

Band Theory in Solids

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

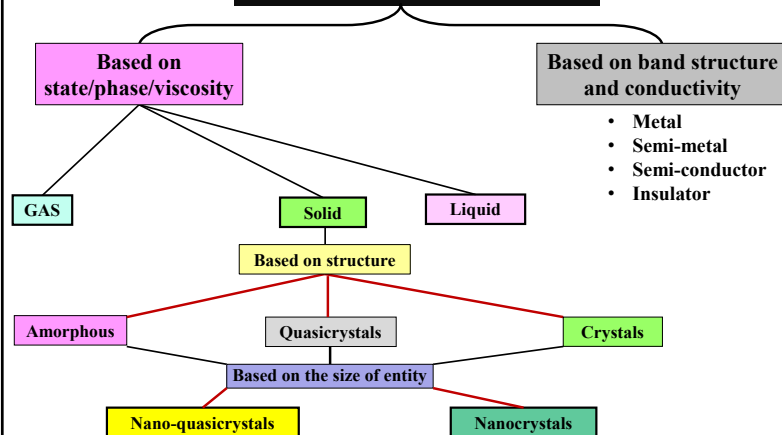
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References

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. Murugesan (**Chapter 46**)
4. *Concepts of Modern Physics* by Arthur Beiser (**Chapter 10**)

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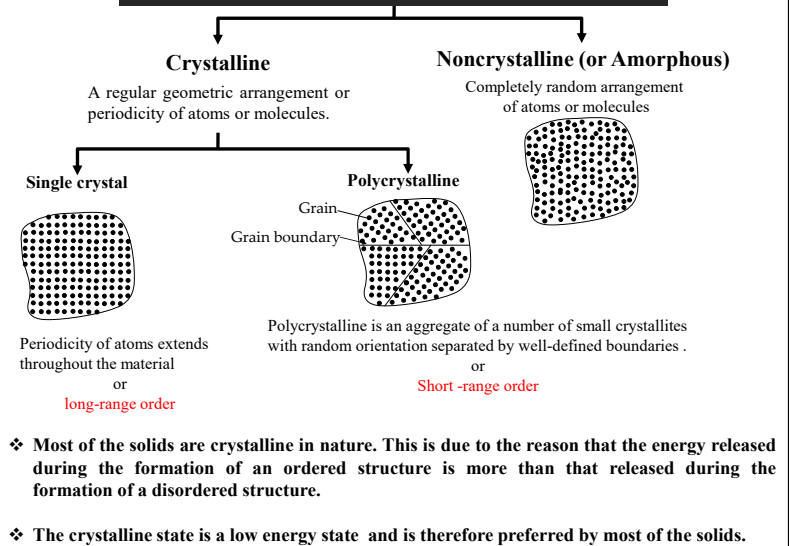
Classification of Materials



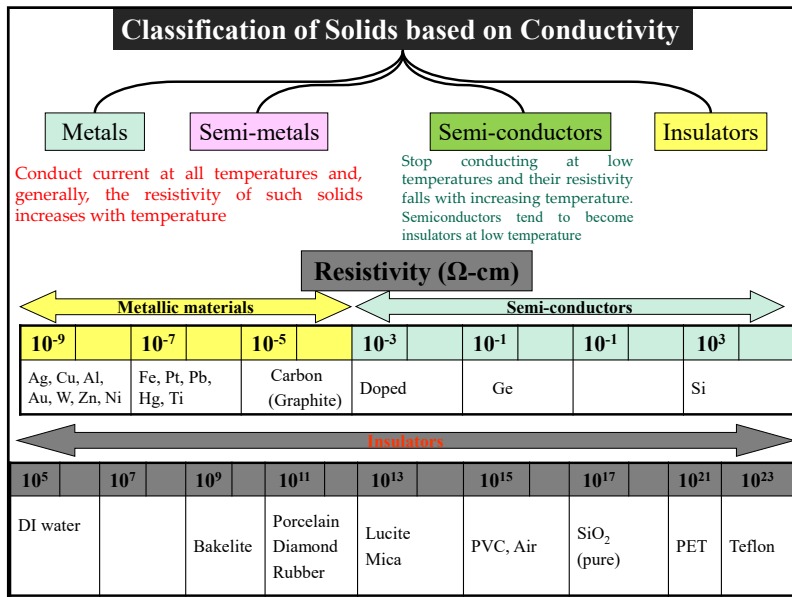
One way of classification does not interfere with another

