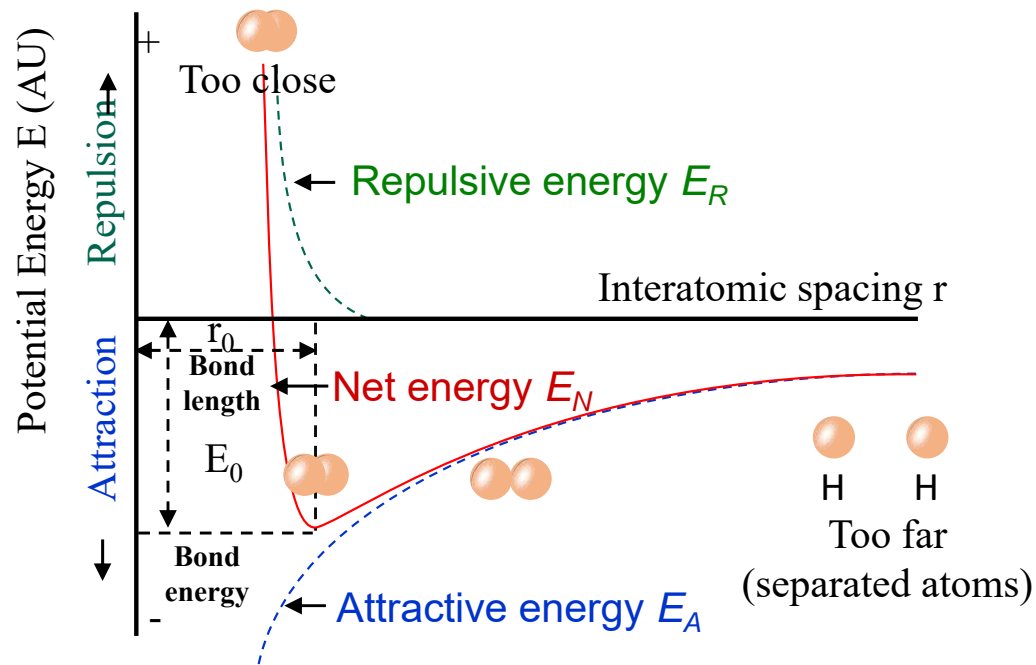
Energy vs. interatomic separation

$$E = E_{att} + E_{rep}$$

$$E = E_A + E_R$$

$$E = -\frac{A}{r^m} + \frac{B}{r^n}$$

- Where A, B, m and n are constants which depend upon the nature of the participating atoms.
- A and B are known as attraction and repulsion constants, respectively.
- The magnitudes of both attractive and repulsive energies increase with decrease in interatomic distance.
- Generally, n>m which indicates that the increase in repulsive energy is faster than the increase in attractive energy particularly for very small values of interatomic distance.
- The repulsive forces are therefore known as short range forces .

- If two molecules are kept at a separation $r = r_o$, they will stay in equilibrium.

- If they are slightly pulled apart so that $r > r_0$, an attractive force will operate between them.

- If they are slightly pushed so that $r < r_o$, a repulsive force will operate.
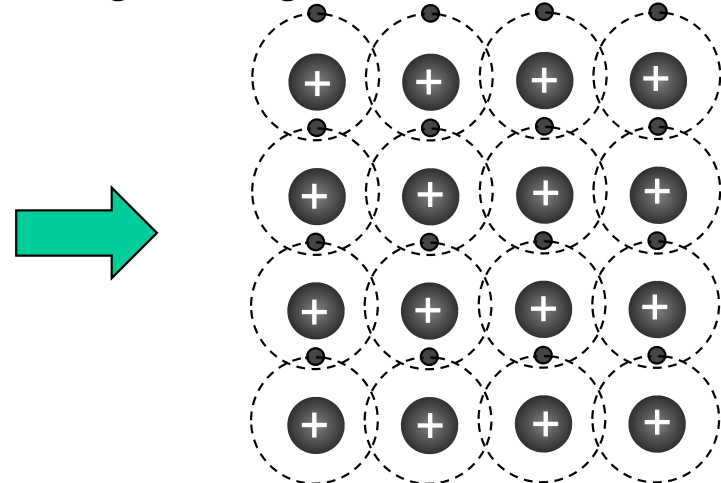
Free Electron Theory

When we bring atoms together to form a metal
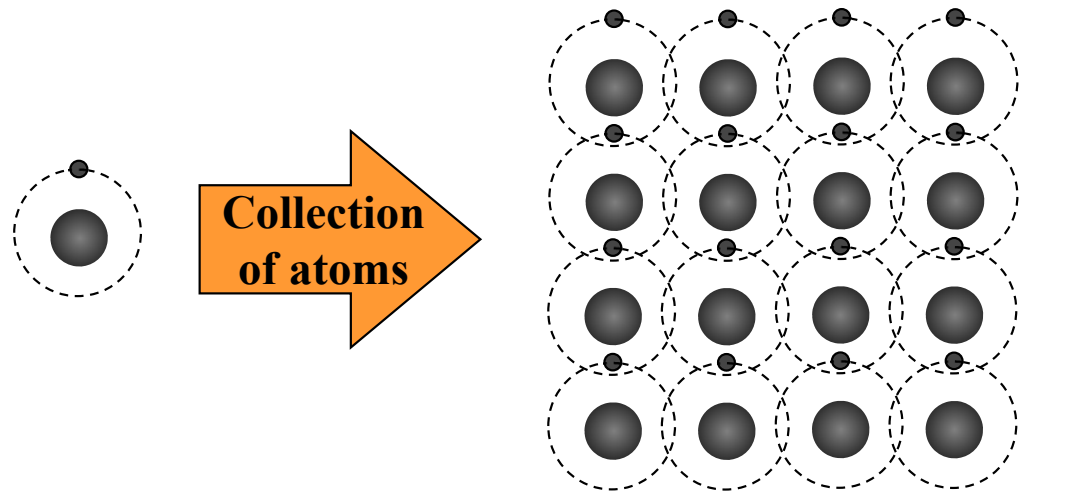
The atomic orbitals of atoms overlap slightly and the valance electrons become no longer attached to a particular ion, but belong to both neighbouring ions at the same time.

Collection of atoms

A valance electron really belongs to the whole crystal, since it can move readily from one ion to its neighbour, and then the neighbour's neighbour, and so on.
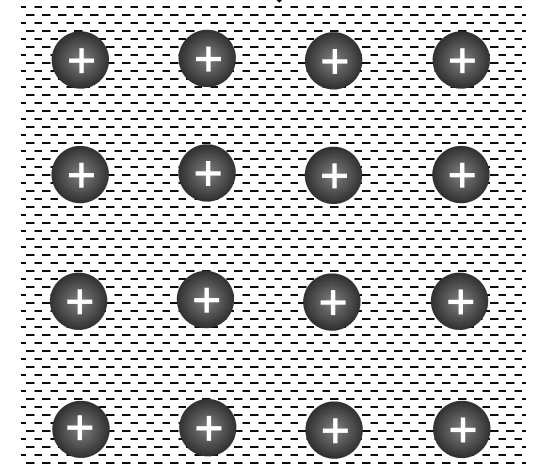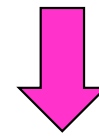
- The removal of the valance electrons leaves a positively charged ion.
- Drude (~1900) assumed that the charge density associated with the positive ion cores is spread uniformly throughout the metal so that the electrons move in a constant electrostatic potential.
- The repulsive force between conduction electrons are ignored.

Free Electron Theory

- Drude, in 1990, postulated that the metals consist of positive ion cores with the valance electrons moving freely among these cores.

- The electrons are bound to move within the metal due to electrostatic attraction between the positive ion cores and the electrons.

- The potential field of these ion cores, which is responsible for such an interaction, is assumed to be constant throughout the metal and the mutual repulsion among the electron is neglected.

- The behaviour of free electrons moving inside the metals is considered to be similar to that of atoms or molecules in perfect gas.

- These free electrons are also referred to as free electron gas and the theory is accordingly named as free electron gas model.

Free Electron Theory
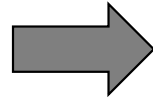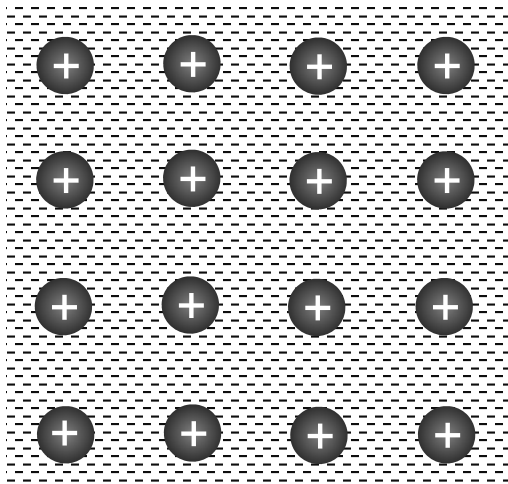
Moving conduction electron

Positive ions at rest
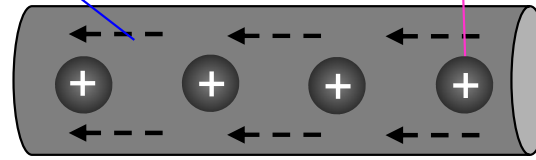
Current carrying conductor

Resistivity vs. Temperature

In general, the motion of free electron is random, but in an electric field, the negatively charged electrons stream in the positive field direction and produce an electric current within the metal.

In order to prevent the electron from accelerating indefinitely, it is assumed in this model that they collide elastically with the metal ions. This lead to a steady-state current, which is proportional to the applied voltage, obeying **Ohm's law**.

ρ

Conductor

Resistivity

ρ_0

0
0   300

Temperature (K)

(a)

ρ

Conductor
(low temperatures)

Resistivity

ρ_0

0
0   20

Temperature (K)

(b)

ρ

Semiconductor

Resistivity

0
0   300
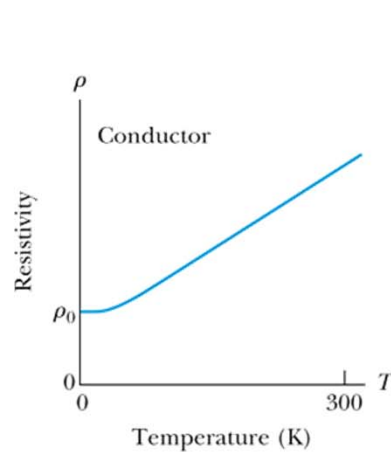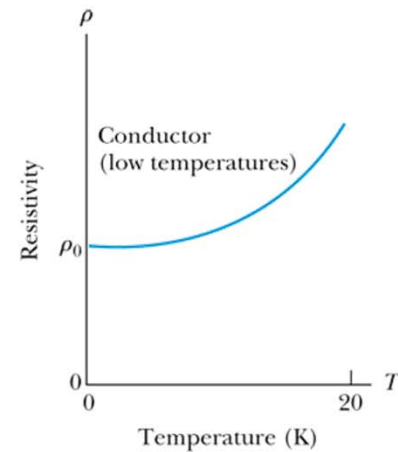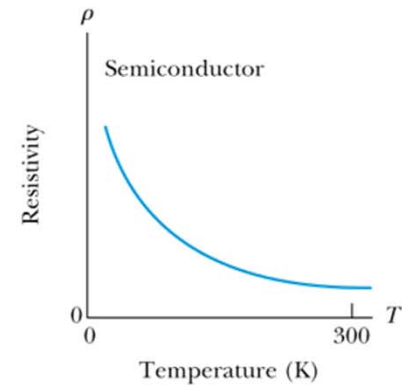
Temperature (K)

(c)

The linear rise in resistivity with increasing temperature except at very low temperatures. (b) at very low temperatures. Notice that the curve flattens and approaches a nonzero resistance as $T \rightarrow 0$. (c) Resistivity versus temperature for a typical semiconductor. The resistivity increases dramatically as $T \rightarrow 0$.

Drawback of Free-electron Model & Introduction of Band Theory of Solids

❖ The free-electron theory was successful in explaining the various electronic and thermal properties of metal such as thermal conductivity, paramagnetism, etc.

❖ It could not explain why certain solids have a large number of free electrons and thus behave as good conductors while certain others have hardly any electrons and, therefore, insulators.

❖ The free-electron model does not apply to semiconductors and insulators, since these materials simply lack of enough free electrons to conduct in a free-electron mode.

❖ It could not account for the variation of resistivity with temperature as well as other properties of semiconductors. In other words, the properties of semiconductors could not be explained based on free-electron theory.
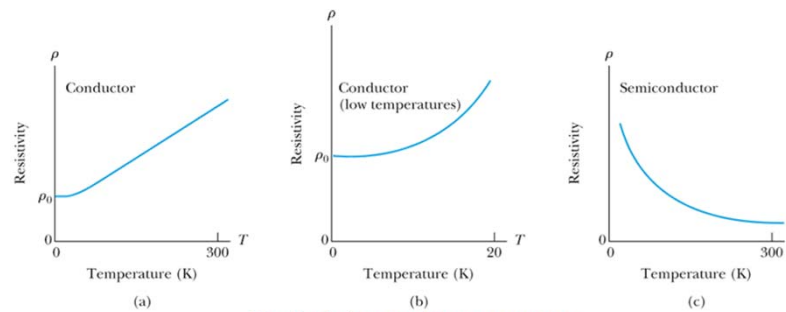
Resistivity *vs.* Temperature

❖ A new theory known as the band theory is introduced.

❖ The essential feature of the band theory is that the allowed energy states for electrons are nearly continuous over certain ranges, called energy bands, with forbidden energy gaps between the bands.

Energy Band Theory

Qualitative Description

Energy bands are composed of closely spaced orbitals

Quantitative Description

Kronig-Penney Model
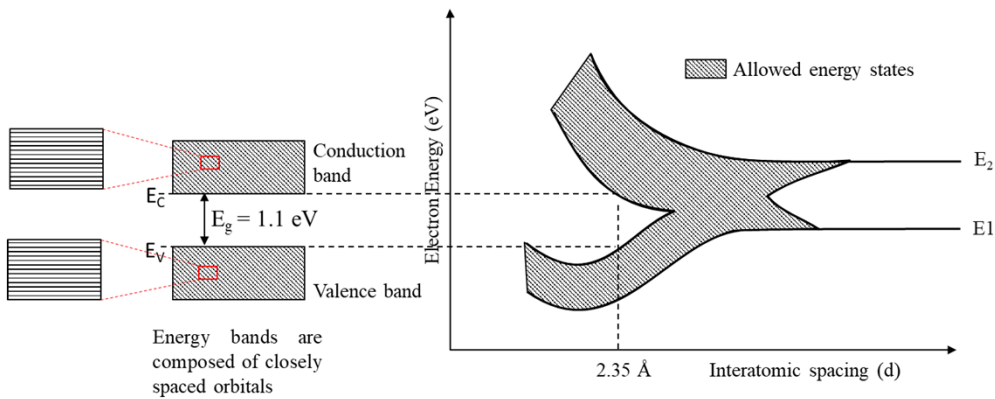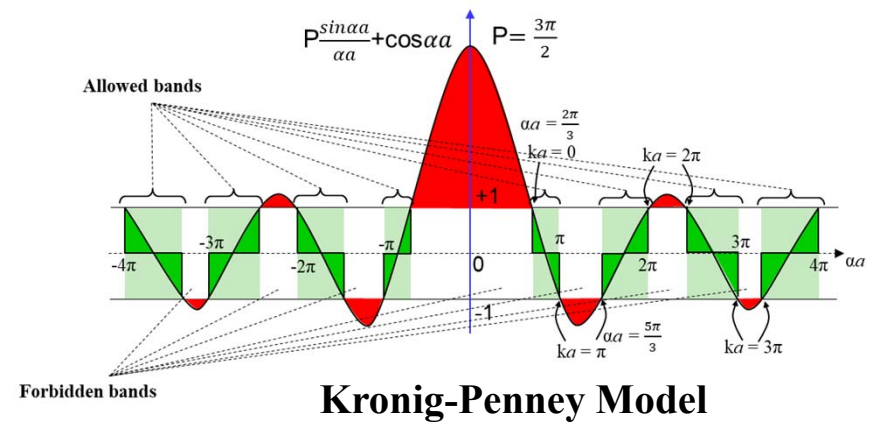
Potential Energy and Potential

The potential energy of the two-charge system is chosen to be zero when they have infinite separation (or very wide separation). Potential energy when separation is r

$$U = \frac{Qq}{4\pi\varepsilon_0 r}$$

The PE depends on the separation between the charges and is independent of the spatial location of the charged particles.

Less separation greater repulsion

$U > 0$

$$U = \frac{Qq}{4\pi\varepsilon_0 r}$$

Spacing r

Greater separation
Less repulsion

$$U = -\frac{Qq}{4\pi\varepsilon_0 r}$$

$U < 0$

Greater separation
Less attraction

Potential Energy E (AU)
Repulsion
Attraction

(a) Potential Energy vs. separation

Less separation
greater attraction

Setting the potential to zero at $r = \infty$ gives the general form of the potential due to a point charge Q

$$V = \frac{Q}{4\pi\varepsilon_0 r} \qquad when\ Q > 0$$

$+V$

Potential V (AU)

Spacing r

$$V = \frac{Q}{4\pi\varepsilon_0 r} \quad when\ Q < 0$$

Single point charge: V = 0 at $r = \infty$

$-V$

(b) Potential vs. separation

As the separation r approaches zero, potential energy becomes infinitely negative or positive, depending on types of charges.

