

According to this we can write all crystal potential

$$V(r) = V_i(r) + V_e(r) \longrightarrow (1)$$

Bloch proved the important theorem that the solution of the Schrodinger equation for a periodic potential must be of a special form

$$\left[\frac{\hbar^2}{2m} \nabla^2 - eV(r) \right] \psi = E\psi \longrightarrow (2)$$

Periodic potential for conduction electron

$$U(r) = -eV(r) \longrightarrow (3)$$

Substitute 3 in 2 we get

$$\left[\frac{\hbar^2}{2m} \nabla^2 - U(r) \right] \psi = E\psi \longrightarrow (4)$$

Solution of Bloch function gives twotype of solution

$$\Psi(r) = U_k(r) e^{\pm \mu \cdot r} \longrightarrow (5)$$

$$\Psi(r) = U_k(r) e^{\pm i \cdot k \cdot r} \longrightarrow (6)$$

The Kronig-Penney Model

In the previous section, we discussed qualitatively the spitting of allowed electron energies as atoms are brought together to form a crystal. The concept of allowed and forbidden energy bands can be developed more rigorously by considering quantum mechanics and Schrodinger's wave equation. It may be easy for the reader to "get lost" in the following derivation, but the result forms the basis for the energy-band theory of semiconductors.

The potential function of a single, no interacting, one-electron atom is shown in Figure 3.5a. Also indicated on the figure are the discrete energy levels allowed for the electron. Figure 3.5b shows the same type of potential function for the case when several atoms are in close proximity arranged in a one-dimensional array. The potential functions of adjacent atoms overlap, and the net potential function for this case is shown in Figure 3.5c. It is this potential function we would need to use in Schrodinger's wave equation to model a one-dimensional single-crystal material.

The solution to Schrodinger's wave equation, for this one-dimensional single crystal lattice, is made more tractable by considering a simple potential function.

Figure 3.6 is the one-dimensional Kronig-Penney model of the **periodic potential**

function, which is used to represent a one-dimensional single-crystal lattice. We need to solve Schrodinger's wave equation in each region. As with previous quantum mechanical problems, the more interesting solution occurs for the case when $E < V_0$, which corresponds to a particle being bound within the crystal. The electrons are contained in the potential wells, but we have the possibility of tunneling between wells. The Kronig-Penney model is an idealized periodic

potential representing a one-dimensional single crystal. but the results will illustrate many of the important features of the quantum behavior of electrons in ;r periodic lattice.

To obtain the solution to Schrodinger's wave equation, we make use of a mathematical theorem by Bloch. The theorem states that all one-electron wave functions,

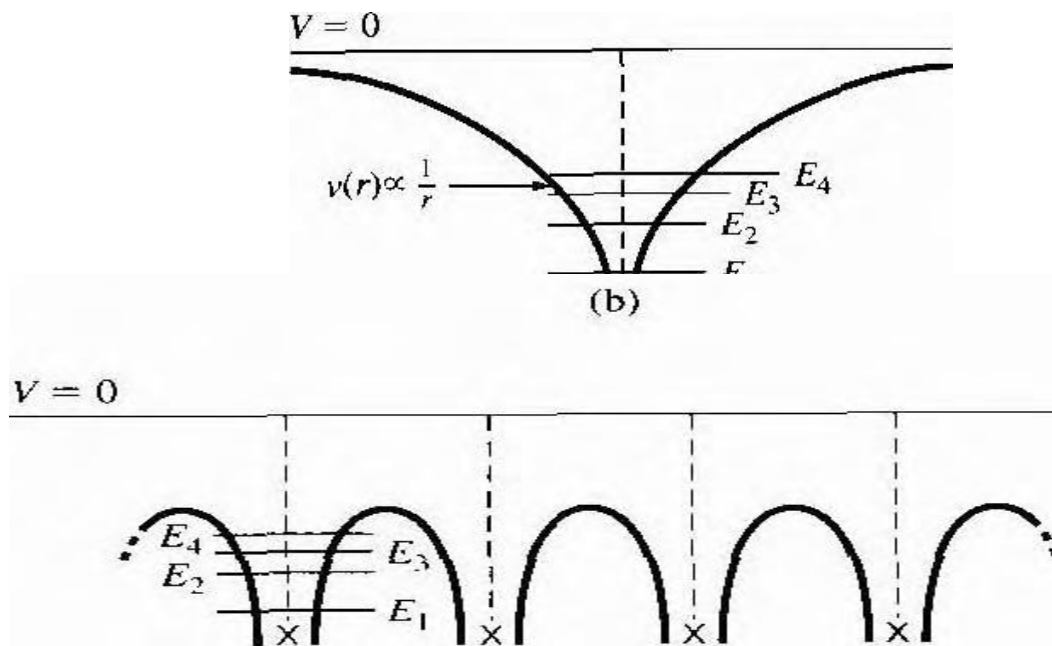


Figure 3 (a) Potential function of a single isolated atom. (b) Overlapping potential functions of adjacent atoms. (c) Net potential function of a one-dimensional single crystal.

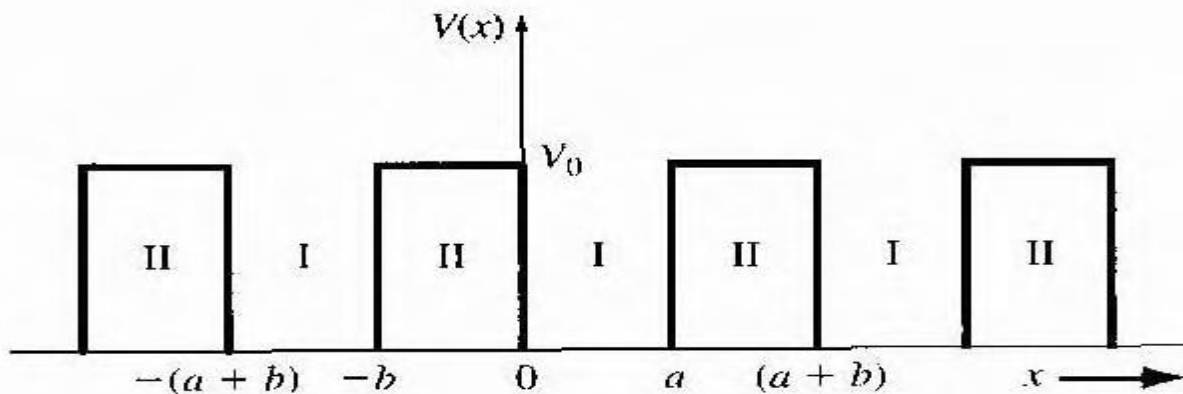


Figure 3 1 The one-dimensional periodic potential function of the Kronig-Penney model for problems involving periodically varying potential energy functions, must be of the form

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

The parameter k is called a constant of motion and will be considered in more detail as we develop the theory. The function $u(x)$ is a periodic function with period $(a + b)$. We stated in Chapter 2 that the total solution to the wave equation is the product of the time-independent solution and the time-dependent solution, or which may be written as

$$\psi(x, t) = u(x)\phi(t)e^{ikx}e^{-\frac{E}{\hbar}t}$$