SRM
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DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

18PYB103J –Semiconductor Physics

Lecture 3

KRONING PENNEY MODEL

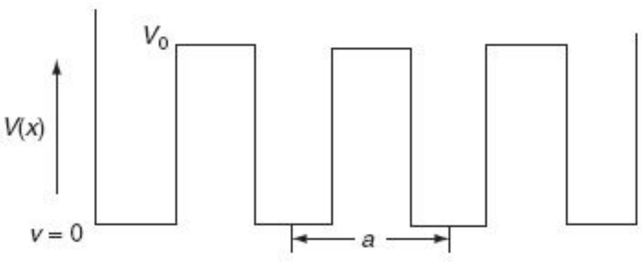
Kroning Penney model :

- According to Kroning and Penney the electrons move in a periodic square well potential.

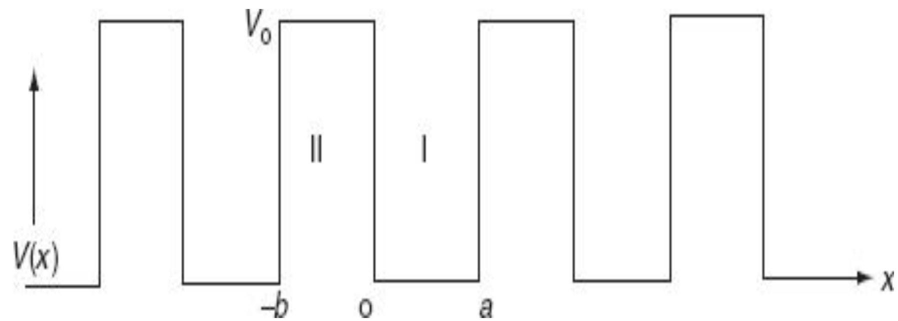
- This potential is produced by the positive ions (ionized atoms) in the lattice.

- The potential is zero near to the nucleus of positive ions and maximum between the adjacent nuclei. The variation of potential is shown in figure.

It is not easy to solve Schrödinger's equation with these potentials. So, Kroning and Penney approximated these potentials inside the crystal to the shape of rectangular steps as shown in Fig. (c). This model is called Kroning-Penney model of potentials.



(c)



The energies of electrons can be known by solving Schrödinger's wave equation in such a lattice. The Schrödinger time-independent wave equation for the motion of an electron along X-direction is given by:

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

The energies and wave functions of electrons associated with this model can be calculated by solving time-independent one-dimensional Schrödinger's wave equations for the two regions I and II as shown in Fig

The Schrödinger's equations are:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$ for 0<x<a............(2)

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left[E - V_o\right]\psi = 0$$ for -b<x<0............(3)

We define two real quantities (say) α and β such that:

$$\alpha^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad \beta^2 = \frac{2m}{\hbar^2}\left(V_0 - E\right) \quad \text{\_\_\_\_\_\_\_\_\_\_} \quad (5.43)$$

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0$$ for 0<x<a

$$\frac{d^2\psi}{dx^2} - \beta^2\psi = 0$$ for -b<x<0

The total wave function is therefore of the form where u(x) is the periodic function as defined by u(x) = u(x + a), and k(x) is the wave number. Rewriting the wave function in such form allows the simplification of the Schrödinger equation, which we now apply to region I, between the barriers where V(x) = 0 and region II, the barrier region where $V(x) = V_0$:

In region I, Schrödinger's equation becomes:

$$\frac{d^2u_I(x)}{dx^2} + 2ik\frac{du_I(x)}{dx} + (\beta^2 - k^2)u_I(x) = 0 \text{ for } 0 < x < a\text{-}b$$

$$\beta = \frac{2\pi}{h}\sqrt{2mE}$$

While in region II, it becomes:

$$\frac{d^2u_{II}(x)}{dx^2} + 2ik\frac{du_{II}(x)}{dx} - (k^2 + \alpha^2)u_{II}(x) = 0 \text{ for } a\text{-}b < x < a$$

$$\alpha = \frac{2\pi}{h}\sqrt{2m(V_0 - E)}$$

$$u_I(x) = (A\cos\beta x + B\sin\beta x)e^{-ikx} \text{ for } 0 < x < a\text{-}b$$

$$u_{II}(x) = (C\cosh\alpha x + D\sin\alpha x)e^{-ikx} \text{ for } a\text{-}b < x < a$$