Potential energy between a nucleus and an electron

Potential energy between a nucleus with atomic number Z and an electron

$$U = -\frac{ze^2}{4\pi\varepsilon_0 r}$$

Valance electron

Nucleus

$U > 0$

$$U = \frac{Qq}{4\pi\varepsilon_0 r}$$

Spacing r

$$U = -\frac{Qq}{4\pi\varepsilon_0 r}$$

$U < 0$

Potential Energy E (AU)

(a) Potential Energy vs. separation

r = 0   Spacing r

$U = 0$
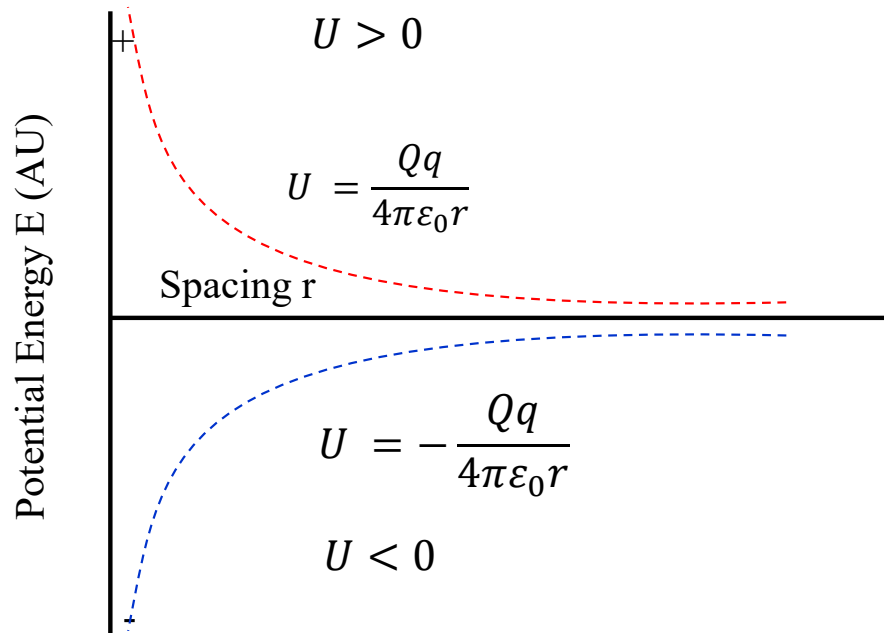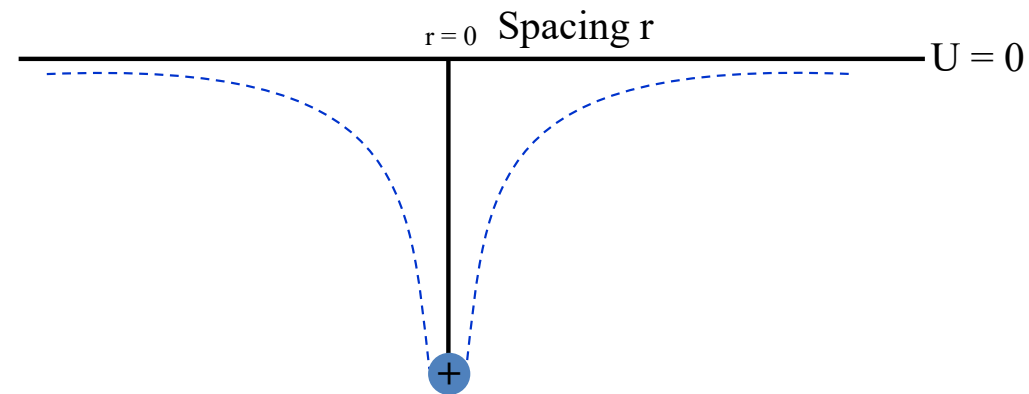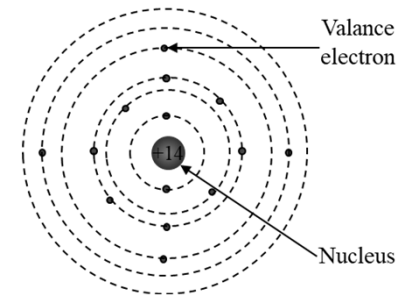
Electronic structure and energy level in a Si atom

First excitation orbits

Valance electron

Valance orbits

Core electron

Inner orbits

Nucleus

+14
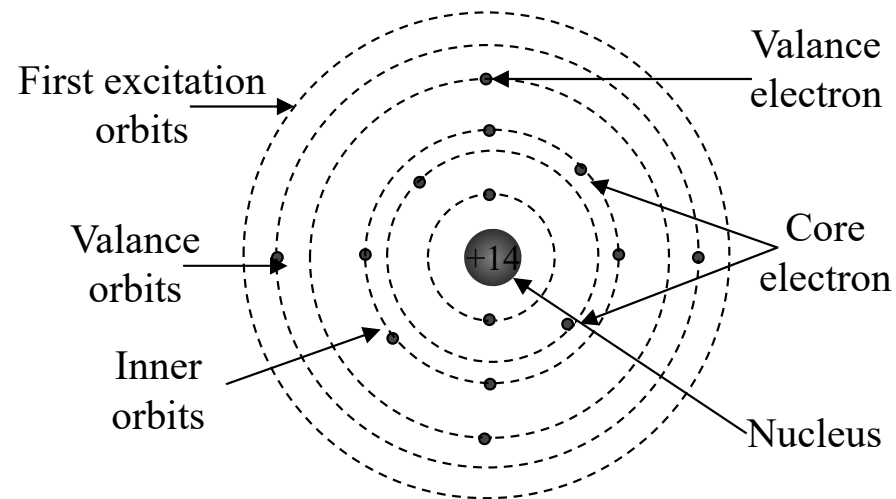
Electronic structure of Si^{14} → 1s^2 2s^2 2p^6 3s^2 3p^2 →[Ne] 3s^2 3p^2

Orbital model: 10 core electrons (n = 1 and 2) and 4 valance electrons (n = 3)

Distance from nucleus

n = 3

n = 2

n = 1

Nucleus

Ionization or zero energy level

Distance

0 Energy

First excitation energy level

3p

3s

Valance level

2p
2s

1s

+ 14
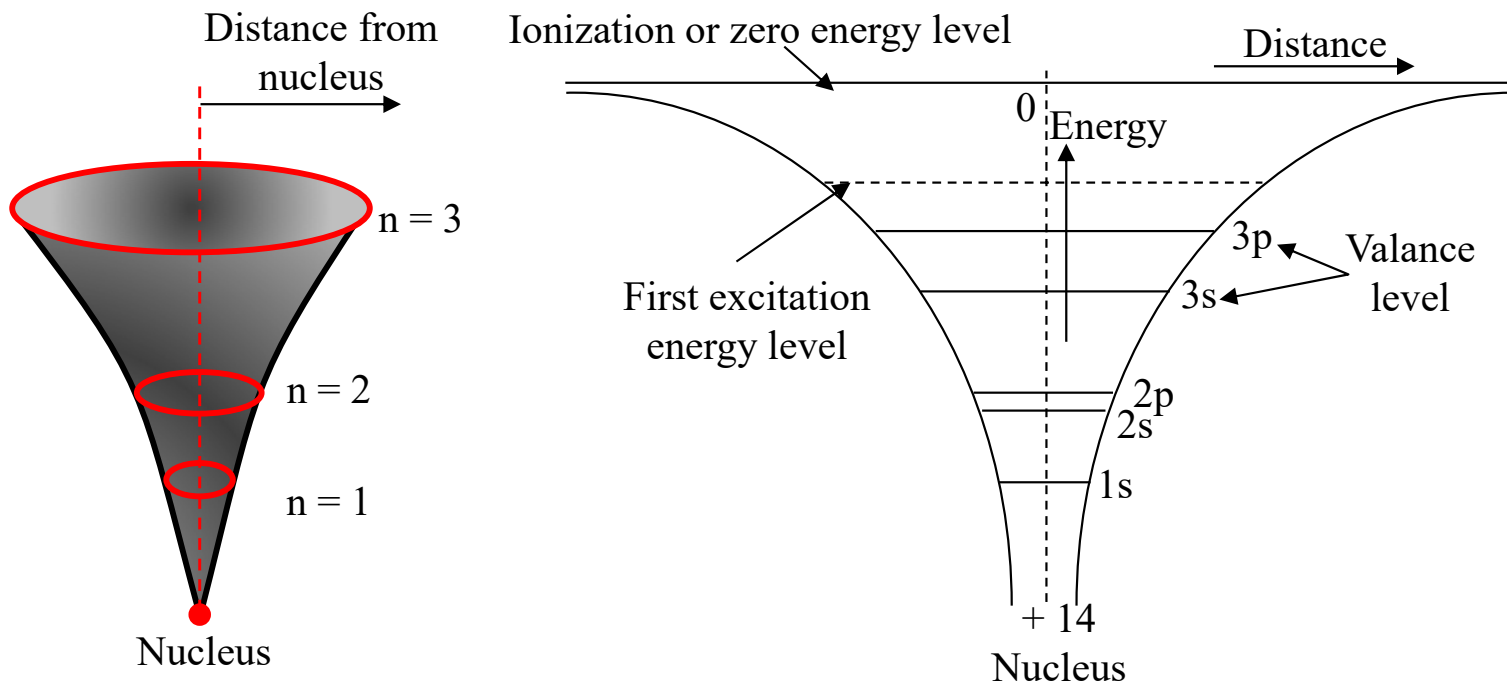
Nucleus

Energy levels in the coulombic potential of nucleus

Coulomb potential varies as 1/r as a function of distance from the charge. The potential energy gradually goes to zero when we approach infinity

Energy Band Theory

➢ When isolated atoms are brought together to form a solid, various interactions occur between neighboring atoms.

➢ The force of attraction and repulsion between atoms find a balance at the proper interatomic spacing for the crystal.

➢ In the process of interaction, important changes occur in the electron energy level configurations and these changes result in the varied electrical properties of solids.

➢ In case of silicon, when the individual atoms are brought close together, the s- and p-orbitals overlap so much that they lose their distinct character. Two 3s and two 3p electrons of outermost shell (or valance shell) interact to form the four hybridized sp^3 electrons (or orbitals). Hybridized sp^3 orbitals point symmetrically in space along the four tetragonal directions.
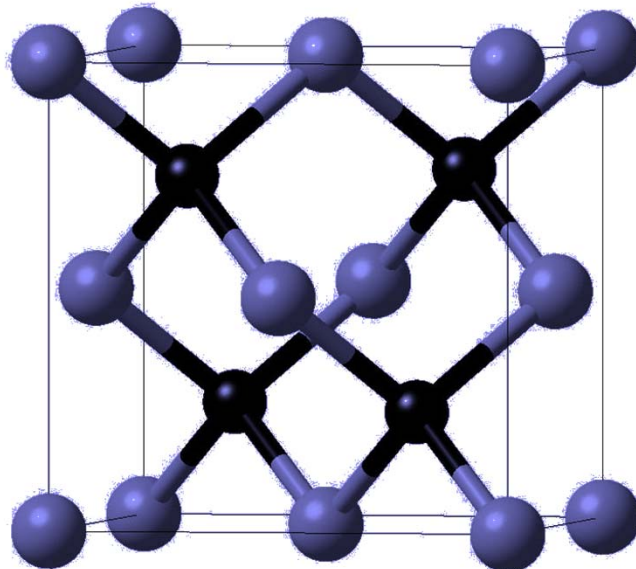
Development of Energy Bands in a Silicon Crystal
(Qualitative Description)

❖ *Pauli exclusion principle* states that no two electrons in an interacting system can have the same set of quantum numbers n, l, m, s.

❖ When the two atoms are completely isolated from each other, there is no interaction of electron wave functions between them.

❖ As the spacing between the two atoms becomes smaller, the initial quantized energy level will split into a band of discrete energy levels in order so that each electron can occupy a distinct quantum state according to *Pauli exclusion principle*
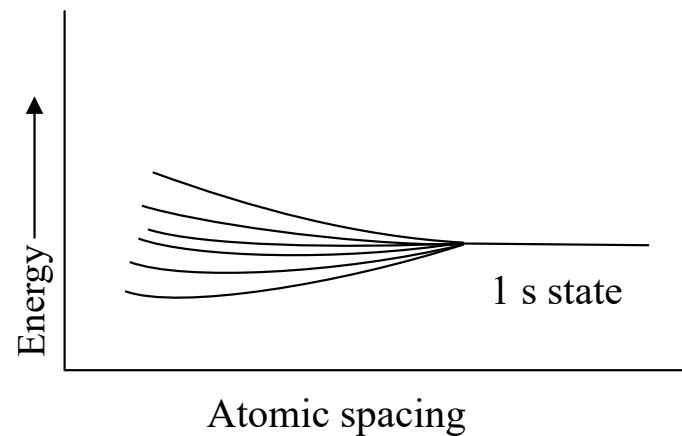
This leads to a splitting of the energy levels consistent with the Pauli exclusion principle.

(Graph: Energy vs. Atomic spacing, showing 1 s state splitting into six energy levels)

Splitting of 1s state of six atoms into a band of six energy levels as the inter-atomic spacing decreases.

Development of Energy Bands in a Silicon Crystal
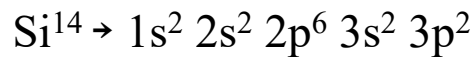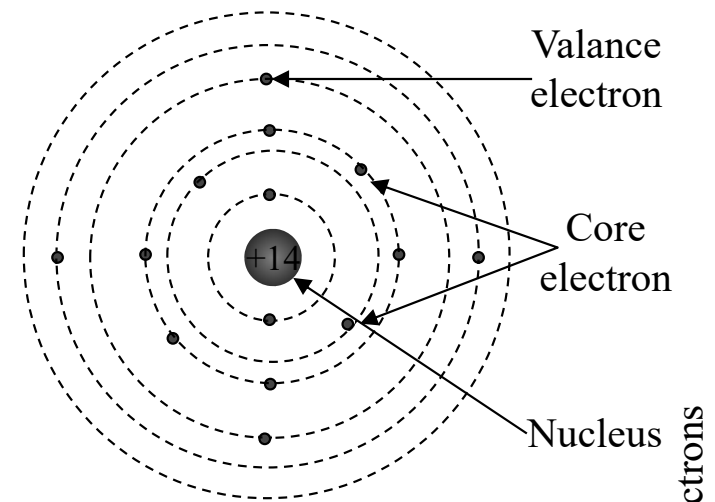
Valance electron

Core electron

Nucleus

+14

$Si^{14} \rightarrow 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$

This leads to a splitting of the energy levels consistent with the Pauli exclusion principle.

Relativistic energy of electrons

4N States
0 Electrons

6N States
2N Electrons

6N States
2N Electrons

Band gap E_g

2N States
2N Electrons

4N States
4N Electrons

2N States
2N Electrons

8N States
4N Electrons

Actual spacing

$r_0 = 2.35$ Å

Relativistic spacing of atoms

s	m	l	n	
$\pm\left(\frac{1}{2}\right)$	+2			
$\pm\left(\frac{1}{2}\right)$	+1			
$\pm\left(\frac{1}{2}\right)$	0	2		
$\pm\left(\frac{1}{2}\right)$	-1			
$\pm\left(\frac{1}{2}\right)$	-2			
$\pm\left(\frac{1}{2}\right)$	+1		3	Outer shell
$\pm\left(\frac{1}{2}\right)$	0	1		
$\pm\left(\frac{1}{2}\right)$	-1			
$\pm\left(\frac{1}{2}\right)$	0	0		
$\pm\left(\frac{1}{2}\right)$	+1			
$\pm\left(\frac{1}{2}\right)$	0	1	2	Middle shell
$\pm\left(\frac{1}{2}\right)$	-1			
$\pm\left(\frac{1}{2}\right)$	0	0		
$\pm\left(\frac{1}{2}\right)$	0	0	1	Inner shell
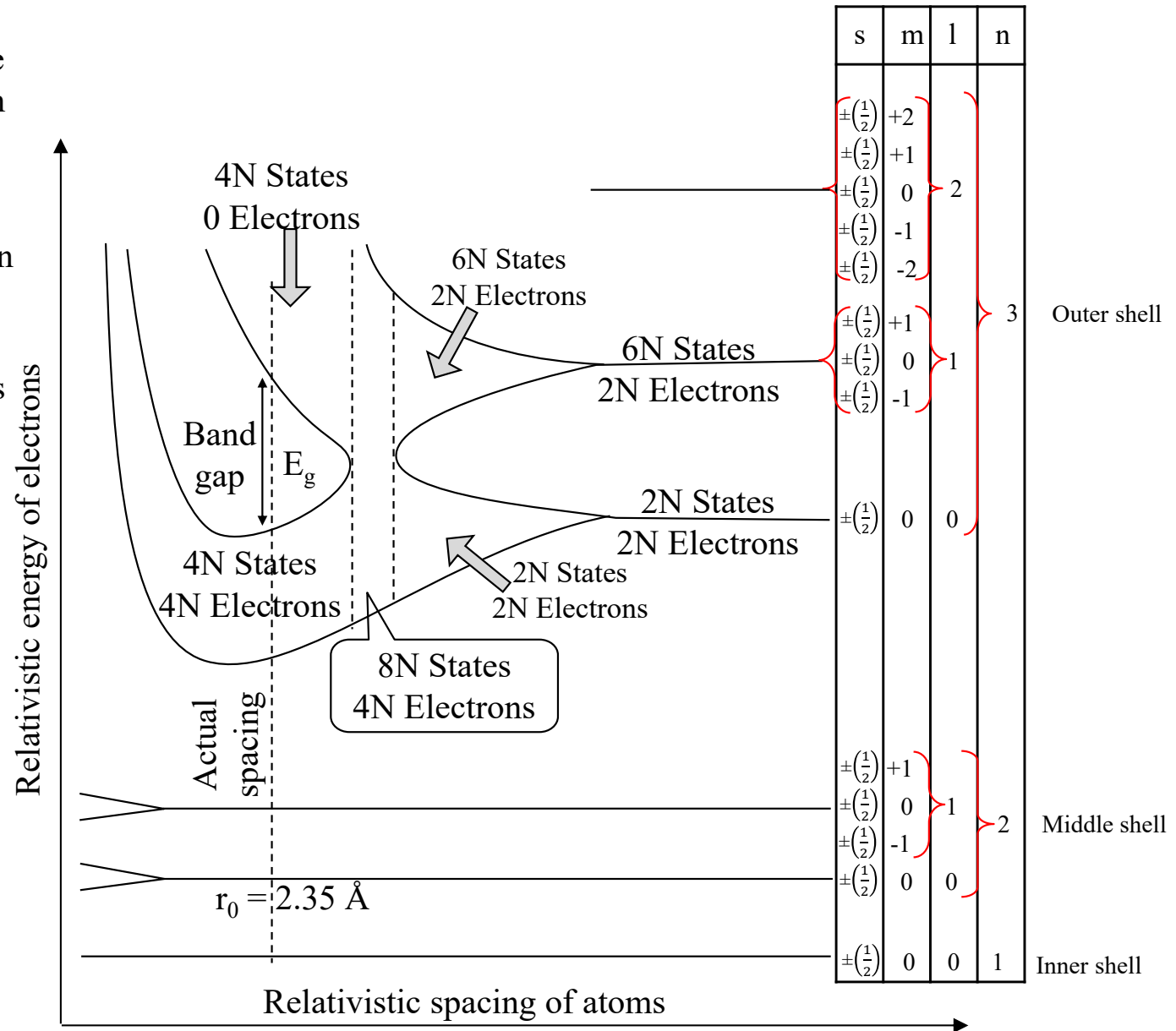
Each atom has available two 1s states, two 2s states, six 2p states, two 3s states, six 3p states, and higher state

Development of Energy Bands in a Silicon Crystal

$Si^{14} \rightarrow 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$

➢ Each atom has available two 1s states, two 2s states, six 2p states, two 3s states, six 3p states, and higher state

➢ Consider an assembly of N Silicon atoms. In this case, there will be 2N, 2N, 6N, 2N, and 6N states of type 1s, 2s, 2p, 3s, and 3p, respectively

➢ When the interatomic distance is large, the energy levels of electrons belonging to various subshells are isolated levels.
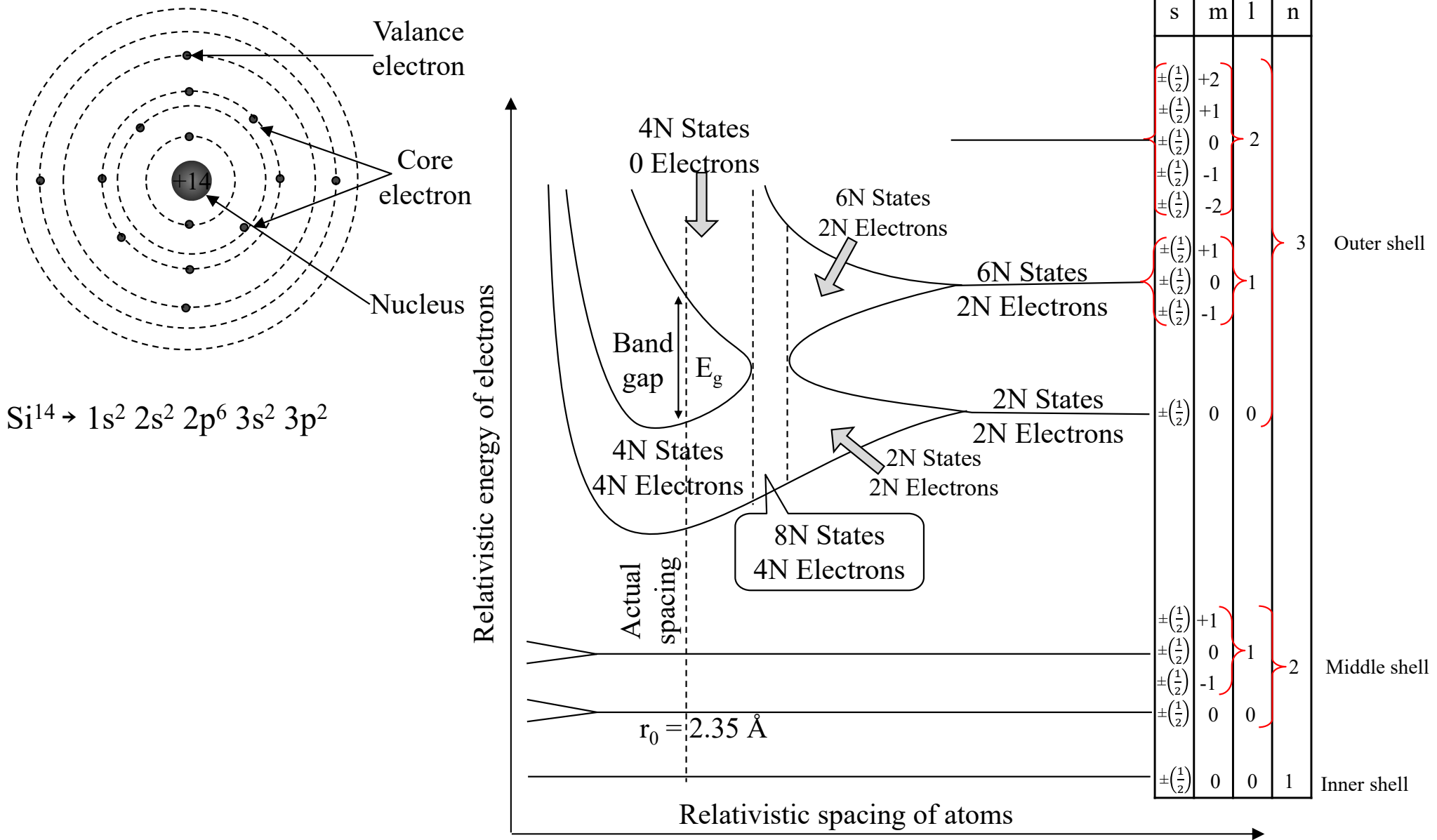
➢ With a reduction in the interatomic spacing, these energy levels split into bands, beginning with the outer (n = 3) shell. As the "3s"and "3p" bands grow, they merge into a single band composed of a mixture of energy levels. This band of "3s-3p" levels contains 8N available states.