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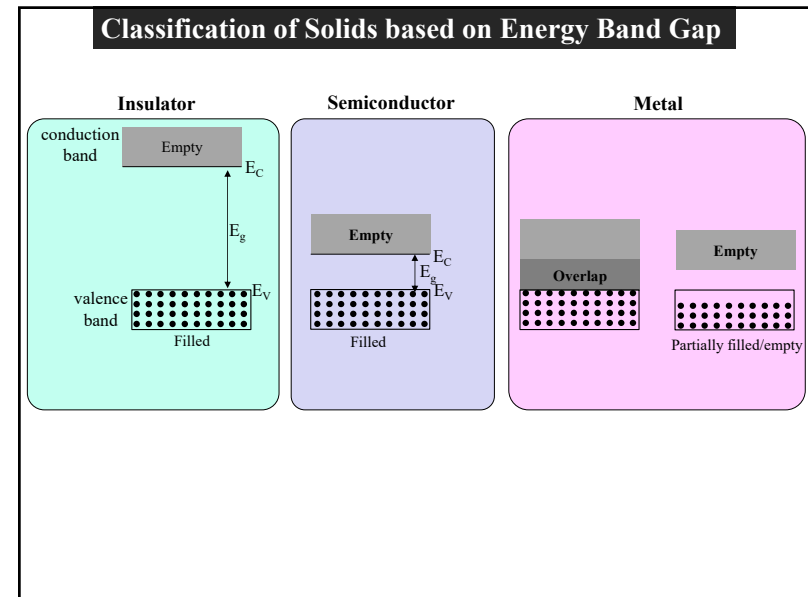
Classification of Solids based on Structures



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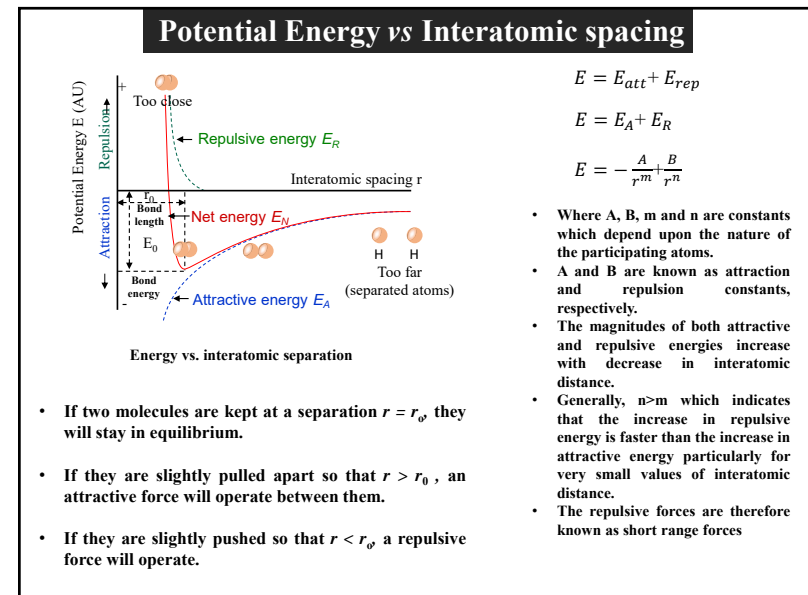


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Bonding Forces in Solids

- ❖ 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.

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Free Electron Theory

When we bring atoms together to form a metal

The atomic orbitals of atoms overlap slightly and the valence electrons become no longer attached to a particular ion, but belong to both neighbouring ions at the same time.

A valence 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 valence 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.

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Free Electron Theory

- Drude, in 1900, postulated that the metals consist of positive ion cores with the valence 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 electrons 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.

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Free Electron Theory

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 leads to a steady-state current, which is proportional to the applied voltage, obeying **Ohm's law**.

Conductor

(a)

Conductor (low temperatures)

(b)

Semiconductor

(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 $T \rightarrow 0$.