Since the potential, $V(x)$, is finite everywhere, the solutions for $u_I(x)$ and $u_{II}(x)$ must be continuous as well as their first derivatives. Continuity at $x = 0$ results in:

$$u_I(0) = u_{II}(0) \text{ so that } A = C$$

and continuity at $x = a\text{-}b$ combined with the requirement that $u(x)$ be periodic results in:

$$u_I(a-b) = u_{II}(-b)$$

so that

$$(A\cos\beta(a-b) + B\sin\beta(a-b))e^{-ik(a-b)} = (C\cosh\alpha b - D\sinh\alpha b)e^{ikb}$$

Continuity of the first derivative at $x = 0$ requires that:

$$\left.\frac{du_I(x)}{dx}\right|_{x=0} = \left.\frac{du_{II}(x)}{dx}\right|_{x=0}$$

The first derivatives of $u_I(x)$ and $u_{II}(x)$ are:

$$\frac{du_I(x)}{dx} = (A\beta\sin\beta x - B\beta\cos\beta x)e^{-ikx} - ik(A\cos\beta x + B\sin\beta x)e^{-ikx}$$

$$\frac{du_{II}(x)}{dx} = (C\alpha\sinh\alpha x + D\alpha\cosh\alpha x)e^{-ikx} - ik(C\cosh\alpha x + D\sinh\alpha x)e^{-ikx}$$

so that (2.3.15) becomes:

$$-B\beta - ikA = D\alpha - ikC$$

Finally, continuity of the first derivative at $x = a\text{-}b$, again combined with the requirement that $u(x)$ is periodic, results in:

$$\left.\frac{du_I(x)}{dx}\right|_{x=a-b} = \left.\frac{du_{II}(x)}{dx}\right|_{x=-b}$$

so that

$$\begin{aligned}
&(A\beta \sin\beta(a-b) - B\beta\cos\beta(a-b))e^{-ik(a-b)} \\
&-ik(A\cos\beta(a-b) + B\sin\beta(a-b))e^{-ik(a-b)} \\
&= (-C\alpha\sinh\alpha b + D\alpha\cosh\alpha b)e^{ikb} - ik(C\cosh\alpha b - D\sinh\alpha b)e^{ikb}
\end{aligned}$$

This equation can be simplified using equation (2.3.14) as:

$$(A\beta\sin\beta(a-b) - B\beta\cos\beta(a-b)) = (-C\alpha\sinh\alpha b + D\alpha\cosh\alpha b)e^{ika}$$

$$\begin{vmatrix}
1 & 0 & -1 & 0 \\
0 & \beta & 0 & \alpha \\
\cos\beta(a-b) & \sin\beta(a-b) & -\cosh\alpha b\exp ika & \sinh\alpha b\exp ika \\
\beta\sin\beta(a-b) & -\beta\cos\beta(a-b) & \alpha\sin\alpha b\exp ika & -\alpha\cosh\alpha b\exp ika
\end{vmatrix} = 0$$

three rows and column, while replacing $\cos\beta(a-b)$ by β_c, $\sin\beta(a-b)$ by β_s, $\cosh\alpha b\ e^{ika}$ by α_c and $\sinh\alpha b\ e^{ika}$ by α_s, which results in:

$$\begin{vmatrix} \beta & 0 & \alpha \\ \beta_s & -\alpha_c & \alpha_s \\ -\beta\beta_c & \alpha\alpha_s & -\alpha\alpha_c \end{vmatrix} = \begin{vmatrix} 0 & \beta & \alpha \\ \beta_c & \beta_s & \alpha_s \\ \beta\beta_s & -\beta\beta_c & -\alpha\alpha_c \end{vmatrix}$$

Working out the determinants and using $\beta_c^2 + \beta_s^2 = 1$, and $\alpha_c^2 - \alpha_s^2 = e^{2ika}$, one finds:

$$(\alpha^2 - \beta^2)\sinh\alpha b \sin\beta(a-b)\exp ika + 2\alpha\beta\cosh\alpha b\cos\beta(a-b)\exp ika = \alpha\beta$$

And finally, substituting β_c, β_s, α_c and α_s:

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