➢ As the interatomic spacing approaches equilibrium spacing of silicon crystal, this band splits into two bands separated by an energy gap, where no allowed energy states for electrons exist, is called forbidden gap.

➢ The upper band (called the conduction band) and the lower band (called the valence band) contain 4N states each.

➢ This energy-band splitting, and the formation of allowed and forbidden bands is the **energy-band theory of single-crystal materials**.

Development of Energy Bands in a Silicon Crystal

$Si^{14} \rightarrow 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$

Valance electron

Core electron

Nucleus

+14

Relativistic energy of electrons

4N States
0 Electrons

6N States
2N Electrons

6N States
2N Electrons

Band gap E_g

2N States
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4N States
4N Electrons

2N States
2N Electrons

8N States
4N Electrons

Actual spacing

$r_0 = 2.35\ \text{Å}$

Relativistic spacing of atoms

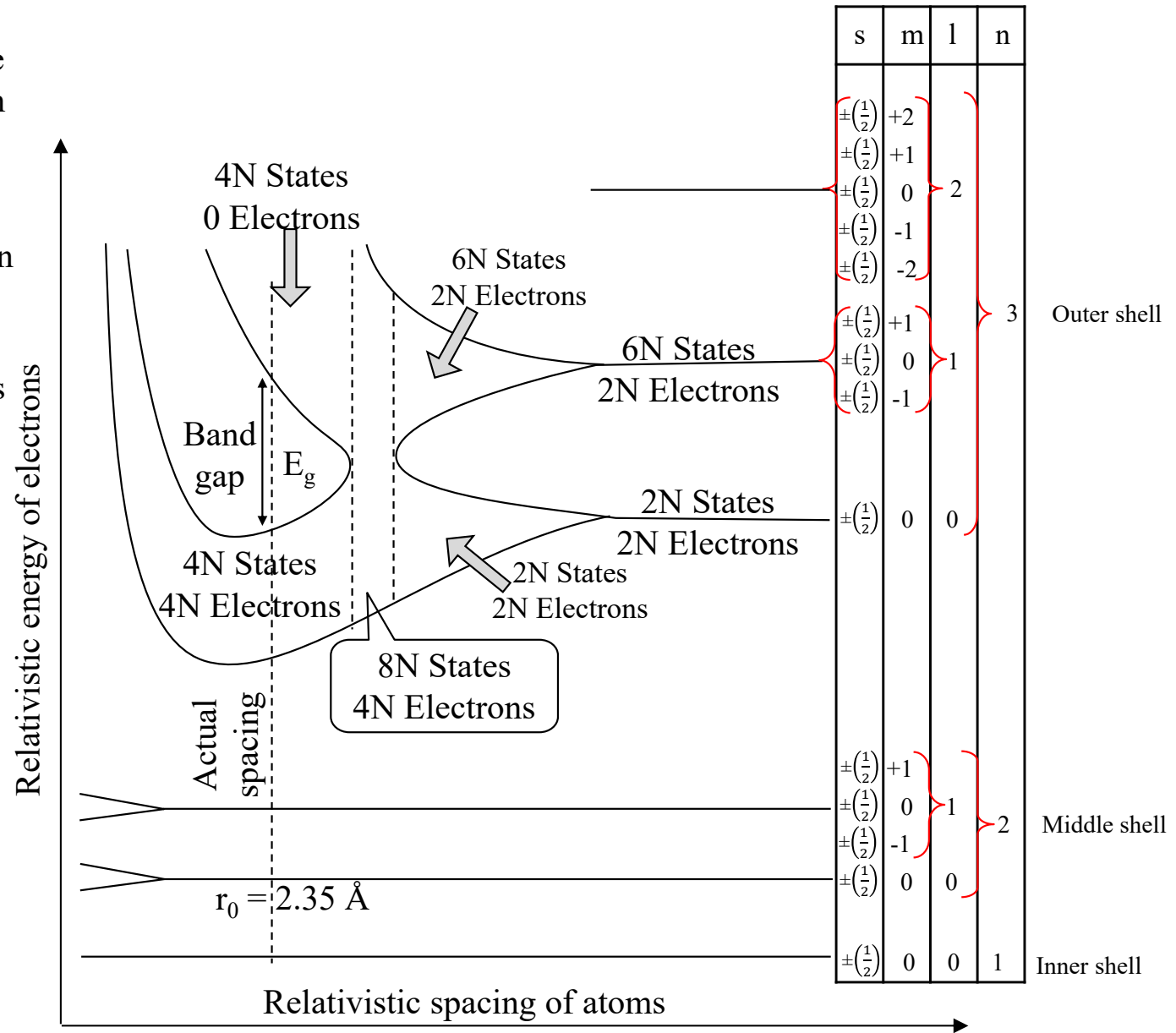| s	m	l	n	
$\pm\left(\frac{1}{2}\right)$	+2			
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$\pm\left(\frac{1}{2}\right)$	0	1		
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$\pm\left(\frac{1}{2}\right)$	0	0	1	Inner shell

The splitting of the atomic energy levels of silicon into bands is followed by the merging of the 3s and 3p bands and a subsequent splitting of these bands as the separation approaches the interatomic equilibrium spacing r_o. At the equilibrium interatomic spacing r_0, the '3s 3p' band splits again into two hybrid bands separated by an energy gap Eg.
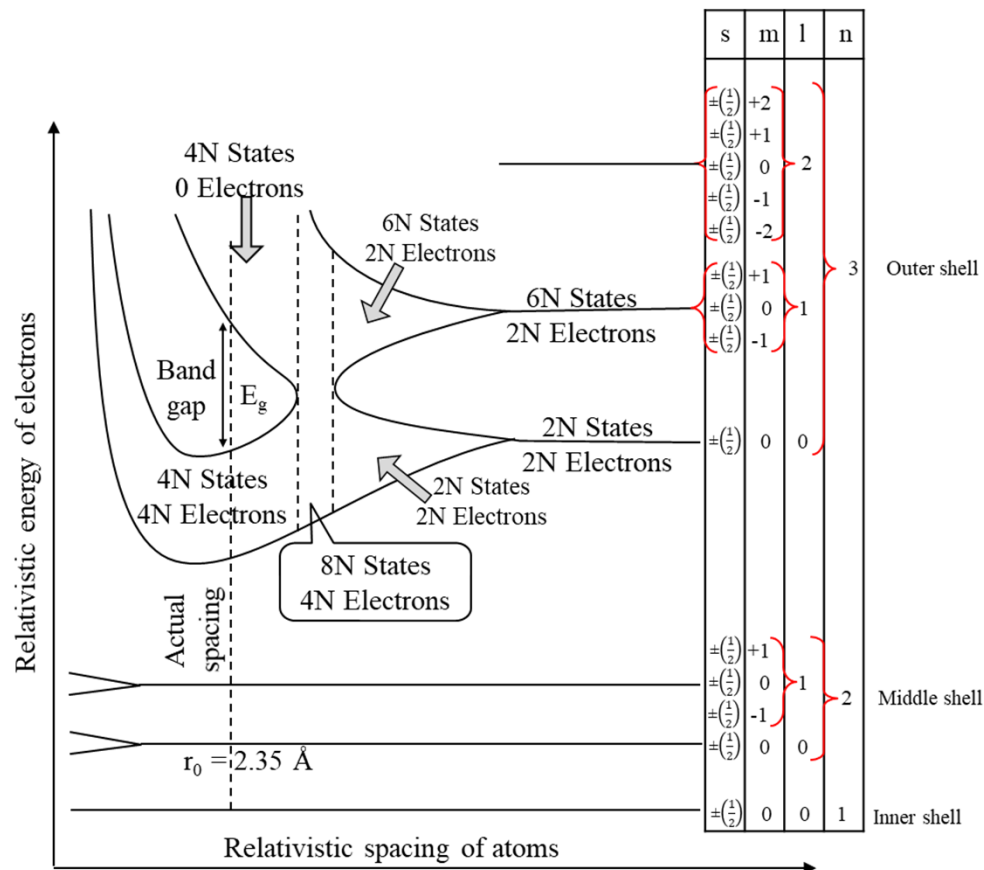
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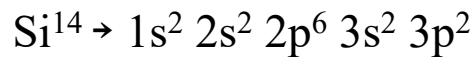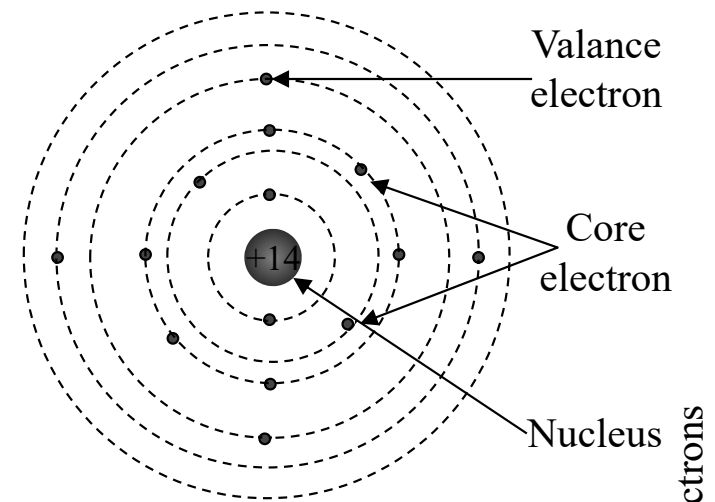
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Core electron

Nucleus

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$\pm\left(\frac{1}{2}\right)$	0	0		
$\pm\left(\frac{1}{2}\right)$	0	0	1	Inner shell

Energy levels in Si as a function of interatomic spacing. The core levels (n = 1,2) in Si are completely filled with electrons. At the actual atomic spacing of the crystal, the 2N electrons in the 3s subshell and the 2N electrons in the 3p subshell undergo *sp3* hybridization, and all end up in the lower *4N* states (valence band), while the higher-lying 4 N states (conduction band) are empty, separated by a band gap.

Energy Band Theory

➢ The lower "1s" band is filled with the 2N electrons which originally resided in the collective 1s states of the isolated atoms. Similarly, the 2s band and the 2p bands will have 2N and 6N electrons in them, respectively.

➢ There are 4N electrons in the original isolated n = 3 shells (2N in 3s states and 2N in 3p states).These 4N electrons must occupy states either in the valence band or in the conduction band.

➢ At 0 K, the electrons will occupy the lowest energy states available to them thus, the 4N states in the valence band will be completely filled, and the 4N states in the conduction band will be completely empty. As we shall see, this arrangement of completely filled and empty energy bands has an important effect on the electrical conductivity of the solid.

Development of Energy Bands in a Silicon Crystal

Energy bands are composed of closely spaced orbitals
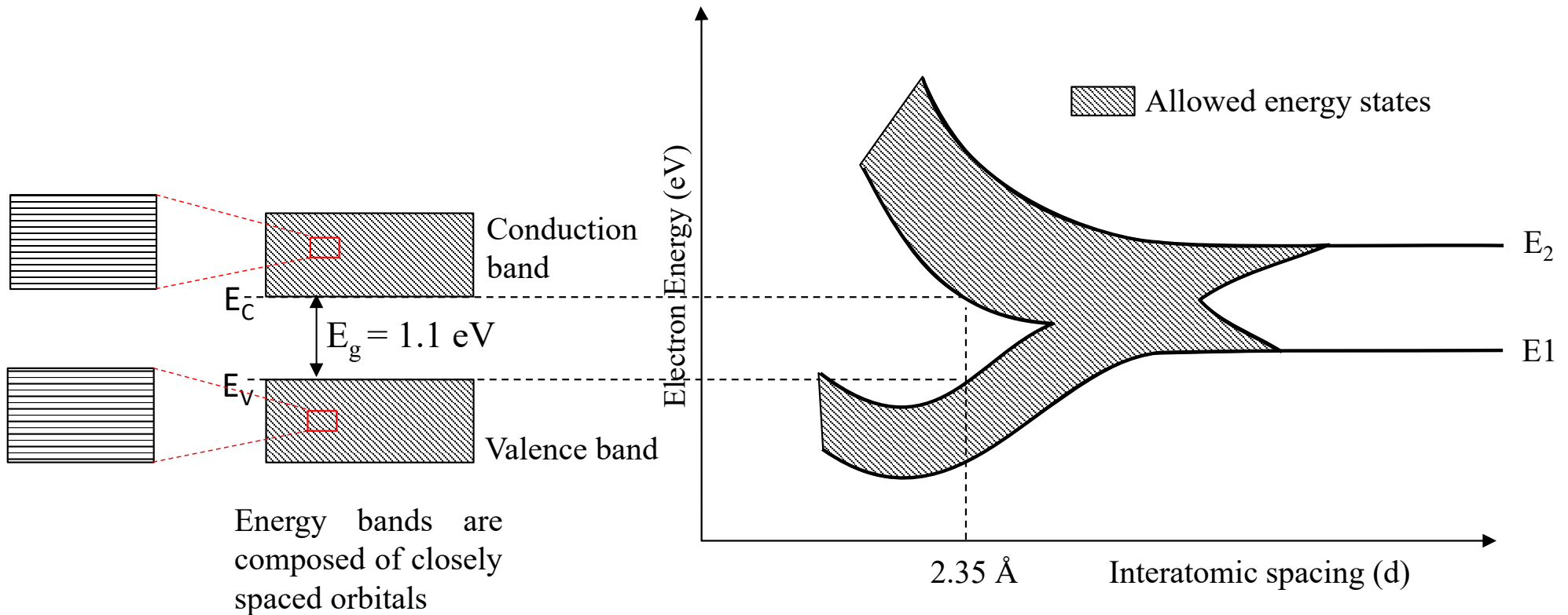
The energy of adjacent levels is so close together that they can be considered as a continuum, an energy band.

The splitting of the atomic energy levels into bands is followed by the merging of the bands and a subsequent splitting of these bands as the separation approaches the interatomic equilibrium spacing r_o. At the equilibrium interatomic spacing r_0, the band splits again into two hybrid bands separated by an energy gap E_g.

Energy Bands
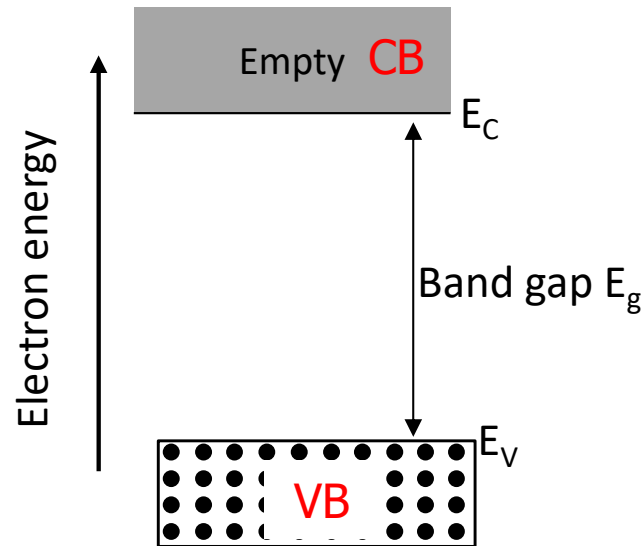
If a band is completely filled with electrons, and the band immediately above it is empty, the material has an energy **band gap**. This band gap is the energy difference between the highest occupied state in the valence band and the lowest unoccupied state in the conduction band. The material is either a semiconductor if the band gap is relatively small, or an insulator if the band gap is relatively large.

The bands are actually composed of a finite number of very closely spaced electron energy levels.

Energy Band Theory

Electronic structure of $Na^{11} \rightarrow 1s^2\ 2s^2\ 2p^6\ 3s^1$
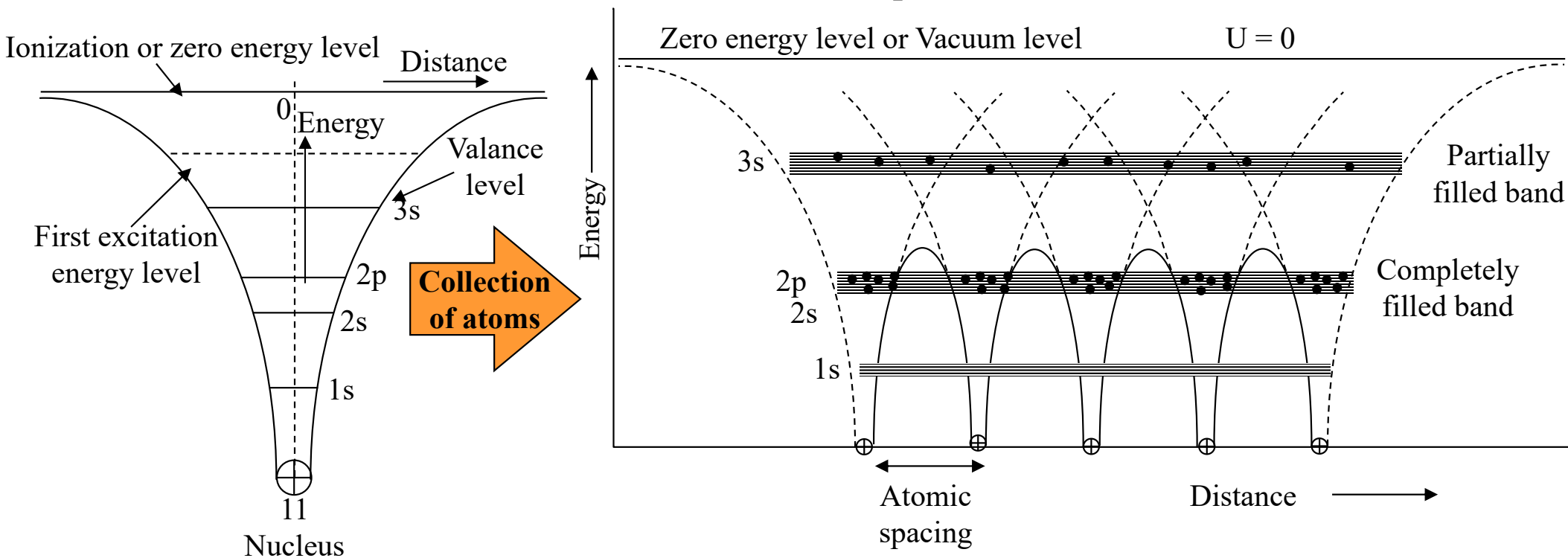
- Consider a crystal containing N atoms that are arranged in a periodic array.
- When the atoms are far apart, there is no interaction between them, and the allowed states of the system are just the states of a single atom repeated N times in space.
- As the interatomic spacing is decreased, the valance orbitals of the atoms begin to overlap and spread into bands.
- The electrons belonging to each atom in the 2s and 2p bands are still separated from neighboring atoms by potential humps and therefore not able to move from one atom to another.
- The band formed by the 3s electrons is only partially filled, and the electrons in this band can move freely from one atom to another because the energies lie above the potential humps.
- Only electrons that are in the highest energy band close to the Fermi level can move freely in the solid.