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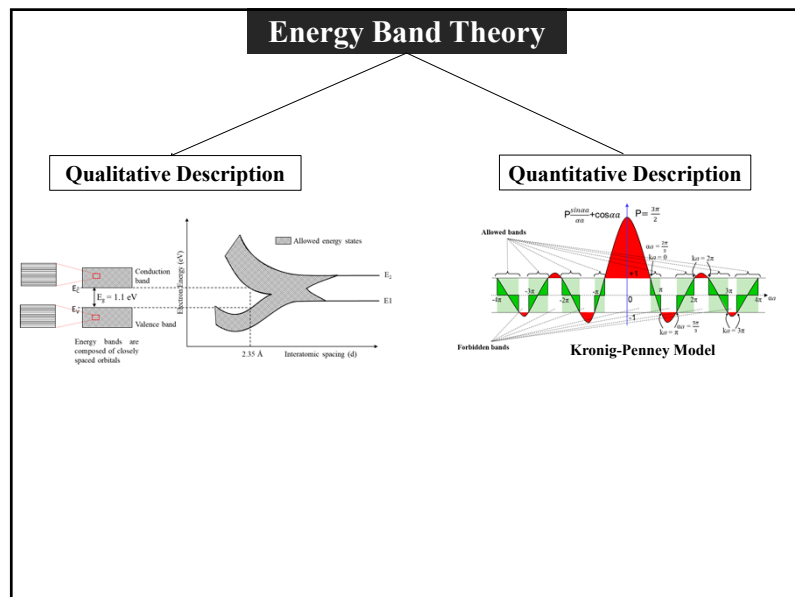
Drawback of Free-electron Model & Introduction of Band Theory of Solids

- ❖ 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.

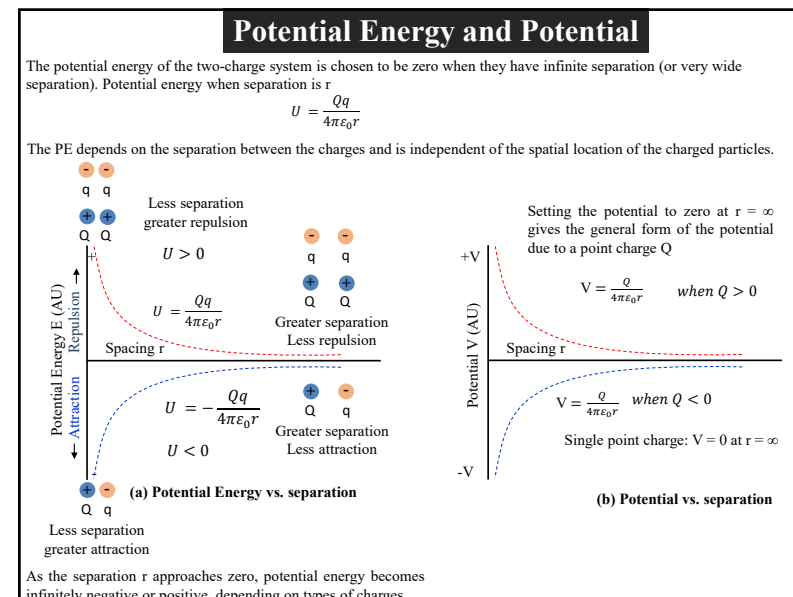
Resistivity vs. Temperature

- ❖ 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.

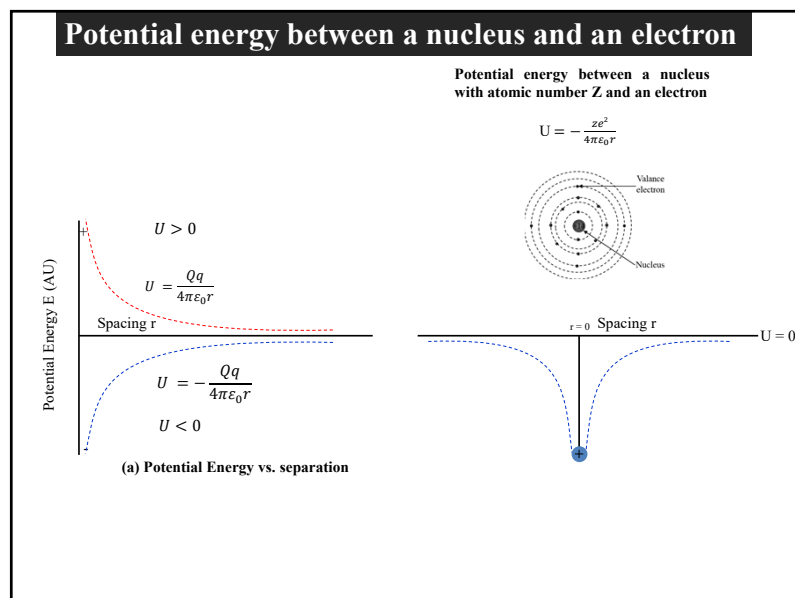
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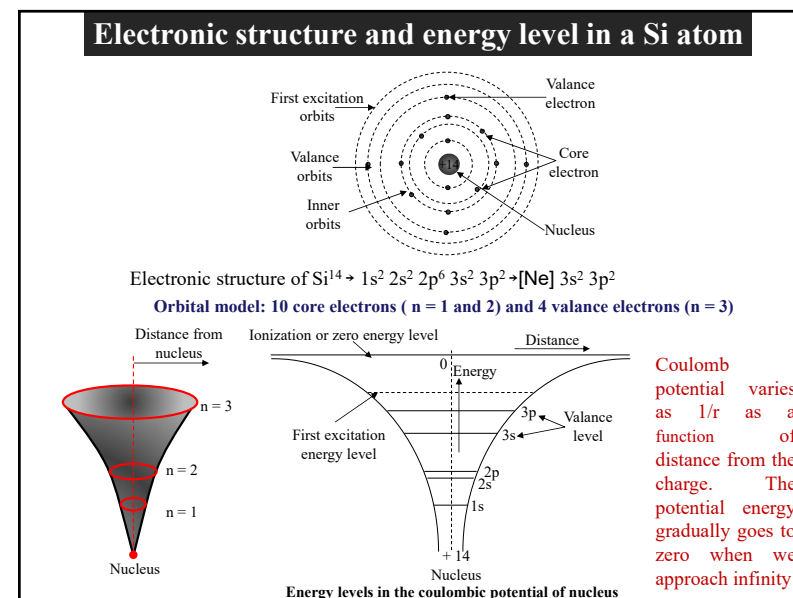
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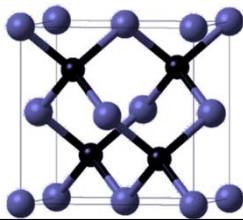
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Energy Band Theory

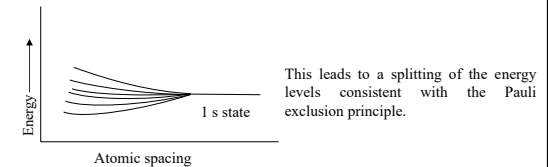
- When isolated atoms are brought together to form a solid, various interactions occur between neighboring atoms.
- The force of attraction and repulsion between atoms find a balance at the proper interatomic spacing for the crystal.
- In the process of interaction, important changes occur in the electron 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.



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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*



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

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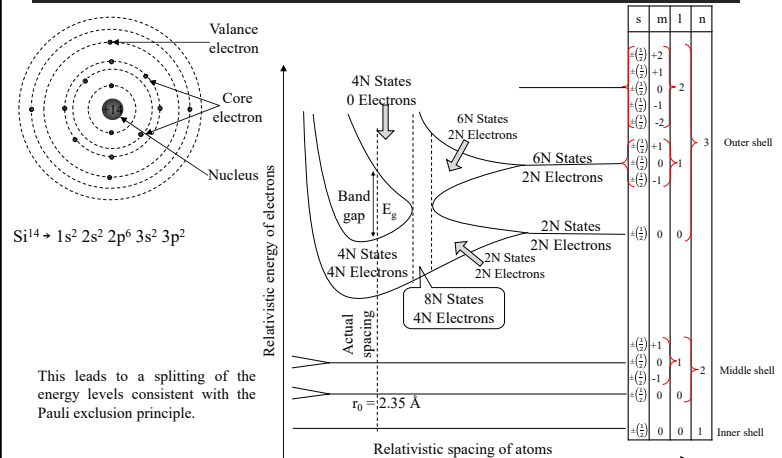
Development of Energy Bands in a Silicon Crystal



- 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, the **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**.

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Development of Energy Bands in a Silicon Crystal

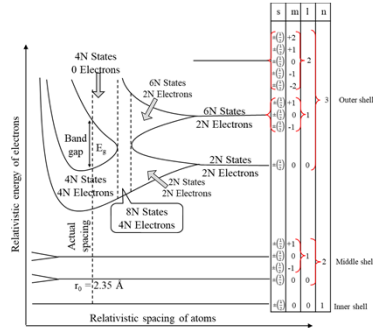


Energy levels in Si as a function of interatomic spacing. The core levels ($n = 1, 2$) in Si are completely filled with electrons. At the actual atomic spacing of the crystal, the $2N$ electrons in the 3s subshell and the $2N$ electrons in the 3p subshell undergo sp^3 hybridization, and all end up in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