Energy Band Theory

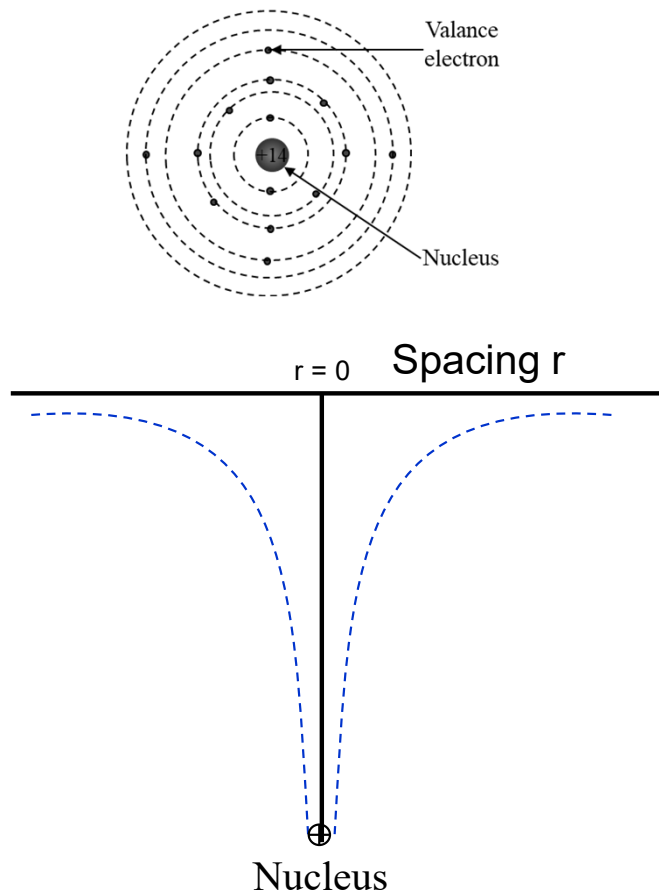Electronic structure of $Si^{14} \rightarrow 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$
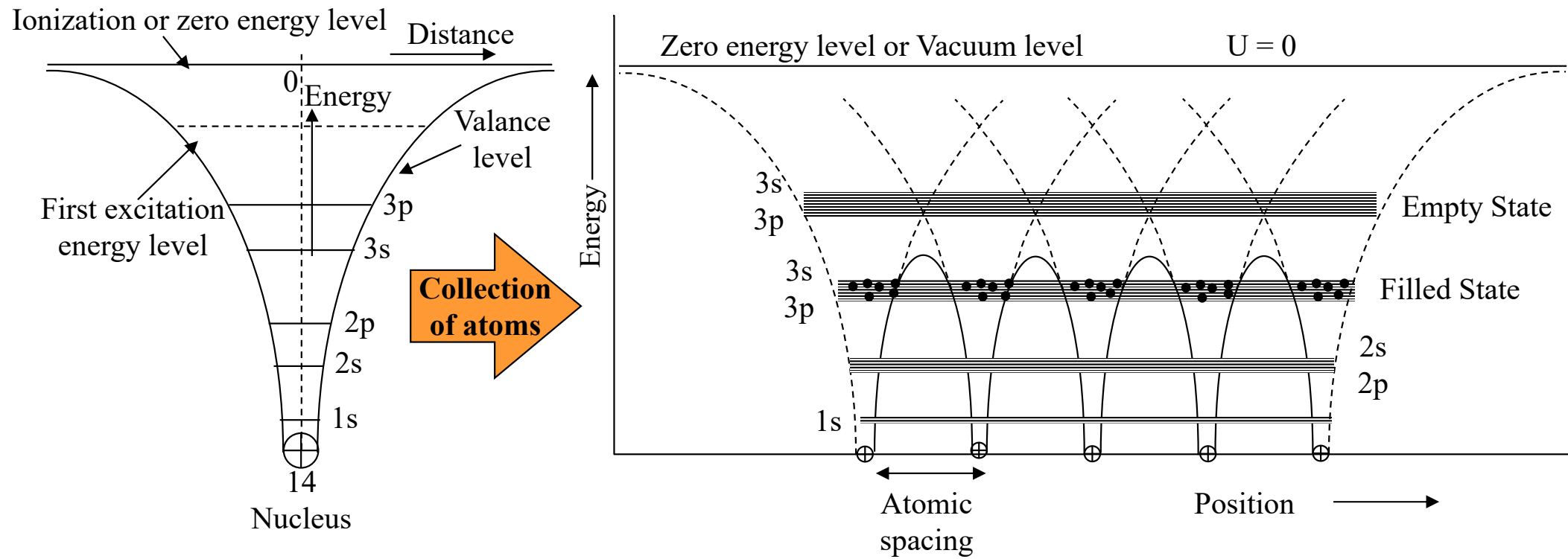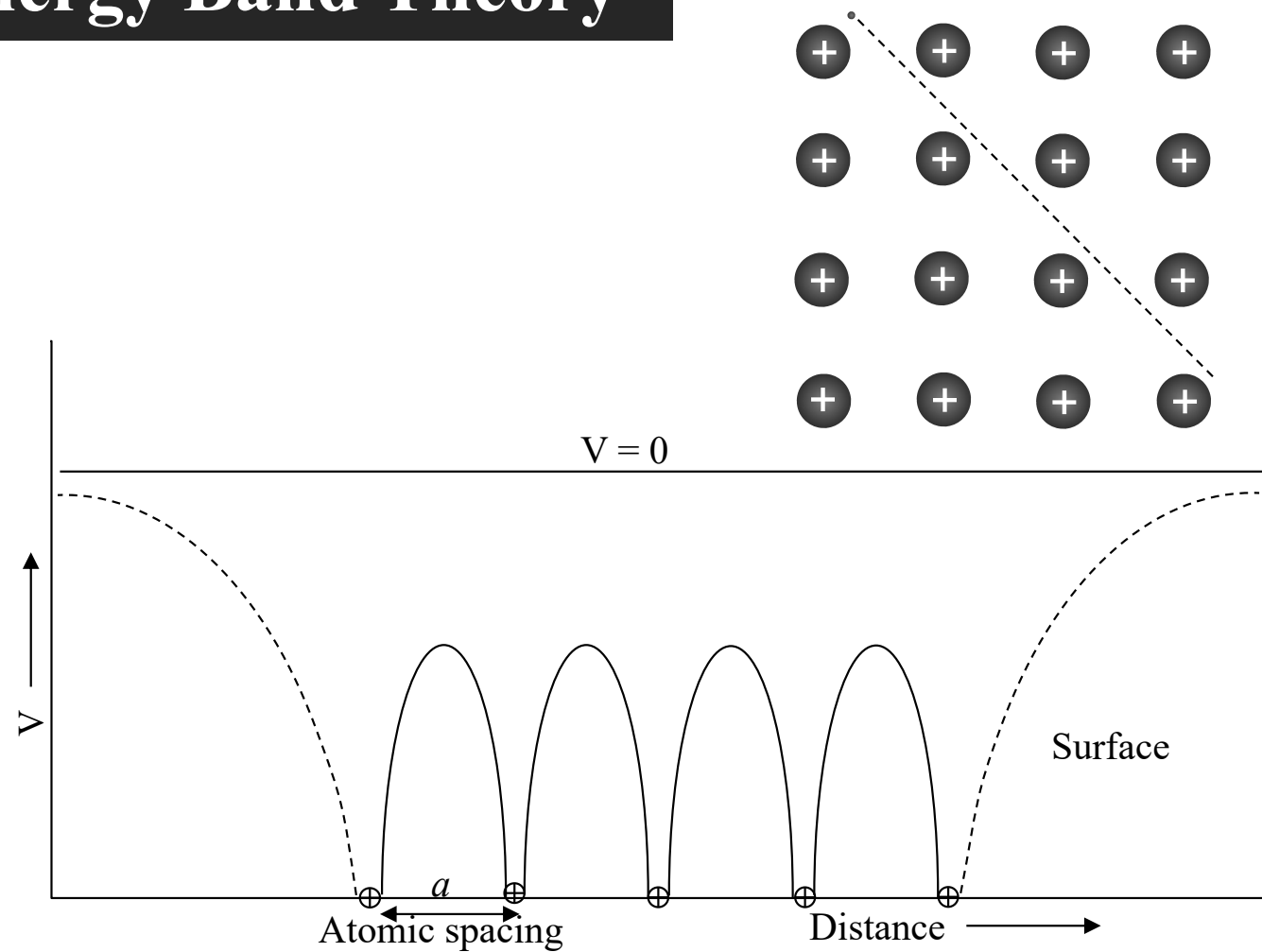
Energy Band Theory
(Quantitative Description)

- Free electron theory was given to explain the properties of solids. The fundamental assumption was electron moves in a constant potential well.

- The free electron theory successfully explained the electric conductivity and thermionic emission of metals, but it was failed to explain the classification of materials as solids, insulators and semiconductors.

- The failure of the free electron model is due to the oversimplified assumption that a conduction electron in a metal experiences a constant or zero potential due to the ion cores and hence is free to move about in a crystal; the motion being restrained only by the surface of the crystal.

- The potential due to ion cores is not constant and may change with position of the electron in the crystal.

- The actual nature of the potential under which an electron moves in a crystal is very complicated.

- To a reasonable approximation, the ion cores may be considered at rest and the potential experienced by an electron in a crystal is assumed to be periodic with period equal to the lattice constant for a one-dimensional case.

- The potential contribution due to all other free electrons may be taken as constant.
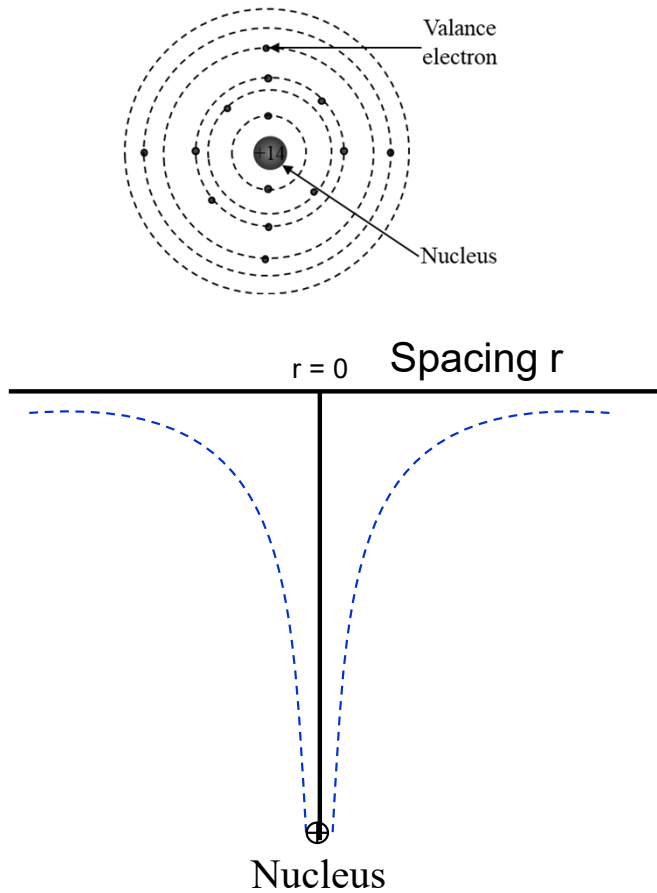
Energy Band Theory

Spacing r

r = 0

Nucleus

Coulombic potential of a nucleus

$V = 0$

a

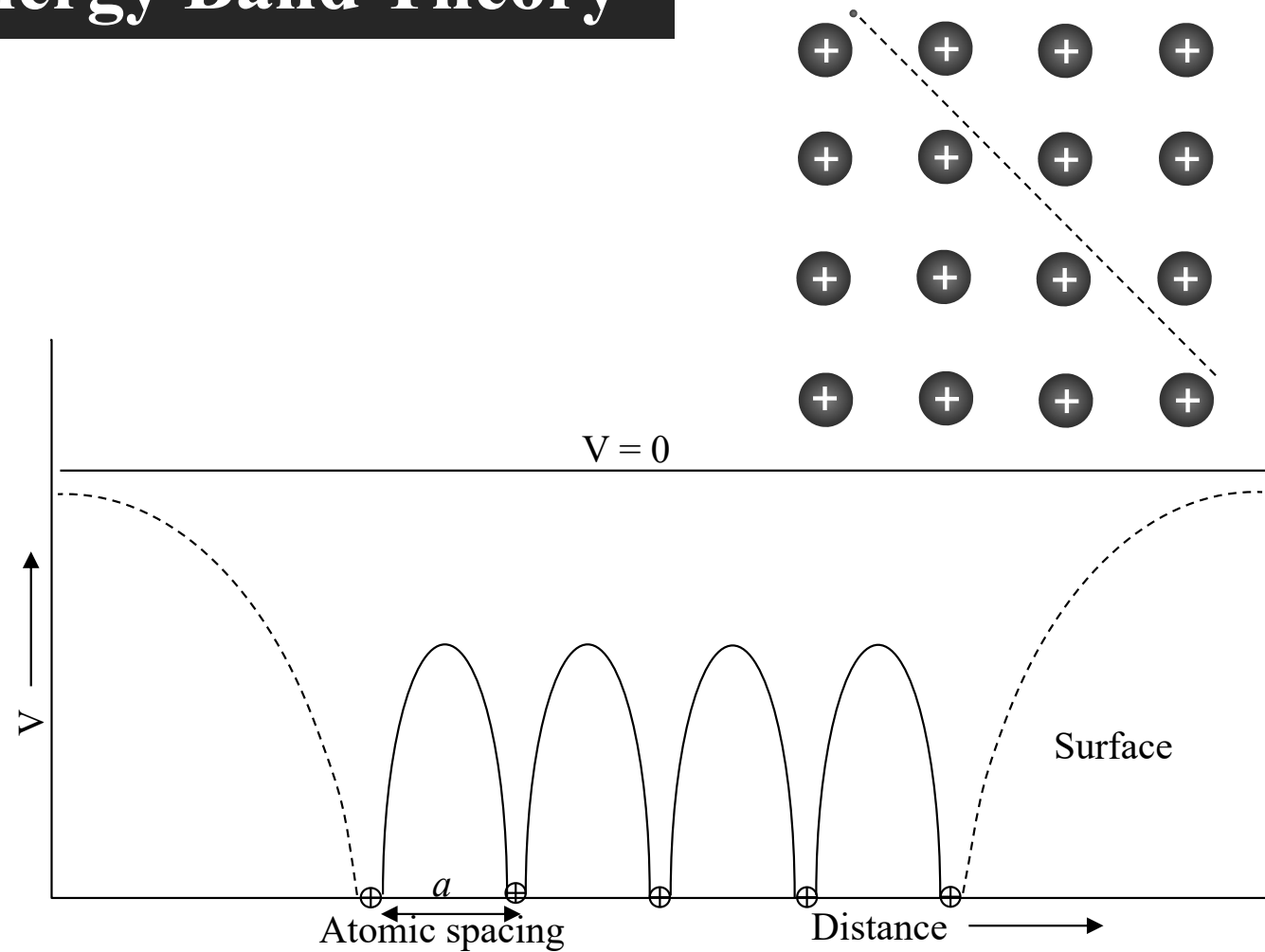Atomic spacing

Distance

Surface

One-dimensional representation of potential experienced by an electron in a periodic crystal lattice with lattice constant a. The potential near the surface is shown on the left and right.

- To explain the properties of metal, insulators and semiconductors, the periodic potential experienced by electron must be accounted.
- The figure shows the periodic potential U that arises from interaction of electrons with the periodic array of ions in a crystal.
- For a free electron, U = 0. Negative potential imply bound electrons.
- Solution of the Schrodinger equation for a periodic potential results in energy bands and bandgaps.

Energy Band Theory

**Coulombic potential of a nucleus**

One-dimensional representation of potential experienced by an electron in a periodic crystal lattice with lattice constant a. The potential near the surface is shown on the left and right.

- This type of periodic potential extends up to infinity in all directions except at the surface of the crystal where, due to interruption in periodicity of the lattice, it has a shape similar to as shown on the right and left-hand edges of the figure.

- This type of potential irregularity may be ignored.

- The periodic potential described above forms the basis of the band theory of solids.

Energy Band Theory

- The behaviour of an electron in the period potential is described by constructing wave functions using one-electron approximation.

- The total wave function for the system is obtained from a combination of wave functions each one of which involves the coordinate of one electron.

- The existence of band gaps is the most important new property which emerges when the free electron model is extended to include the effect of periodic potential of the ion cores.

- The band gaps result from the interaction of the conduction electron waves with ion cores of the crystal and are of decisive significance to determine whether a solid is a conductor, a semiconductor or an insulator.

- To solve this problem the basic assumption of free electron theory was modified by Bloch.

- Bloch proposed that the electron inside the material are not in constant potential, but they are moving in periodic potential well as per the periodicity of lattice.

- Let us first determine the electron wave function for a periodic lattice.

The Bloch Theorem
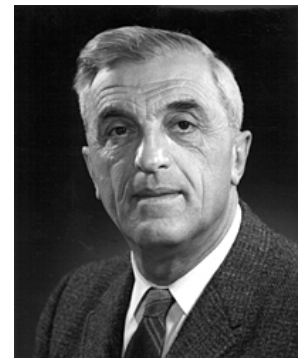
Felix Bloch
(23 Oct 1905-10 Sept 1983)
Swiss-American physicist
Nobel Prize for Physics: 1952

The one-dimensional Schrodinger equation for a free electron moving in a constant potential V_0

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0$$

The solutions to this equation are plane waves of the type

$$\psi(x) = e^{\pm ikx}$$

Where $\quad (E - V_0) = \dfrac{\hbar^2 k^2}{2m} = \dfrac{p^2}{2m} = Ekin$

Schrodinger equation for an electron moving in a one-dimensional periodic potential, $V(x)$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi = 0$$

Since the potential is periodic with period equal to the lattice constant a

$$V(x) = V(x + a)$$

The Bloch Theorem

There is an important theorem known as the Bloch theorem concerned with the solution to

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi = 0.$$

Bloch's theorem states that solutions to the Schrödinger equation in a periodic potential take the form of a plane wave modulated by a periodic function.

Hence, the solutions to $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi = 0$ are plane waves of the type $\psi(x) = e^{\pm ikx}$ which are modulated by a function $u_k(x)$ having the same periodicity as that of the lattice.

Thus, the solutions are of the form $\psi(x) = e^{\pm ikx} u_k(x)$ with $u_k(x) = u_k(x+a)$

Functions of this form are known as Bloch functions (or Bloch states) and serve as a suitable basis for the wave functions or states of electrons in crystalline solids.

Kronig-Penney Model

Ralph Kronig
(10 March 1904-16 Nov. 1995), German physicist.
He is noted for the discovery of particle spin and for
his theory of X-ray absorption spectroscopy.

William George Penney, Baron Penney
(24 June 1909-3 March 1991), English mathematician

- R. de L. Kronig and W. G. Penney developed a useful one-dimensional model of the interaction between the electrons and the lattice of atoms (i.e., electron lattice interaction) in 1931.

- They assumed that an electron experiences an infinite one-dimensional array of finite potential wells.

- The size of the wells is roughly to the lattice spacing.

- They explained mainly band in solids and classification of semiconductor and insulators.