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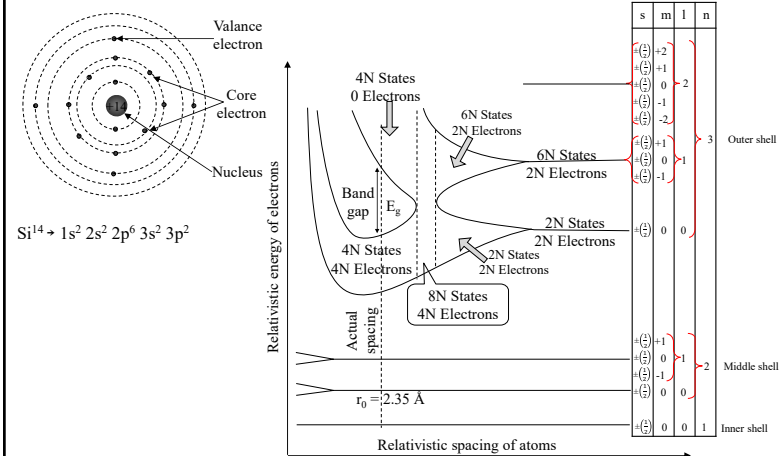
Energy Band Theory

- 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.



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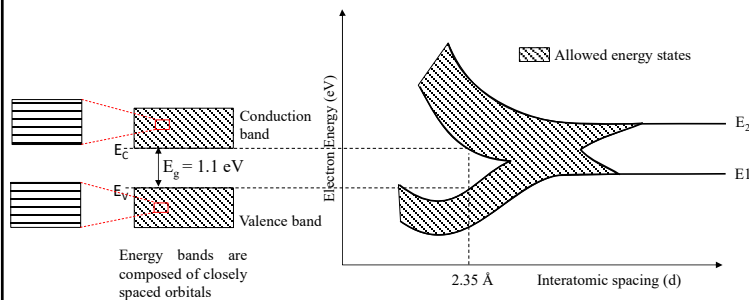
Development of Energy Bands in a Silicon Crystal



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_0 . At the equilibrium interatomic spacing r_0 , the '3s 3p' band splits again into two hybrid bands separated by an energy gap E_g .

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Development of Energy Bands in a Silicon Crystal

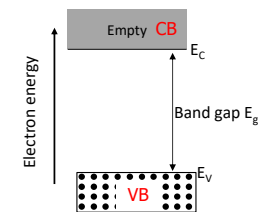


The energy of adjacent levels is so close together that they can be considered as a continuum, an energy band.

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_0 . At the equilibrium interatomic spacing r_0 , the band splits again into two hybrid bands separated by an energy gap E_g .

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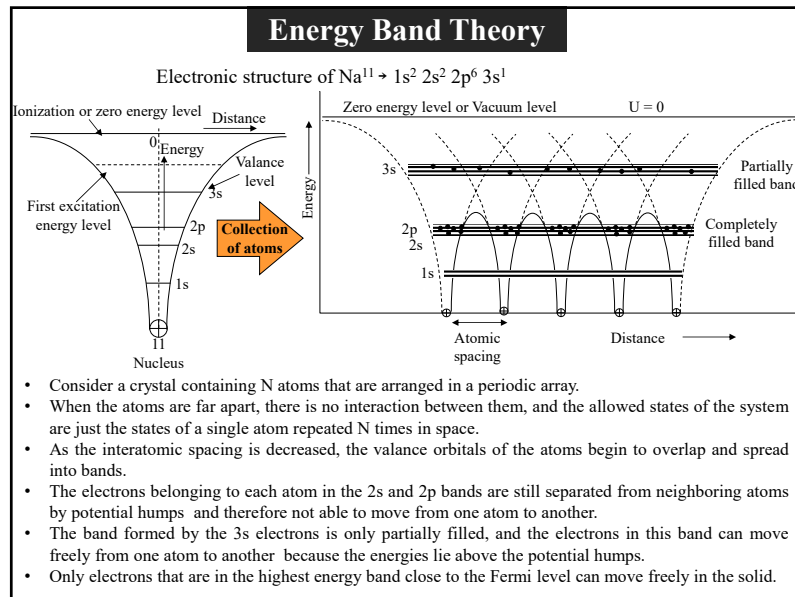
Energy Bands



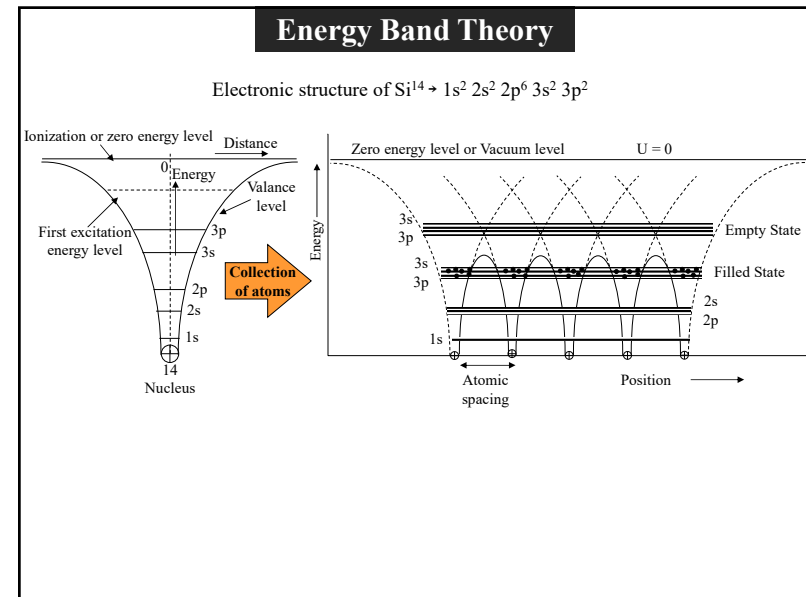
If a band is completely filled with electrons, and the band immediately above it is empty, the material has an energy **band gap**. This band gap is the energy difference between the highest occupied state in the valence band and the lowest unoccupied state in the conduction band. The material is either 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.

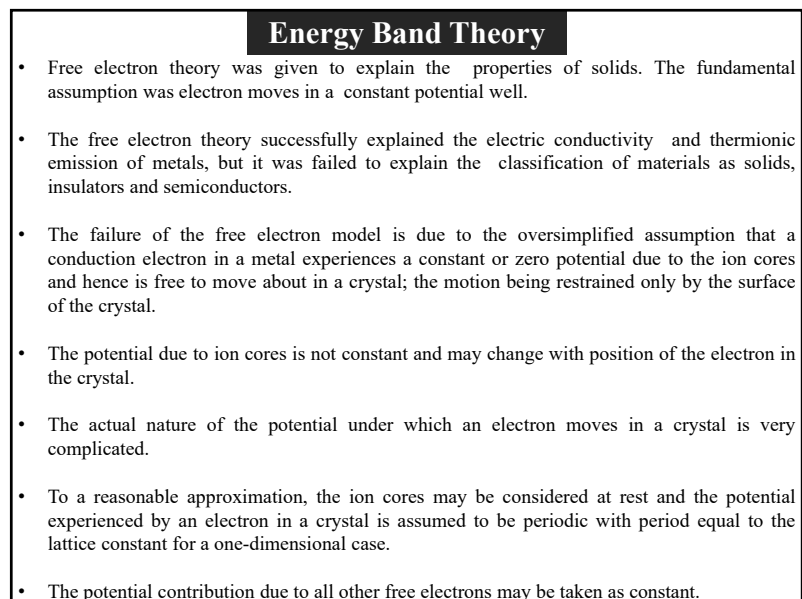
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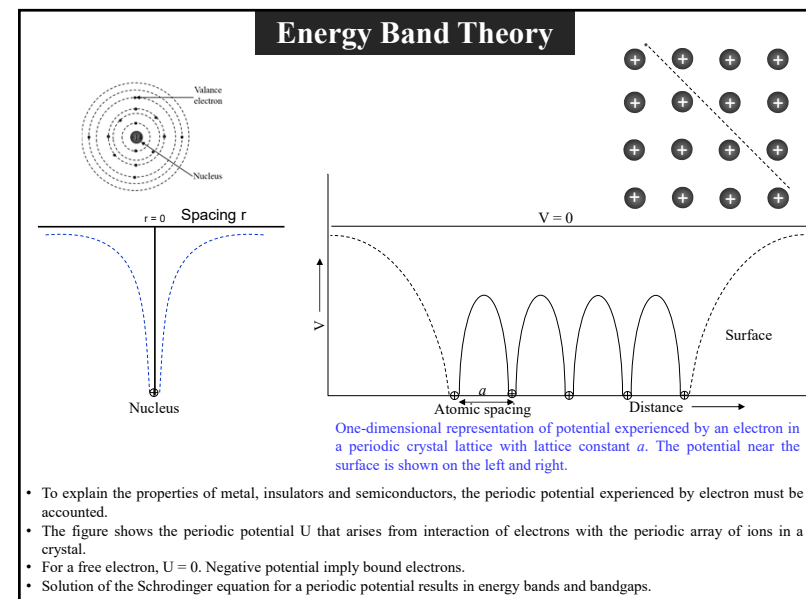
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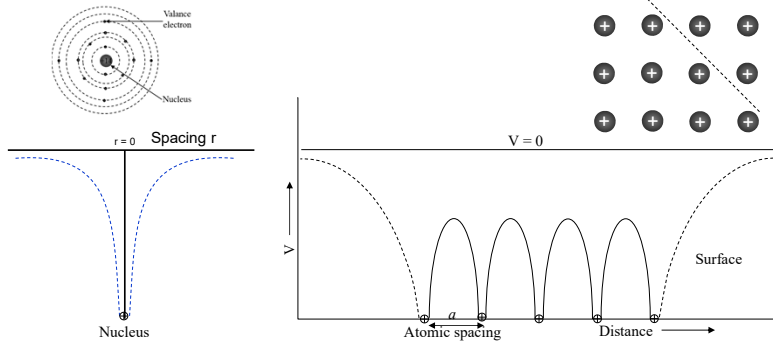