Kronig-Penney Model
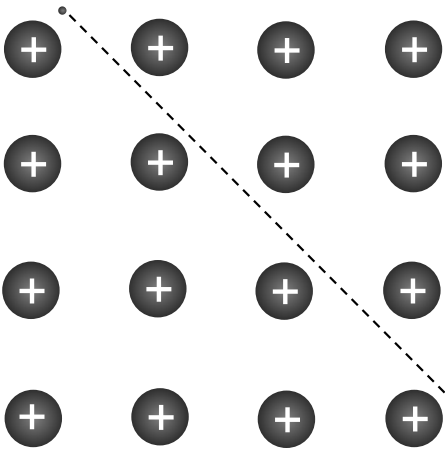
- The potential energy of an electron is a linear array of positive nuclei is assumed to have the form of a periodic array of square well with period of $(a+b)$.
- At the bottom of a well, i.e., for $0<x<a$, the electron is assumed to be in the vicinity of a nucleus and the potential energy is taken as zero, whereas outside a well, i.e., for $-b<x<0$, the potential energy assumed to be V_0.
- Although this model employs a very crude approximation to the type of periodic potential existing inside a lattice, it is very useful to illustrate various important features of the quantum behavior of electrons in the periodic lattice.

Original crystal potential

Approximate crystal potential

V_0 II   I V_{max}

V_{min}

$-b$ $0\ a$ $a+b$
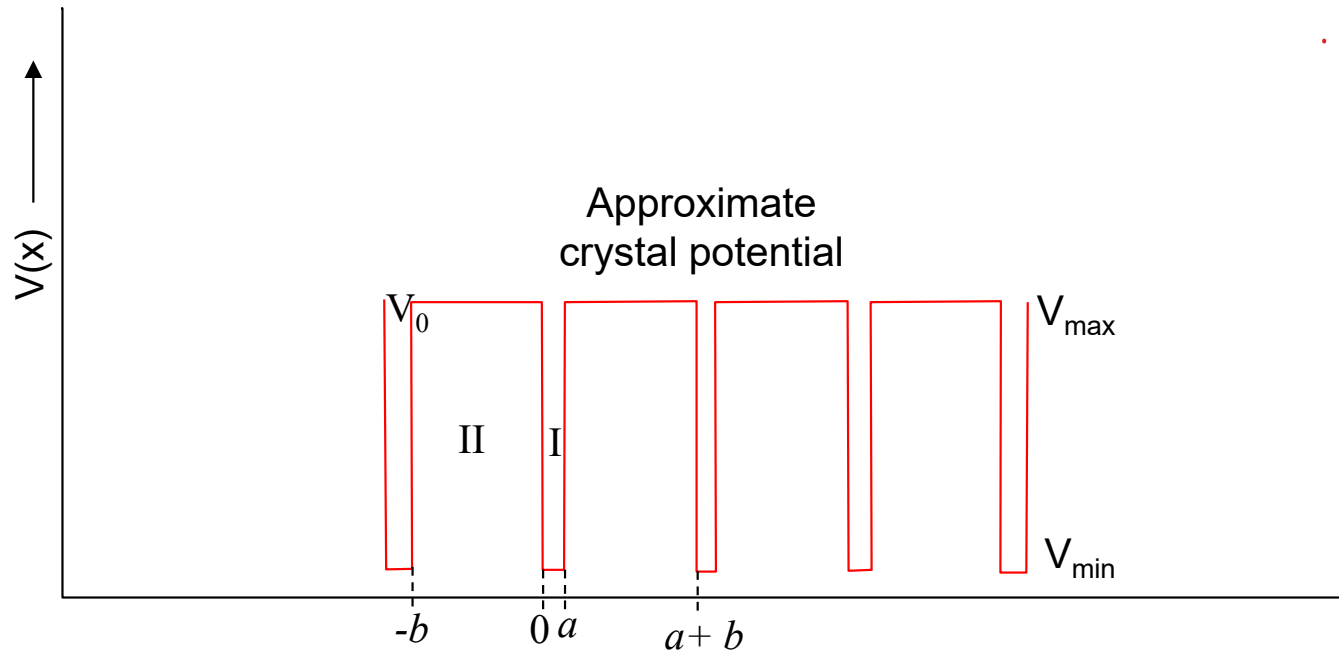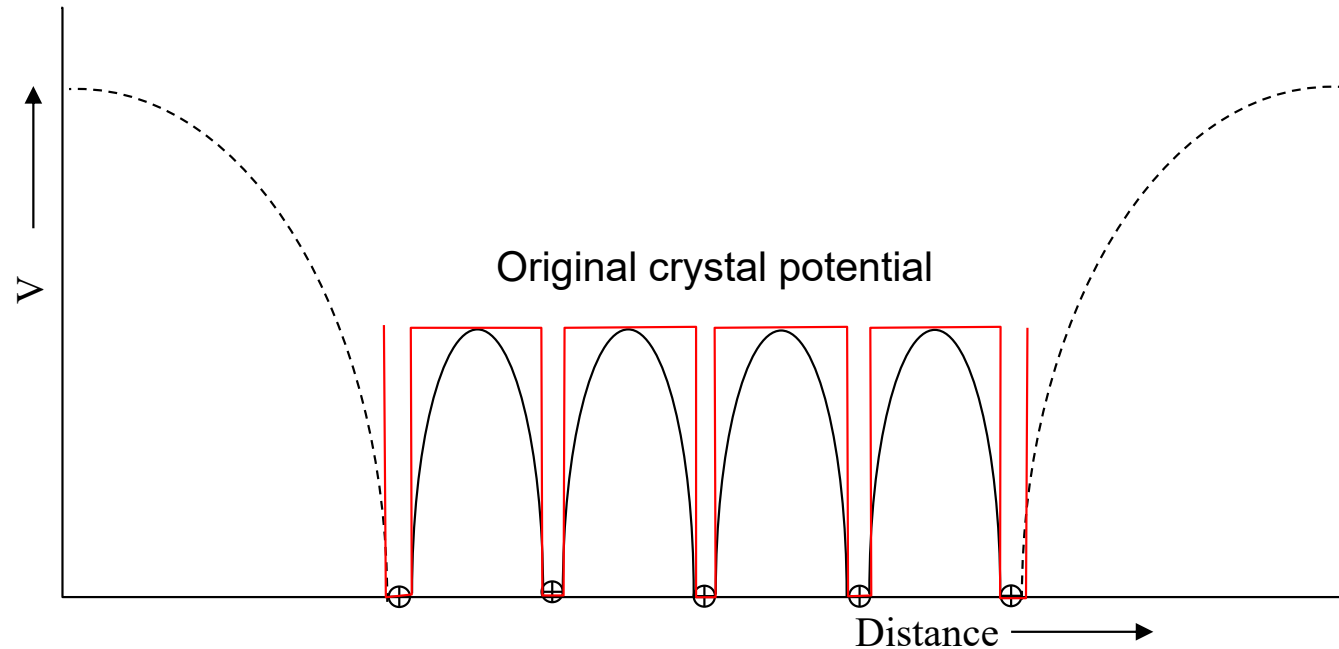
One-dimensional periodic potential used by Kronig and Penney

Kronig-Penney Model

An effective way to understand the energy gap in semiconductors is to model the interaction between the electrons and the lattice of atoms.
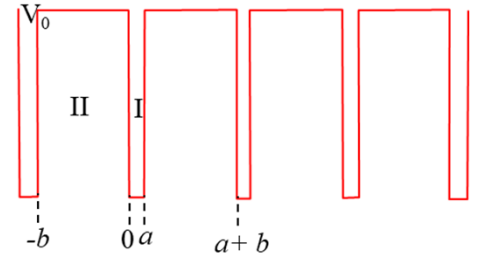
The Schrodinger's wave equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

For I-Region ($0<x<a$), V = 0

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

For II-Region ($-b<x<0$), V = V_0

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0$$

Assuming that the energy E of the electrons is less than V_0, we define two real quantities α and β as

$$\boxed{\alpha^2 = \frac{2mE}{\hbar^2}} \qquad \boxed{\beta^2 = \frac{2m(V_0 - E)}{\hbar^2}}$$

For I-Region ($0<x<a$), V = 0

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0 \Rightarrow \boxed{\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0}$$

For II-Region ($-b<x<0$), V = V_0

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0 \Rightarrow \boxed{\frac{d^2\psi}{dx^2} - \beta^2\psi = 0}$$

Kronig-Penney Model

Since the potential is periodic, the wave function must be of the form of Bloch function according to Bloch theorem

$$\psi(x) = e^{ikx}u_k(x)$$

Where $u_k(x)$ is the periodic function in x with periodicity of $(a+b)$ i.e.

$$u_k(x) = uk(x + a + b)$$

$$\checkmark \psi(x) = uk(x)e^{ikx}$$

$$\boxed{\frac{d\psi}{dx} = ike^{ikx}u_k(x) + e^{ikx}\frac{du_k}{dx}}$$

$$\frac{d^2\psi}{dx^2} = -k^2 e^{ikx}u_k(x) + 2ike^{ikx}\frac{du_k}{dx} + e^{ikx}\frac{d^2u_k}{dx^2}$$

$$\boxed{\frac{d^2\psi}{dx^2} = e^{ikx}\left(\frac{d^2u_k}{dx^2} + 2ik\frac{du_k}{dx} - k^2u_k\right)}$$

For I-Region $(0<x<a)$, $u_k \rightarrow u_1$

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0 \Rightarrow e^{ikx}\left(\frac{d^2u_1}{dx^2} + 2ik\frac{du_1}{dx} - k^2u_1\right) + \alpha^2 u_1 e^{ikx} = 0$$

$$e^{ikx}\left\{\frac{d^2u_1}{dx^2} + 2ik\frac{du_1}{dx} + (\alpha^2 - k^2)u_1\right\} = 0$$

$$\frac{d^2u_1}{dx^2} + 2ik\frac{du_1}{dx} + (\alpha^2 - k^2)u_1 = 0$$
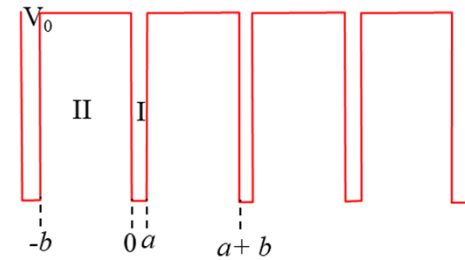
$$\psi(x) = e^{ikx} u_k(x)$$

Kronig-Penney Model

For I-Region ($0<x<a$), $u_k \rightarrow u_1$

$$\frac{d^2 u_1}{dx^2} + 2ik \frac{du_1}{dx} + (\alpha^2 - k^2)u_1 = 0 \quad \checkmark$$

For II-Region ($-b<x<0$), $u_k \rightarrow u_2$ $\quad \frac{d^2\psi}{dx^2} = e^{ikx}\left(\frac{d^2 u_k}{dx^2} + 2ik \frac{du_k}{dx} - k^2 u_k\right)$

$$\frac{d^2\psi}{dx^2} - \beta^2\psi = 0 \implies \frac{d^2 u_2}{dx^2} + 2ik \frac{du_2}{dx} - (\beta^2 + k^2)u_2 = 0 \quad \checkmark$$

These are second order linear differential equations

Homogeneous linear differential equation

The general form of a linear ordinary differential equation with constant coefficients

$$\frac{d^n y}{dx^n} + k_n \frac{d^{n-1} y}{dx^{n-1}} + --------- k_1 y = 0$$

Let $D \equiv \frac{d}{dx}$ $D^n \equiv \frac{d^n}{dx^n}$

The symbolic form of the equation

$$(D^n + k_n D^{n-1} + k_{n-1} D^{n-2} + \ldots\ldots\ldots + k_2 D + k_1) y = 0$$

Let the roots of this equation are $m_1, m_2, m_3 \ldots\ldots m_n$

$$(D - m_n)(D - m_{n-1}) \ldots\ldots\ldots (D - m_1) = 0$$

The solution of the equation

$$y = c_1 e^{m_1 x} + c_2 e^{m_2 x} + \ldots\ldots\ldots + c_n e^{m_n x}$$

Where $c_1, c_2, c_3 \ldots\ldots c_n$ are arbitrary coefficients

Kronig-Penney Model

$$ax^2 + bx + c = 0$$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

For I-Region $(0 < x < a)$, $u_k \rightarrow u_1$

$$\frac{d^2 u_1}{dx^2} + 2ik \frac{du_1}{dx} + (\alpha^2 - k^2)u_1 = 0$$
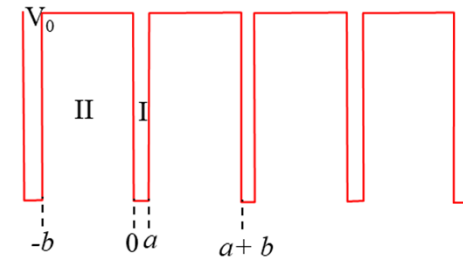
Roots of this equation
$i(a - k) \ \& \ -i(a + k)$

For II-Region $(-b < x < 0)$, $u_k \rightarrow u_2$

$$\frac{d^2\psi}{dx^2} = e^{ikx}\left(\frac{d^2 u_k}{dx^2} + 2ik \frac{du_k}{dx} - k^2 u_k\right)$$

$$\frac{d^2\psi}{dx^2} - \beta^2\psi = 0 \implies \frac{d^2 u_2}{dx^2} + 2ik \frac{du_2}{dx} - (\beta^2 + k^2)u_2 = 0$$

Roots of this equation
$(\beta - ik) \ \& \ -(\beta + ik)$

These are second order linear differential equations

The general solutions of these equations are

$$u_1 = Ae^{i(\alpha - k)x} + Be^{-i(\alpha + k)x} \quad \text{For I-Region } (0 < x < a), V = 0$$

$$u_2 = Ce^{(\beta - ik)x} + De^{-(\beta + ik)x} \quad \text{For II-Region } (-b < x < 0), V = V_0$$

Where A, B, C and D are constants which can be determined using boundary conditions

Since the electrons are not free if their energies are less than the height V_0 of each of the potentials, but the electron is essentially free in the gap $0 < x < a$

In the region between $a < x < a + b$ the electron can tunnel through, and the wave function loses its oscillatory solution and becomes exponential.

Matching solutions at the boundary

Kronig-Penney Model
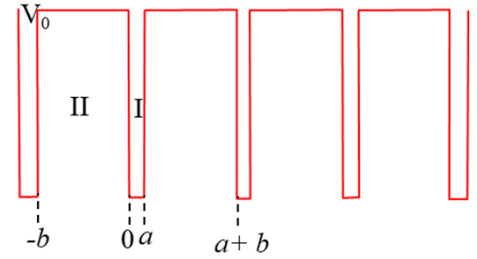
The wave function ψ and its derivative $\frac{d\psi}{dx}$, and hence u and $\frac{du}{dx}$ must be continuous

$$\boxed{u_1(0) = u_2(0)}$$

$$\boxed{\left(\frac{du_1}{dx}\right)_{x=0} = \left(\frac{du_2}{dx}\right)_{x=0}}$$

According to the periodicity of $u_k(x)$

$$\boxed{u_1(a) = u_2(-b)}$$

$$\boxed{\left(\frac{du_1}{dx}\right)_{x=a} = \left(\frac{du_2}{dx}\right)_{x=-b}}$$

Apply these boundary conditions to following equations

$$u_1 = Ae^{i(\alpha-k)x} + Be^{-i(\alpha+k)x}$$

$$u_2 = Ce^{(\beta-ik)x} + Be^{-(\beta+ik)x}$$

We get following four linear homogeneous equations

$$A + B = C + D$$

$$Ai(\alpha - k) - Bi(\alpha + k) += C(\beta - ik) - D(\beta + ik)$$

$$Ae^{i(\alpha-k)a} + Be^{-i(\alpha+k)a} = Ce^{-(\beta-ik)b} + D\ e^{(\beta+ik)b}$$

$$Ai(\alpha - k)e^{i(\alpha-k)a} - Bi(\alpha + k)e^{-i(\alpha+k)a} = C(\beta - ik)e^{-(\beta-ik)b} - Di(\beta + ik)e^{(\beta+ik)b}$$

Kronig-Penney Model

$$A + B = C + D$$

$$Ai(\alpha - k) - Bi(\alpha + k) += C(\beta - ik) - D(\beta + ik)$$

$$Ae^{i(\alpha-k)a} + Be^{-i(\alpha+k)a} = Ce^{-(\beta-ik)b} + D\ e^{(\beta+ik)b}$$

$$Ai(\alpha - k)e^{i(\alpha-k)a} - Bi(\alpha + k)e^{-i(\alpha+k)a} = C(\beta - ik)e^{-(\beta-ik)b} - Di(\beta + ik)e^{(\beta+ik)b}$$

These equations are used to determine the constants A, B, C and D. A non-zero solution to these equations exists only if the determinant of the coefficients of A, B, C and D vanishes i.e.

$$\begin{vmatrix} 1 & 1 & 1 & 1 \\ i(\alpha - k) & -i(\alpha + k) & (\beta - ik) & -(\beta + ik) \\ e^{i(\alpha-k)a} & e^{-i(\alpha+k)a} & e^{-(\beta-ik)b} & e^{(\beta+ik)b} \\ i(\alpha - k)e^{i(\alpha-k)a} & -i(\alpha + k)e^{-i(\alpha+k)a} & (\beta - ik)e^{-(\beta-ik)b} & -i(\beta + ik)e^{(\beta+ik)b} \end{vmatrix} = 0$$

On solving this determinant, we obtain

$$\frac{\beta^2 + \alpha^2}{2\beta\alpha} sinh\beta b sin\alpha a + cosh\beta b cos\alpha a = cos k(a + b)$$

Kronig-Penney Model

$$\frac{\beta^2 + \alpha^2}{2\beta\alpha} \boxed{sinh\beta b} sin\alpha a + \boxed{cosh\beta b} cos\alpha a = cosk(a+b)$$
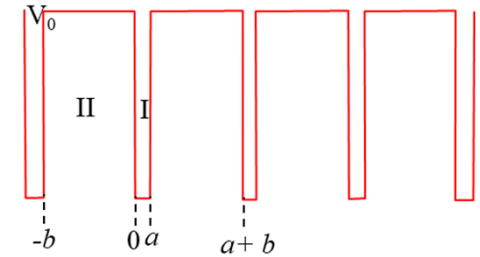
To simplify this equation, Kronig and Penney considered the case when V_0 tends to infinity and b approaches zero but the product $V_0 b$ remains finite, i.e., the potential barriers become delta functions. Under these circumstances, the model is modified to the one of a series of wells separated by infinitely thin potential barriers. The quantity lim $V_0 b$ for $V_0 \to \infty$ and b→0 is called the barrier strength.

As b→0, sinhβb→ βb and coshβb→1.

$$\delta(x) = \begin{cases} 0 & x \neq 0 \\ \infty & x = 0 \end{cases} \quad \text{and} \quad \int_{-\infty}^{\infty} \delta(x)dx = 1$$

From $\alpha^2 = \dfrac{2mE}{\hbar^2}$ and $\beta^2 = \dfrac{2m(V_0 - E)}{\hbar^2}$

$$\frac{\beta^2 + \alpha^2}{2\beta\alpha} = \frac{mV_0}{\beta\alpha\hbar^2}$$

$$\frac{mV_0}{\beta\alpha\hbar^2}\beta b sin\alpha a + cos\alpha a = coska \implies \frac{mV_0 b}{\alpha\hbar^2} sin\alpha a + cos\alpha a = coska$$

$$\implies \frac{mV_0 ba}{\hbar^2 \alpha a} sin\alpha a + cos\alpha a = coska$$
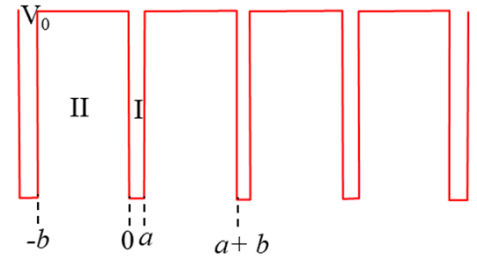
Kronig-Penney Model

$$\frac{mV_0 ba}{\hbar^2 \alpha a} \, sin\alpha a + cos\alpha a = coska$$

$$\frac{mV_0 ba}{\hbar^2} \frac{sin\alpha a}{\alpha a} + cos\alpha a = coska$$

Let $\frac{mV_0 ba}{\hbar^2} = P$

Which is a measure of the area $V_0 b$ of the potential barrier. Thus increasing P has the physical meaning of binding an electron more strongly to a particular potential well. In other words, P is the measure of strength with which electrons in a crystal are attracted to positive ions on the crystal lattice sites.

$$P\frac{sin\alpha a}{\alpha a} + cos\alpha a = coska$$

This is the condition which must be satisfied for the solutions to the wave equation to exit. Since $coska$ lies between +1 and -1, the left hand side should assume only those values of αa for which its values lies between +1 and -1. Such values of αa, therefore, represent wave like solutions of the type of $\psi(x) = e^{ikx}u_k(x)$ and are allowed. The other values of αa are not allowed.