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Energy Band Theory



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-hand edge 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.

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Energy Band Theory

- The behaviour of an electron in the periodic 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.

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The Bloch Theorem

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

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

$$\text{Where } (E - V_0) = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m} = E_{kin}$$

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

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



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

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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.

$$\psi(x) = e^{\pm ikx} u_k(x) \quad \text{with } u_k(x) = u_k(x + a)$$

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.

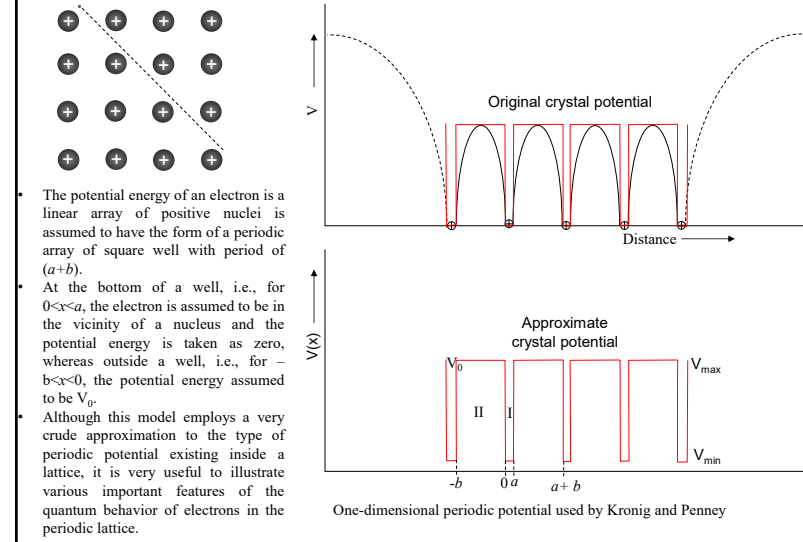
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Kronig-Penney Model

- 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.

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Kronig-Penney Model



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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

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

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

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

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

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

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

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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.

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

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

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

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

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

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

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

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

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

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Kronig-Penney Model

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

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

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

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

The general solutions of these equations are

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

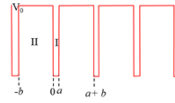
$$u_2 = Ce^{i(\beta-ik)x} + De^{-(\beta+ik)x} \quad \text{For II-Region } (-b < x < 0), V = V_0$$

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



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Kronig-Penney Model

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

$$u_1(0) = u_2(0)$$

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

According to the periodicity of $u_k(x)$

$$u_1(a) = u_2(-b)$$

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

Apply these boundary conditions to following equations

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

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

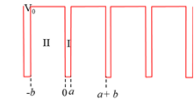
We get following four linear homogeneous equations

$$A + B = C + D$$

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

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

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



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Kronig-Penney Model

$$A + B = C + D$$

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

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

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

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.

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

On solving this determinant, we obtain

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

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Kronig-Penney Model

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

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 $\lim_{V_0 \rightarrow \infty, b \rightarrow 0} V_0 b$ is called the barrier strength.

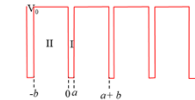
As $b \rightarrow 0$, $\sinh\beta b \rightarrow \beta b$ and $\cosh\beta b \rightarrow 1$.