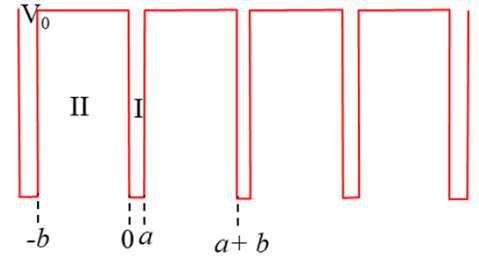# Kronig-Penney Model

$$\frac{mV_0ba}{\hbar^2\alpha a}\, sin\alpha a + cos\alpha a = cos ka$$

Let $\dfrac{mV_0ba}{\hbar^2} = P$

Which is a measure of the area V_0b of the potential barrier. Thus increasing P has the physical meaning of binding an electron more strongly to a particular potential well. In other words, P is the measure of strength with which electrons in a crystal are attracted to positive ions on the crystal lattice sites.

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Kronig-Penney Model

$$P\frac{sin\alpha a}{\alpha a} + cos\alpha a = cos ka \qquad P = \frac{3\pi}{2}$$

$$P\frac{sin\alpha a}{\alpha a} + cos\alpha a = cos ka$$
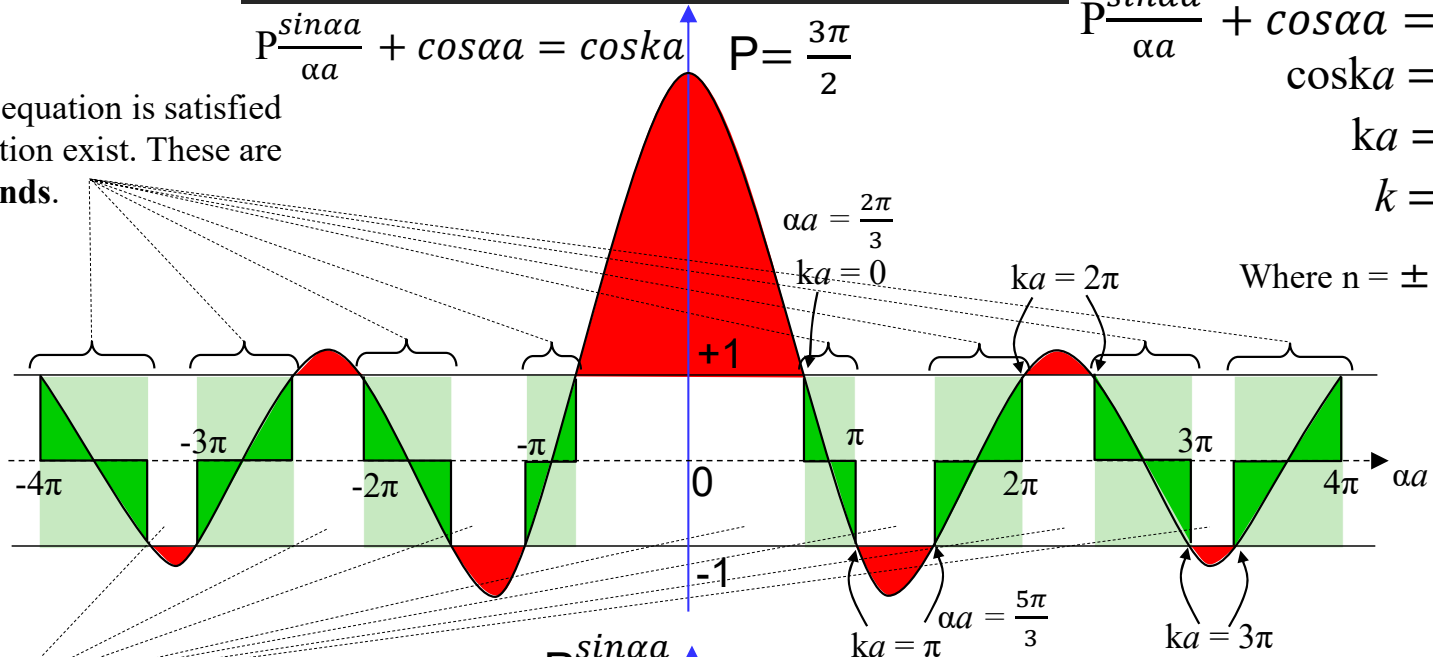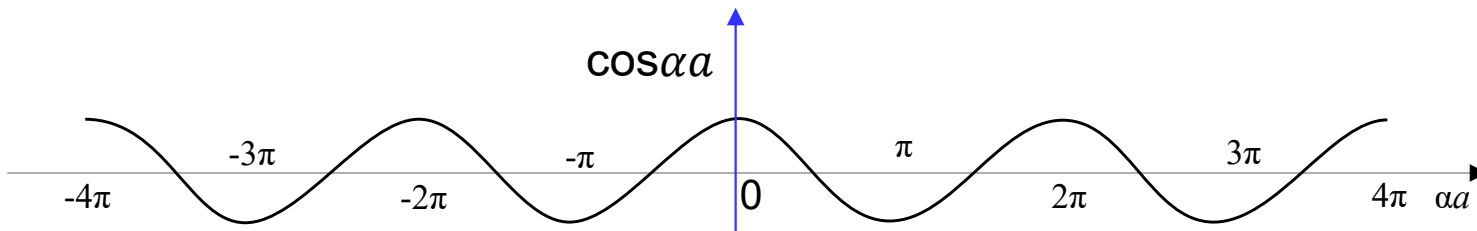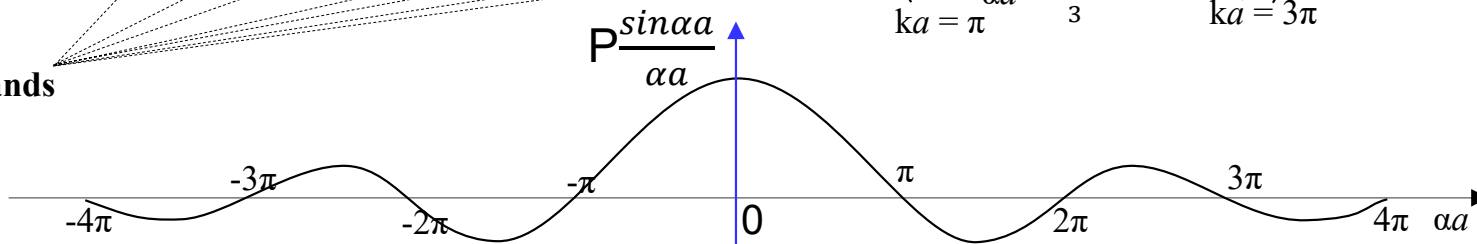$$cos ka = cos(\pm n\pi)$$
$$ka = \pm n\pi$$
$$k = \pm \frac{n\pi}{a}$$

Region where the equation is satisfied and therefore solution exist. These are called **allowed bands**.

Where n = $\pm 1, \pm 2, \pm 3$ ....)

$\alpha a = \frac{2\pi}{3}$

$ka = 0$

$ka = 2\pi$

Forbidden bands

$\alpha a = \frac{5\pi}{3}$

$ka = \pi$

$ka = 3\pi$

It suggest that the first forbidden band in the energy spectrum will appear at $k = \pm\frac{\pi}{a}$.
The second forbidden band will appear at $k = \pm\frac{2\pi}{a}$.

$P\frac{sin\alpha a}{\alpha a}$

$cos\alpha a$

Plot of $P\frac{sin\alpha a}{\alpha a}$+$cos\alpha a$ versus αa for P = $\frac{3\pi}{2}$. The vertical axis lying between -1 and +1, as indicated by the horizontal lines, represents the values acceptable to the left hand side.

In general, as the energy increases (αa increases because $\alpha^2 = \frac{2mE}{\hbar^2}$), each successive band gets wider, and each successive gap gets narrower.

Kronig-Penney Model

$$P = \frac{mV_0 ba}{\hbar^2}$$

$$P\frac{sin\alpha a}{\alpha a} + cos\alpha a$$

$$P = \frac{3\pi}{2}$$

$$P\frac{sin\alpha a}{\alpha a} + cos\alpha a = cos k a$$
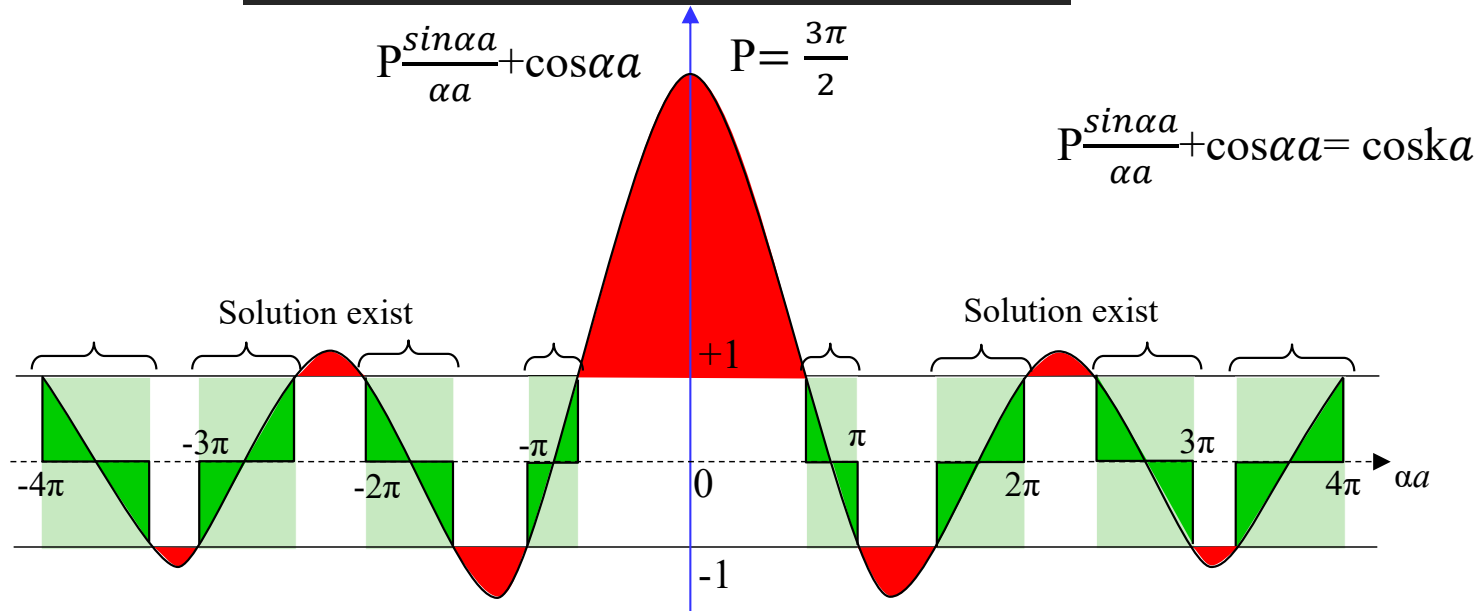
Since α^2 is proportional to the energy E (i.e. $\alpha^2 = \frac{2mE}{\hbar^2}$), the abscissa is measure of the energy. The following conclusions may be drawn from above figure:

- The energy spectrum of the electrons consists of alternate regions of allowed energy bands (solid lines on abscissa) and forbidden energy bands (broken lines).
- The width of the allowed energy bands increases with αa or the energy.
- The width of a particular allowed energy band decreases with increase in the P value i.e., with increase in the binding energy of the electrons.

$$P\frac{sin\alpha a}{\alpha a} + cos\alpha a = cos k a \implies \frac{sin\alpha a}{\alpha a} + \frac{cos\alpha a}{P} = \frac{cos k a}{P}$$

- As P→∞

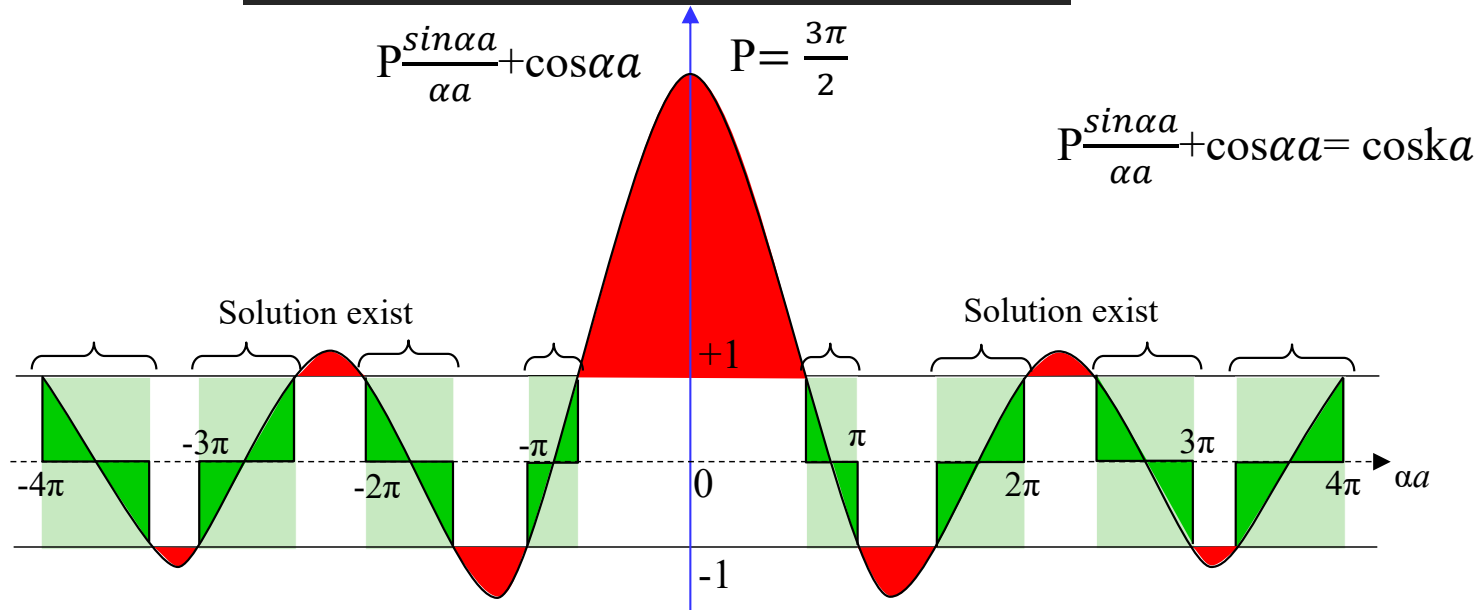$$\frac{sin\alpha a}{\alpha a} = 0 \implies sin\alpha a = 0 \implies sin\alpha a = sin(\pm n\pi) \implies \alpha a = \pm n\pi \implies \alpha^2 = \frac{n^2\pi^2}{a^2}$$

Where n is an integer

Kronig-Penney Model

$$P = \frac{mV_0 ba}{\hbar^2}$$

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$$P = \frac{3\pi}{2}$$

$$P\frac{sin\alpha a}{\alpha a} + cos\alpha a = cos k a$$

$$\alpha^2 = \frac{2mE}{\hbar^2}$$

$$\alpha^2 = \frac{n^2\pi^2}{a^2} \quad => \quad \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2} \quad \Rightarrow \quad E = \frac{\pi^2\hbar^2}{2ma^2}n^2$$

Where n is an integer
(i.e. n = 1, 2 ,3 ....)

This expression gives the energy levels of a particle in a constant potential box of atomic dimensions. This is what is expected physically as, for large P, the tunnelling through the barrier becomes difficult.

• As P→∞, the allowed energy bands are compressed into energy levels and a line spectrum is resulted. In such a case, $P\frac{sin\alpha a}{\alpha a} + cos\alpha a = cos k a$ has solutions only if $sin\alpha a = 0$

Kronig-Penney Model

In the other extreme case i.e. when P→0, the equation $P\frac{sin\alpha a}{\alpha a}+cos\alpha a= cos k a$ becomes

$$\cos\alpha a = \cos k a$$
$$\alpha = k$$
$$\alpha^2 = k^2$$

$$\boxed{\alpha^2 = \frac{2mE}{\hbar^2}}$$

$$\Rightarrow \frac{2mE}{\hbar^2} = k^2 \quad \Rightarrow E = \frac{k^2\hbar^2}{2m} \quad \Rightarrow E = \frac{P^2}{2m} \qquad \text{This is kinetic energy.}$$

Which is applicable to completely free electrons for which all the energies are allowed. This is again an expected result as, for P approaching zero, the electrons become free and, therefore, the free electron model involving quasi-continuous energy level becomes applicable.

Kronig-Penney Model

When P→0

$$\Rightarrow E = \frac{P^2}{2m}$$ This is kinetic energy.

Whe P→∞

$$\Rightarrow E = \frac{\pi^2 \hbar^2}{2ma^2} n^2$$

These results are summarized in following figure, which shows the energy spectrum as a function of P. On the extreme left, i.e. for P = 0, the energy spectrum is quasi-continuous and on the extreme right, i.e. for P = ∞, a line spectrum is resulted. For any other value of P, the position and width of the allowed and forbidden bands are obtained by drawing a vertical line.
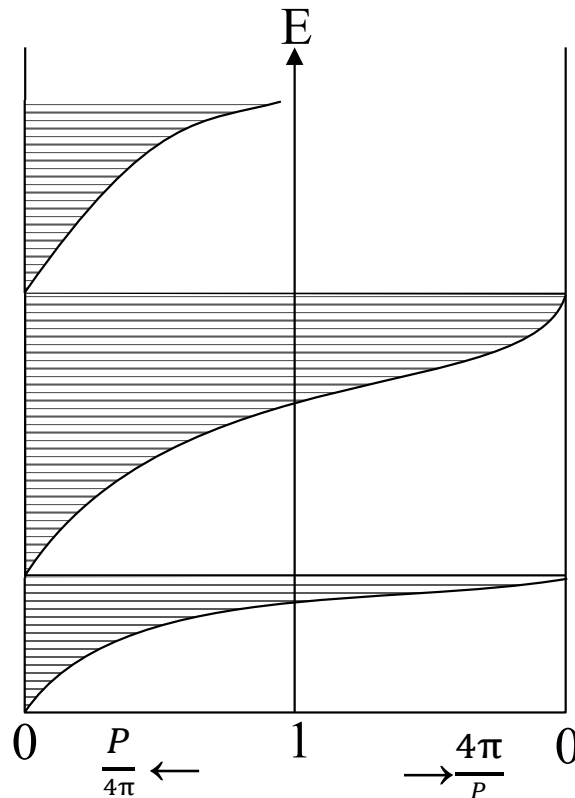
We have established the existence of bands and gaps, we can qualitatively explain the differences between metals, semiconductors, and insulators.

Allowed (shaded) and forbidden (open) energy ranges as a function of P

Wave equation as per Kronig and Penney model

$$\frac{mV_0ba}{\hbar^2\alpha a} \, sin\alpha a + cos\alpha a = cos k a \quad => \text{P}\frac{sin\alpha a}{\alpha a} + cos\alpha a = cos k a \qquad \boxed{\text{Where P} = \frac{mV_0ba}{\hbar^2}}$$

In this case, coska takes a specific value for each allowed energy value E.

coska is an even periodic function of k and remains unchanged if k is replaced by k+$\frac{2\pi n}{a}$, where n is an integer

It means that the energy E is also an even periodic function of k with period $\frac{2\pi}{a}$.

- Periodic representation of energy E for the first few allowed band.
- This can be obtained by a periodic repetition of the region $-\frac{\pi}{a}<k<\frac{\pi}{a}$ i.e., the first Brillouin zone and is known as the periodic or repeated zone scheme.
- In this scheme, k is not uniquely defined as, for each value of E, there exist a number of k values.
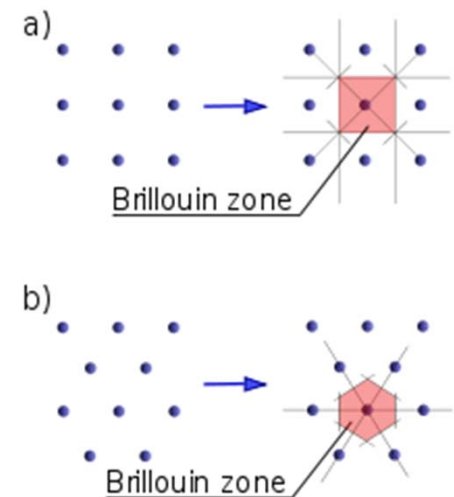- Therefore, it is convenient to introduce the following two schemes:
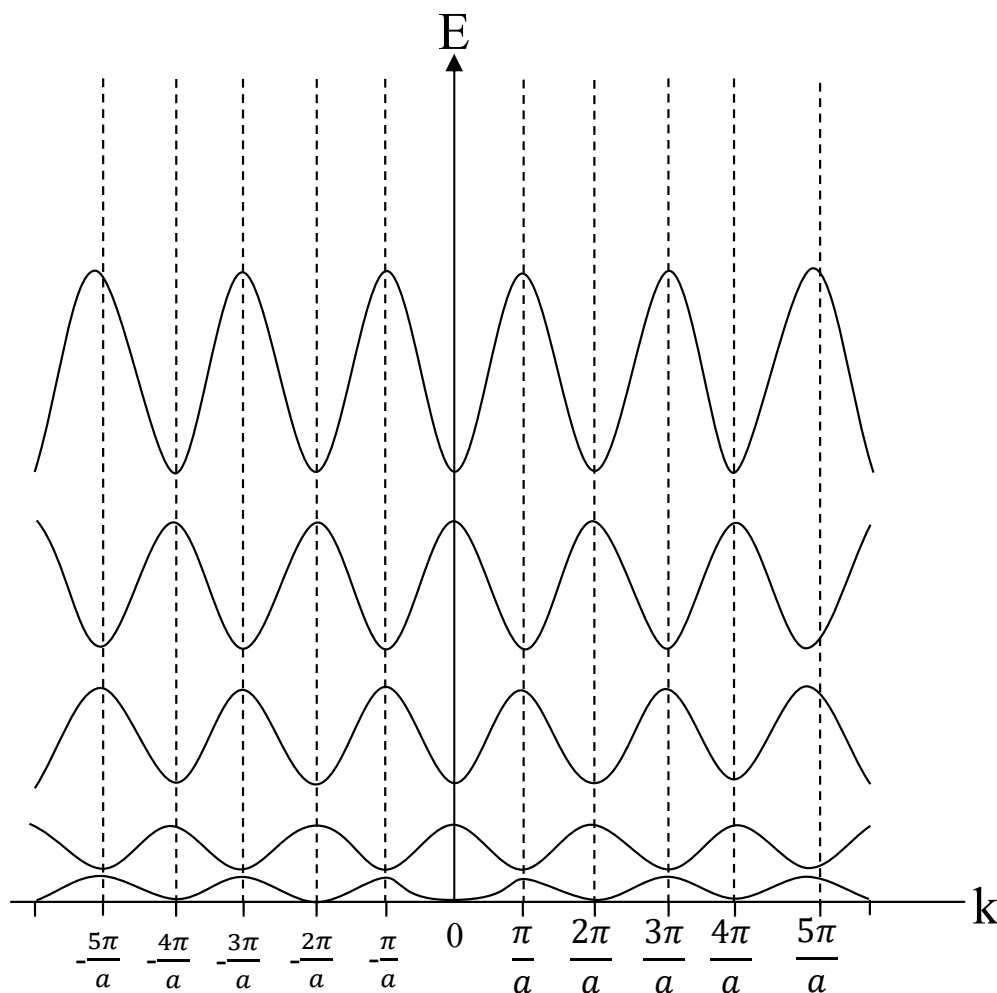
    (a) The extended zone scheme.
   (b) The reduced zone scheme.

In mathematics and solid-state physics, the first Brillouin zone is a uniquely defined **primitive cell in reciprocal space**. In the same way the Bravais lattice is divided up into **Wigner–Seitz cells in the real lattice**, the reciprocal lattice is broken up into Brillouin zones. The boundaries of this cell are given by planes related to points on the reciprocal lattice.

The reciprocal lattices (dots) and corresponding first Brillouin zones of (a) square lattice and (b) hexagonal lattice.

The repeated zone scheme

- A curve of E vs k in the extended zone scheme shown by red colour lines, while the dotted parabolic curve presented by blue color lines corresponds to free electrons in a constant potential.
- The E-k curve of the extended zone scheme has discontinuities at k $= \pm \frac{n\pi}{a}$, where n = 1, 2 ,3,..
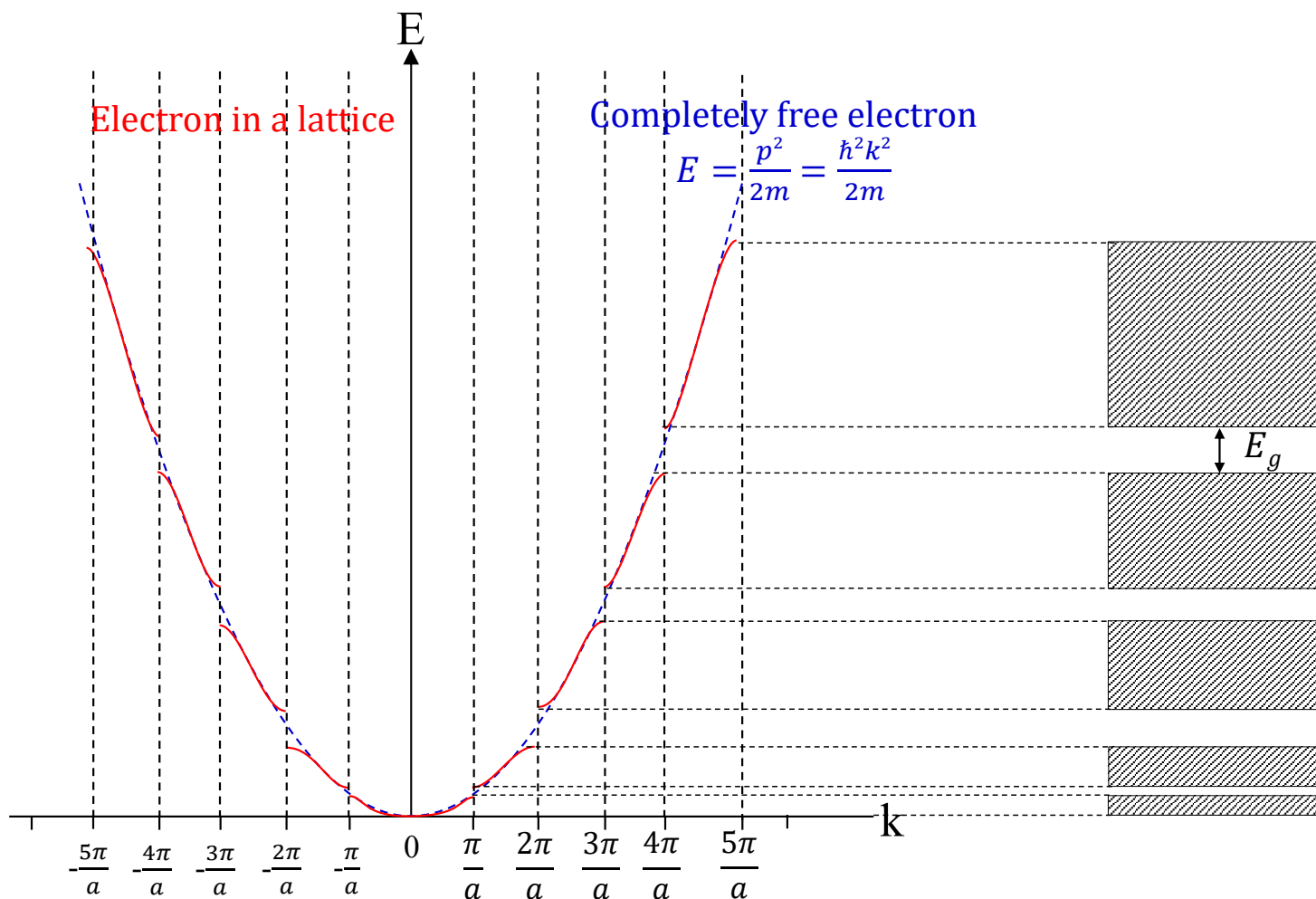
These values of k define the boundaries of the Brillouin zone extends from $-\frac{\pi}{a}$ to $\frac{\pi}{a}$, the second one extends from $\frac{\pi}{a}$ to $\frac{2\pi}{a}$ and from $-\frac{\pi}{a}$ to $-\frac{2\pi}{a}$, and so on.
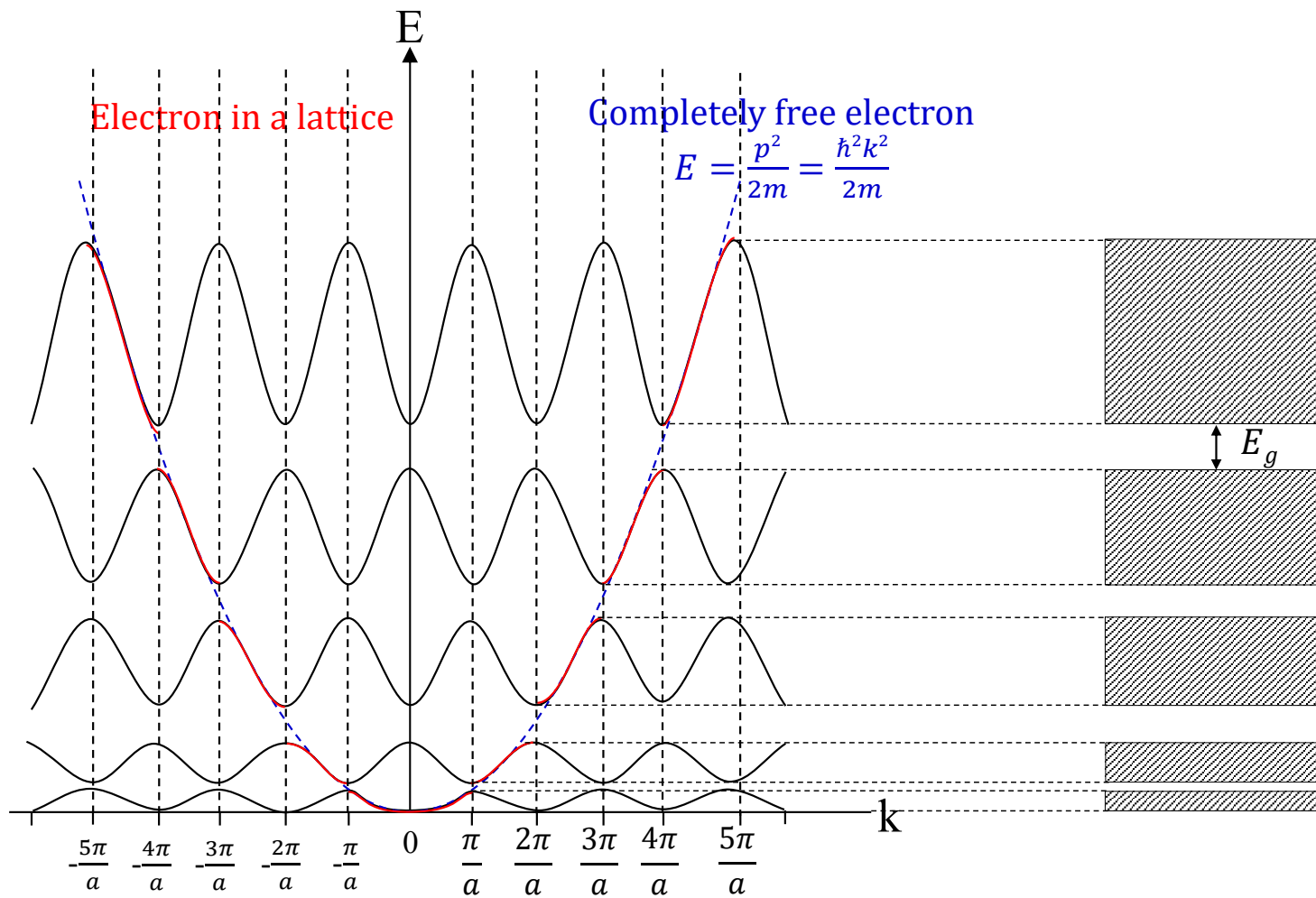
$$k = \pm \frac{n\pi}{a}$$

$$k = \frac{2\pi}{\lambda}$$

$$n\lambda = 2a$$

This is the Bragg's law of reflection for normal incidence.

Hence for k $= \pm \frac{n\pi}{a}$, the electrons suffer Bragg reflection which results in discontinuities in the E-k curve.

Electron in a lattice

Completely free electron

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

E_g

$\frac{5\pi}{a}$ $\frac{4\pi}{a}$ $\frac{3\pi}{a}$ $\frac{2\pi}{a}$ $\frac{\pi}{a}$ 0 $\frac{\pi}{a}$ $\frac{2\pi}{a}$ $\frac{3\pi}{a}$ $\frac{4\pi}{a}$ $\frac{5\pi}{a}$

The extended zone scheme

Electron in a lattice

Completely free electron

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

E_g

$-\frac{5\pi}{a}$ $-\frac{4\pi}{a}$ $-\frac{3\pi}{a}$ $-\frac{2\pi}{a}$ $-\frac{\pi}{a}$ 0 $\frac{\pi}{a}$ $\frac{2\pi}{a}$ $\frac{3\pi}{a}$ $\frac{4\pi}{a}$ $\frac{5\pi}{a}$

E

k

E-k curve in the reduced zone is obtained by reducing the contents of the other zones so as to correspond, in general, to the first zone, i.e. to the region $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$. The wave vector k belonging to this region is called the reduced wave vector.
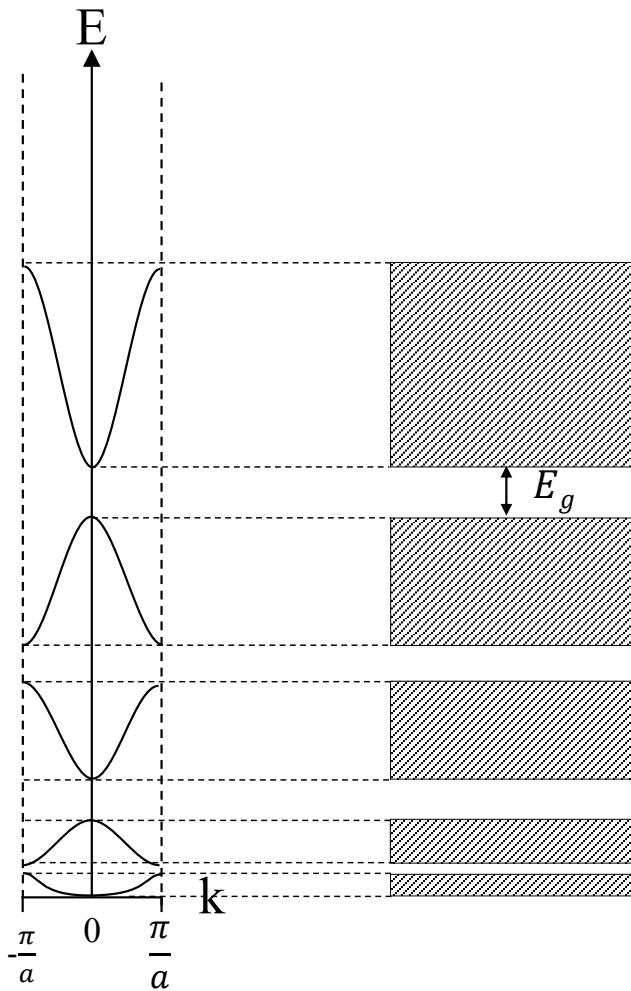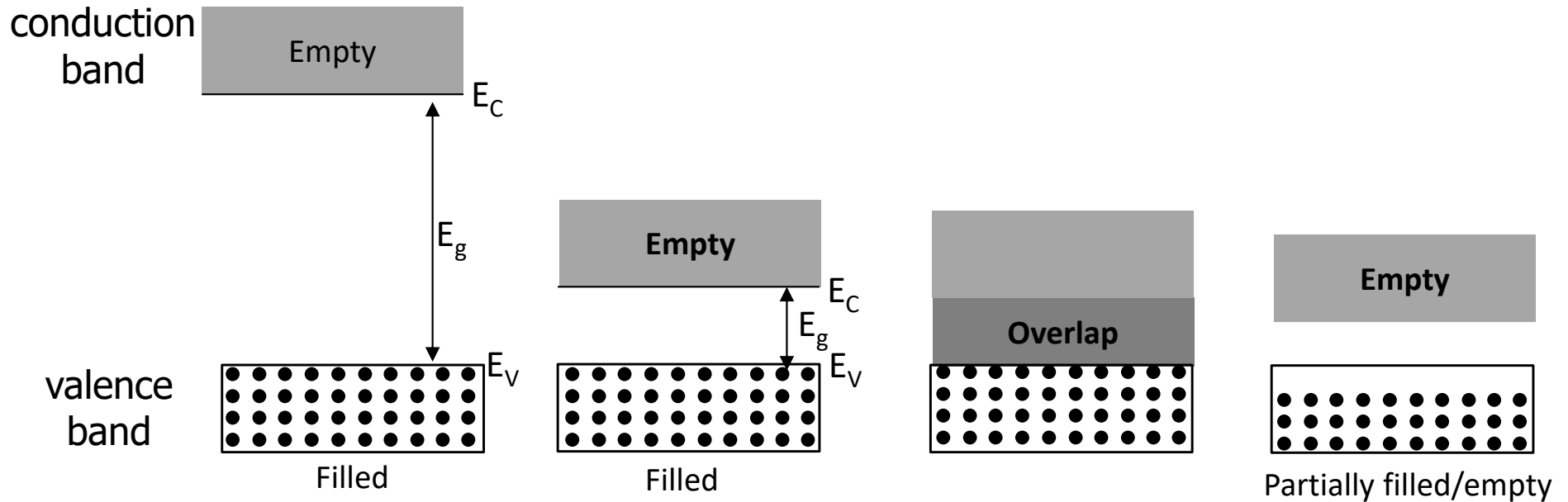

Reduced zone scheme

Energy vs Wave-Vector Relationship –Different Representations

Band structure of a one-dimensional crystal

(a) **Repeated zone scheme** *(b)* **Extended zone scheme** **(c) Reduced zone scheme** *(d)* **Energy band**
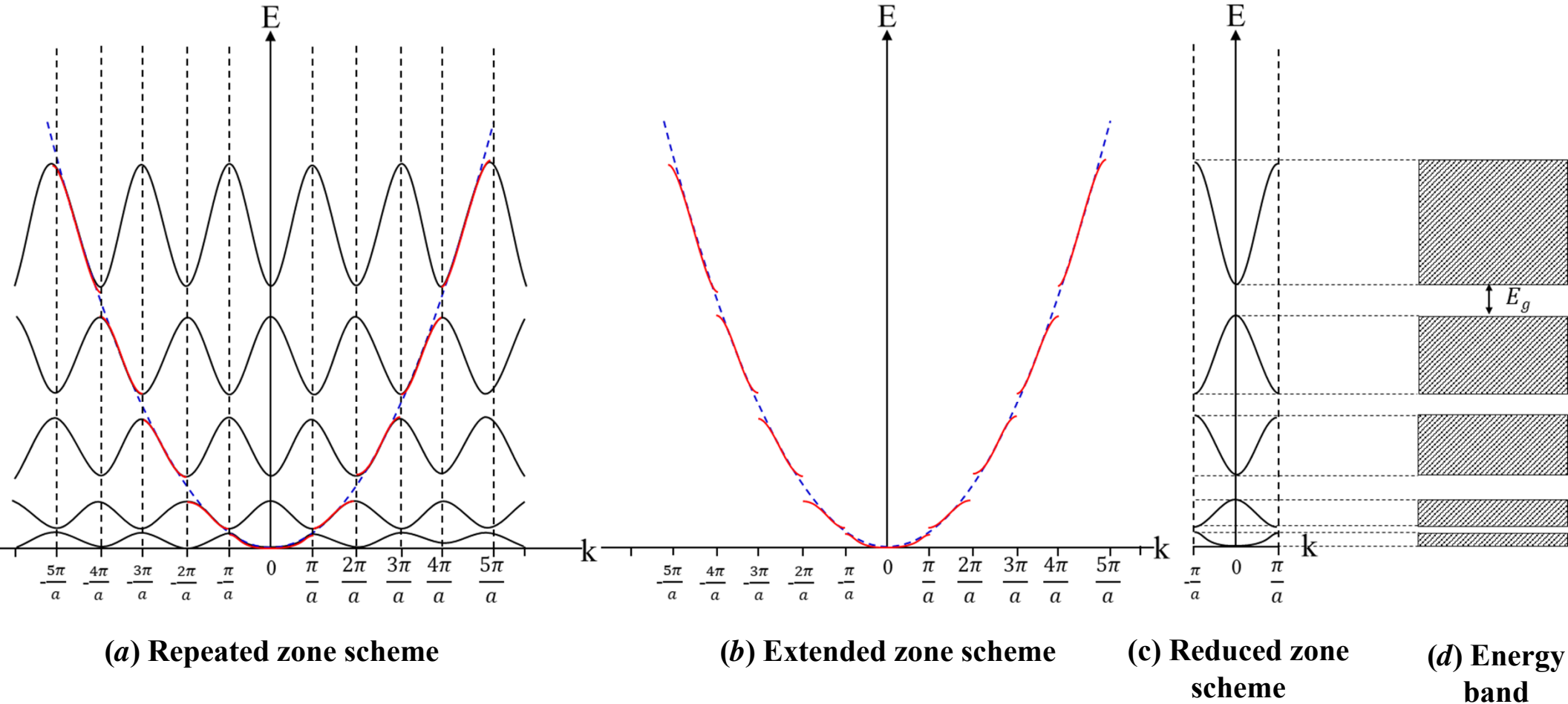
E *vs* k curves in three different zone schemes drawn on the same scale. The dotted parabolic curve of blue color corresponds to free electrons in a constant potential.