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

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

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

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



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Kronig-Penney Model

$$\frac{mV_0b}{\alpha\hbar^2} \sin aa + \cos aa = \cos ka$$

$$\text{Let } \frac{mV_0ba}{\hbar^2} = P$$

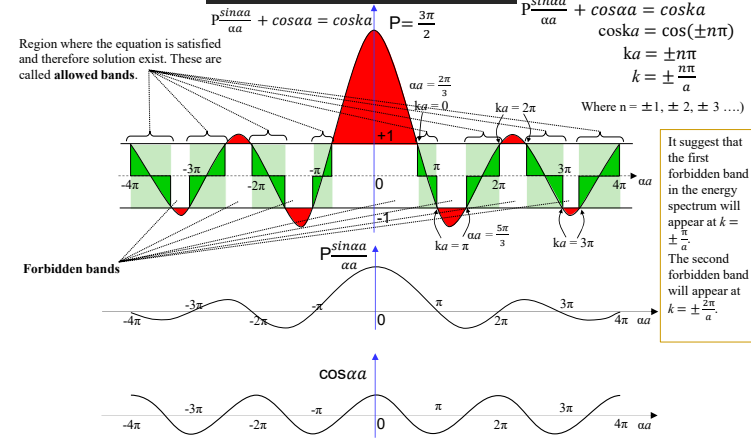
Which is a measure of the area V_0b of the potential barrier. Thus increasing P has the physical meaning of binding an electron more strongly to a particular potential well. In other words, P is the measure of strength with which electrons in a crystal are attracted to positive ions on the crystal lattice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

$$P \frac{\sin aa}{aa} + \cos aa = \cos ka$$

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

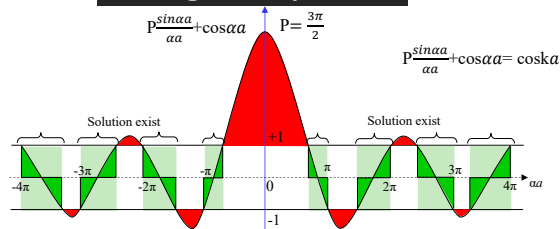
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Kronig-Penney Model



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Kronig-Penney Model



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

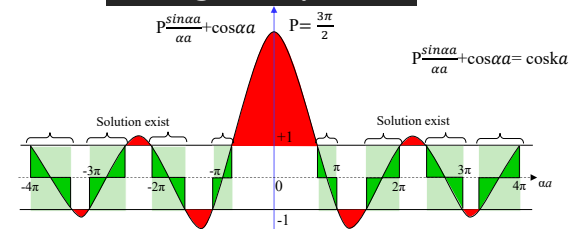
- The energy spectrum of the electrons consists of alternate regions of allowed energy bands (solid lines on abscissa) and forbidden energy bands (broken lines).
- The width of the allowed energy bands increases with aa or the energy.
- The width of a particular allowed energy band decreases with increase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

$$P \frac{\sin aa}{aa} + \cos aa = \cos ka \Rightarrow \frac{\sin aa}{aa} + \frac{\cos aa}{P} = \frac{\cos ka}{P}$$

- As $P \rightarrow \infty$
 $\frac{\sin aa}{aa} = 0 \Rightarrow \sin aa = 0 \Rightarrow \sin(\pm n\pi) \Rightarrow aa = \pm n\pi \Rightarrow a^2 = \frac{n^2\pi^2}{a^2}$
 Where n is an integer

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Kronig-Penney Model



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

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

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 $P \rightarrow \infty$, the allowed energy bands are compressed into energy levels and a line spectrum is resulted. In such a case, $P \frac{\sin aa}{aa} + \cos aa = \cos ka$ has solutions only if $\sin aa = 0$

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Kronig-Penney Model

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

$$\cos \alpha a = \cos ka$$

$$\alpha = k$$

$$\alpha^2 = k^2$$

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

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

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.

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Kronig-Penney Model

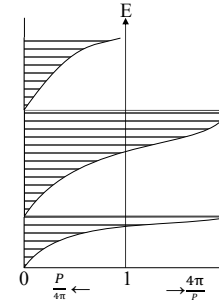
When $P \rightarrow 0$

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

When $P \rightarrow \infty$

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

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 $P = \infty$, 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.



Now that we have established the existence of bands and gaps, we can qualitatively explain the differences between metals, semiconductors, and insulators.

The position and occupation of the highest band or two of the solid determine the conductivity

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

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