Classification of Material on the Basis of Energy Band Gap

conduction band

Empty

E_C

E_g

Empty

E_C

E_g

valence band

Empty

Overlap

Empty

Filled E_V

Filled E_V

Partially filled/empty

Band Theory and Conductivity

Band theory helps us to understand what makes a conductor, insulator, or semiconductor.

- Good conductors like copper can be understood using the free electron.

- It is also possible to make a conductor using a material with its highest band filled, in which case no electron in that band can be considered free.

- If this filled band overlaps with the next higher band, however (so that effectively there is no gap between these two bands) then an applied electric field can make an electron from the filled band jump to the higher level.
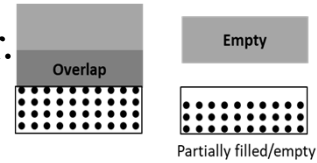
This allows conduction to take place, although typically with slightly higher resistance than in normal metals. Such materials are known as **semimetals**.

The band structures of insulators and semiconductors resemble each other qualitatively. Normally there exists in both insulators and semiconductors a filled energy band (referred to as the **valence band**) separated from the next higher band (referred to as the **conduction band**) by an energy gap.
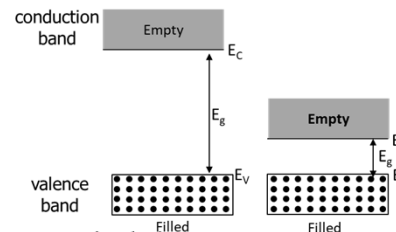
If this gap is at least several electron volts, the material is an **insulator**. It is too difficult for an applied field to overcome that large energy gap, and thermal excitations lack the energy to promote sufficient numbers of electrons to the conduction band.

For smaller energy gaps (around 1 electron volt), it is possible for enough electrons to be excited thermally into the conduction band, so that an applied electric field can produce a modest current. The result is a semiconductor.

# Classification of Materials on the Basis of Energy Band Gap

➤ Every solid has its own characteristic energy band structure. This variation in band structure is responsible for the wide range of electrical characteristics observed in various materials.

➤ For electrons to move under an applied electric field, there must be states available to them.

➤ A completely filled band cannot contribute to current transport; neither can a completely empty band.

➤ Thus, semiconductors at 0 K are perfect insulators.

➤ With thermal or optical excitation, some of these electrons can be excited from the valence band to the conduction band, and then they can contribute to the current transport process.

➤ At temperatures other than 0 K, the magnitude of the band gap separates an insulator from a semiconductor, e.g., at 300 K,   (diamond) = 5.6 eV (insulator), and   (Silicon) = 1.12 eV (semiconductor).

➤ Number of electrons available for conduction can be increased greatly in semiconductors by reasonable amount of thermal or optical energy.

➤ In metals, the bands are either partially filled, or they overlap, thus electrons and empty states coexist great electrical conductivity.

Classification of Materials on the Basis of Energy Band Gap
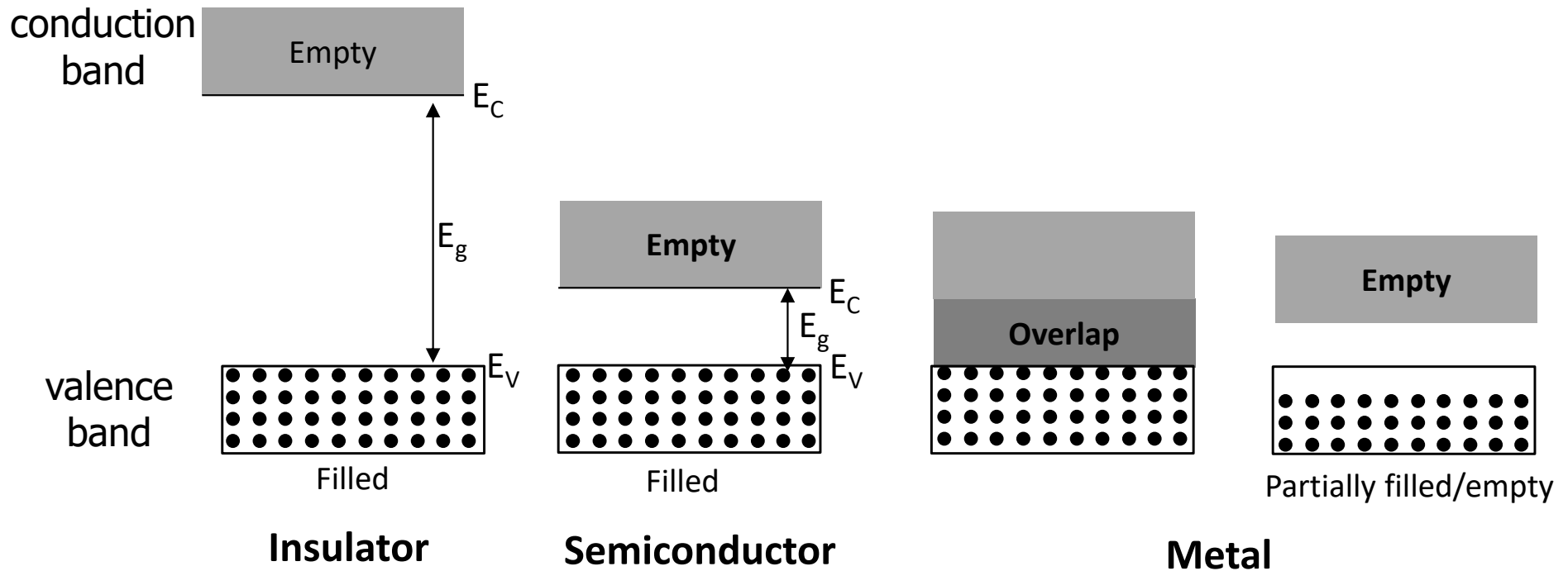
- The difference between insulators and semiconductor materials lies in the size of the band gap E_g, which is much smaller in semiconductors than in insulators.
- In metals the bands either overlap or are only partially filled. Thus electrons and empty energy states are intermixed with-in the bands so that electrons can move freely under the influence of an electric field.
- A rough rule of thumb: a band gap of less than 3 eV gives rise to a semiconductor.
- These band structures are schematic. Real bands are not boxes or lines.

Optical Properties of Solids
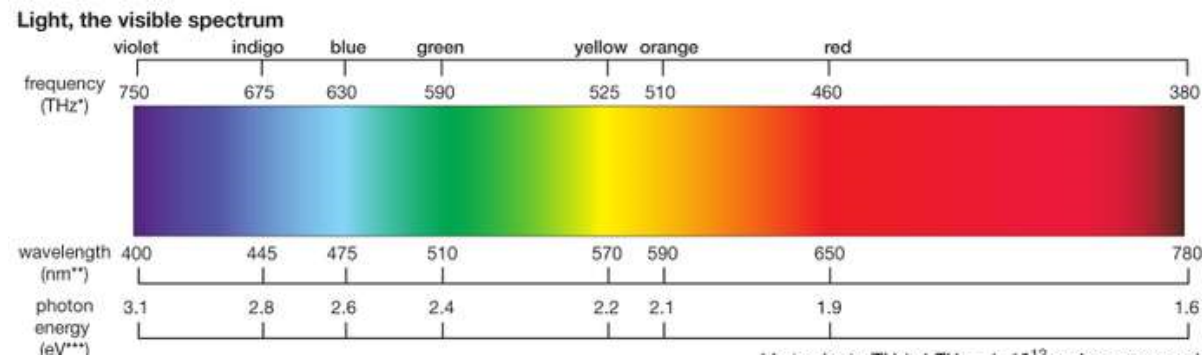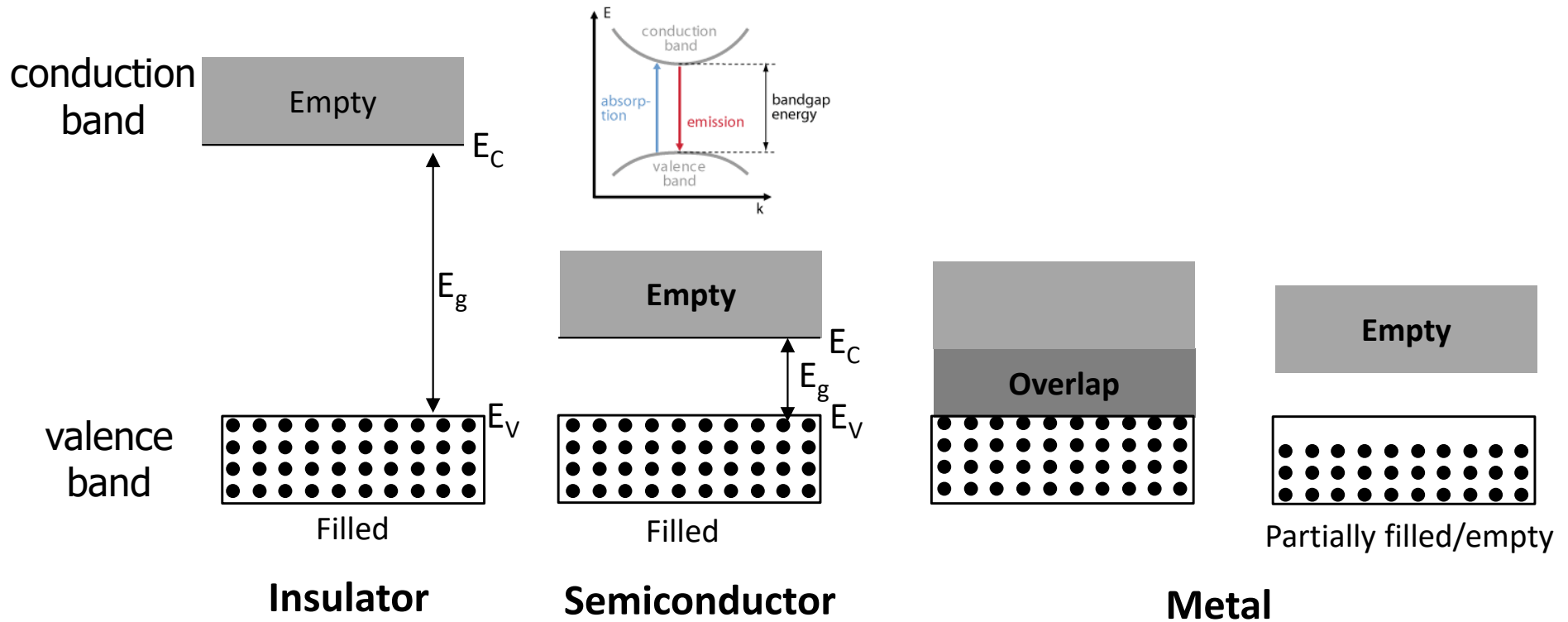
* **Optical properties are closely related to band structures.**

* **Visible photons have energies ranging from about 1 eV to about 3 eV.**

* **Metals can absorb visible photons because there are many empty states for electrons to move.**

* **In diamond, the valence band is full, and the conduction band is empty.**

* **A 3 eV photon cannot excite an electron across the 6 eV band gap. Diamond cannot absorb visible photons. Diamonds are transparent.**

Why does resistivity of semiconductors decrease with increase in temperature?

➢ At 0 K, the valence band is completely filled, and the conduction band is completely empty and therefore semi-conductors shows high resistivity (or behave like insulator) at low temperatures.

➢ As the temperature of the semi-conductor is increased, the electrons in the valence band gain sufficient thermal energies to jump to the conduction band. As the number of electrons in the conduction band increases, so conductivity increases and resistivity decreases

➢ After excitation to the conduction band, an electron is surrounded by a large number of empty states, e.g., the equilibrium number of EHPs at 300 K in Si is $\sim 10^{10}/cm^3$, whereas the Si atom density is $\sim 10^{22}/cm^3$

➢ The electrons in the conduction band are free to move about via the many available empty states.

$$n_i = N_C e^{-(E_c - E_i)/kT}$$

$$p_i = N_V e^{-(E_i - E_v)/kT}$$
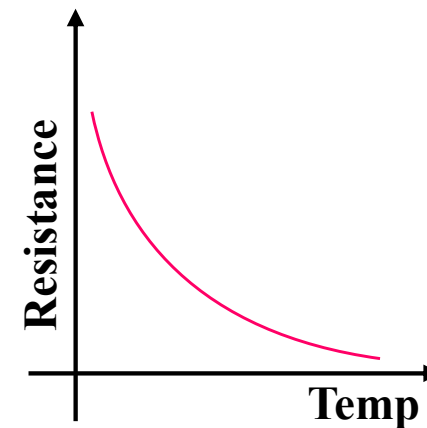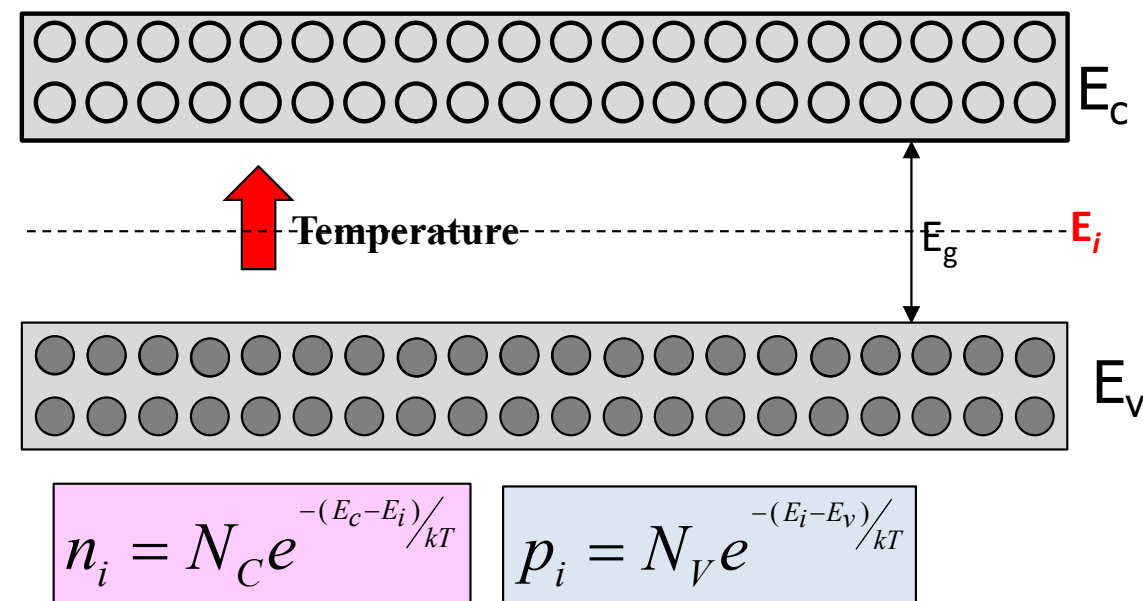
N_C and N_V are the effective density of states in the CB and VB, respectively

Intrinsic and Extrinsic Semiconductors

Intrinsic (pure or undoped) semiconductor: Intrinsic semiconductors are pure in form, no form of impurity is added to them

Extrinsic (or doped) semiconductor: An extrinsic semiconductor is one that has been doped.
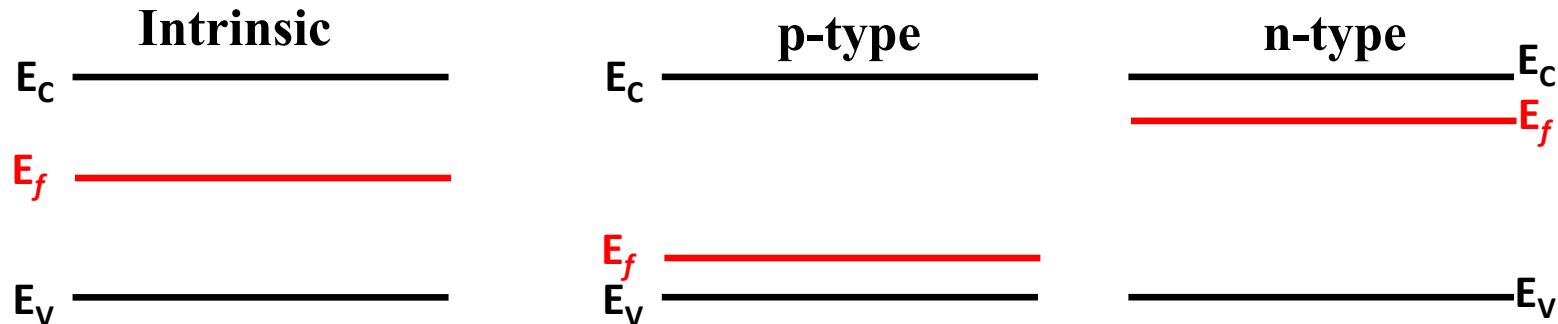
The **Fermi-Dirac distribution function** gives the probability of occupancy of an energy state E if the state exists.

$$f(E) = \frac{1}{1 + e^{(E-E_f)/kT}}$$

k : Boltzmann's constant

f(E) : Fermi-Dirac distribution function

E_f : Fermi level

➢ **An energy state at the Fermi level has a probability of ½ of being occupied by an electron.**

➢ **At 0K every available energy state upto E_f is filled with electron, and all states above E_f are empty.**

➢ **At T>0K, some probability exists for states above the Fermi level to be filled**