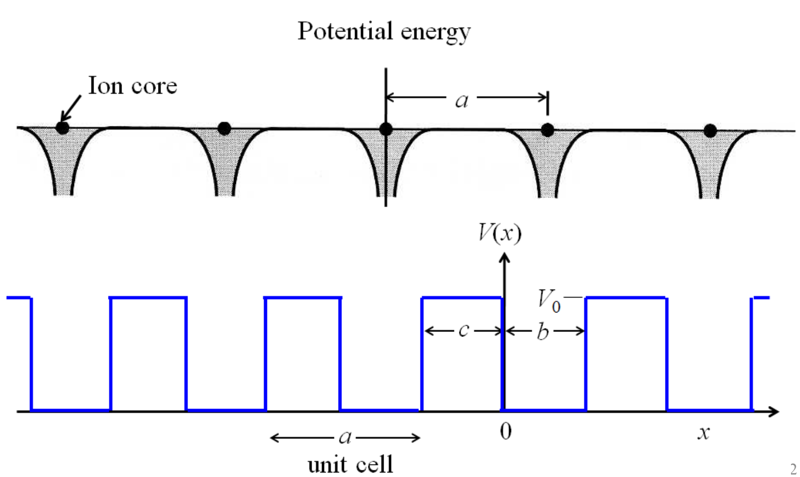
KRONIG-PENNY MODEL

1

Kronig-Penny Model: Periodic Potential

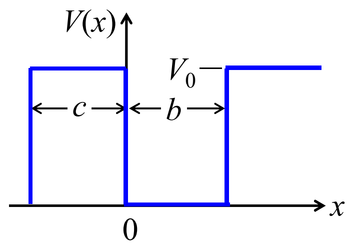
- One electron approximation: Each valence electron is considered independent and only acted upon by the periodic positive ions.



2

2

Schrodinger's Equation



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

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

- Wavefunction will be of Bloch form: $\psi(x)=e^{ikx}u(x)$

  → $u(x)$ has the periodicity of the lattice.

3

3

Schrodinger's Equation

- After substitution

$$\frac{d^2}{dx^2}e^{ikx}u(x)+\frac{2m}{\hbar^2}\left[\varepsilon-V(x)\right]e^{ikx}u(x)=0$$

$$\frac{d}{dx}\left[ike^{ikx}u(x)+e^{ikx}\frac{du(x)}{dx}\right]+\frac{2m}{\hbar^2}\left[\varepsilon-V(x)\right]e^{ikx}u(x)=0$$

$$(ik)^2e^{ikx}u(x)+ike^{ikx}\frac{du(x)}{dx}+ike^{ikx}\frac{du(x)}{dx}+e^{ikx}\frac{d^2u(x)}{dx^2}$$

$$+\frac{2m}{\hbar^2}\left[\varepsilon-V(x)\right]e^{ikx}u(x)=0$$

$$\frac{d^2u(x)}{dx^2}+2ik\frac{du(x)}{dx}-k^2u(x)+\frac{2m}{\hbar^2}\left[\varepsilon-V(x)\right]u(x)=0$$

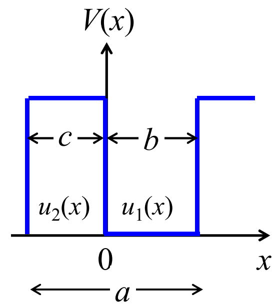
$$\frac{d^2u(x)}{dx^2}+2ik\frac{du(x)}{dx}-\left[k^2-\alpha^2+\frac{2mV(x)}{\hbar^2}\right]u(x)=0,\quad \alpha^2=\frac{2m\varepsilon}{\hbar^2}$$

4

4

Potential Well and Barrier

$$\frac{d^2u(x)}{dx^2} + 2ik\frac{du(x)}{dx} - \left[k^2 - \alpha^2 + \frac{2mV(x)}{\hbar^2}\right]u(x) = 0$$



$0 < x < b:$

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

$-c < x < 0:$

$$\frac{d^2u_2(x)}{dx^2} + 2ik\frac{du}{dx} - \left(k^2 - \beta^2\right)u_2(x) = 0$$

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

5

5

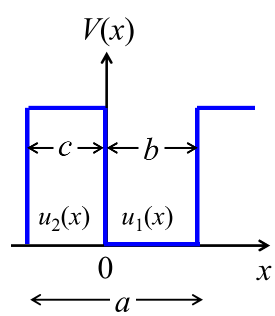
Solutions

$0 < x < b:$

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

$-c < x < 0:$

$$u_2(x) = Ce^{i(\beta - k)x} + De^{-i(\beta + k)x}$$



A, B, C, D are constants and must be determined.

Apply Boundary Conditions:

Wavefunctions and their derivatives must be continuous at all points.

6

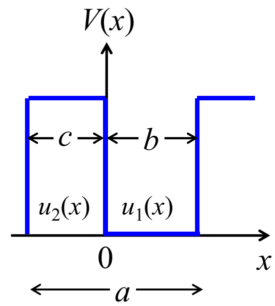
6

Boundary Conditions

- At $x = 0$

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

$$\Rightarrow \quad A + B = C + D$$



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

$$\Rightarrow \quad i(\alpha - k)A - i(\alpha + k)B = i(\beta - k)C - i(\beta + k)D$$

7

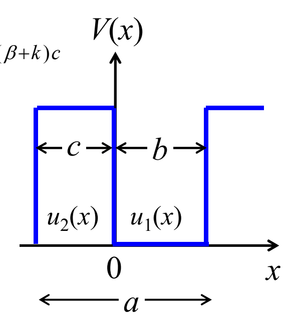
7

Boundary Conditions

- At $x = b$

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

$$\Rightarrow \quad Ae^{i(\alpha-k)b} + Be^{-i(\alpha+k)b} = Ce^{-i(\beta-k)c} + De^{i(\beta+k)c}$$



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

$$\Rightarrow \quad i(\alpha - k)Ae^{i(\alpha-k)b} - i(\alpha + k)Be^{-i(\alpha+k)b}$$
$$= i(\beta - k)Ce^{-i(\beta-k)c} - i(\beta + k)De^{i(\beta+k)c}$$

8

8

Solutions

$$A + B = C + D$$
$$i(\alpha - k)A - i(\alpha + k)B = i(\beta - k)C - i(\beta + k)D$$
$$Ae^{i(\alpha-k)b} + Be^{-i(\alpha+k)b} = Ce^{-i(\beta-k)c} + De^{i(\beta+k)c}$$
$$i(\alpha - k)Ae^{i(\alpha-k)b} - i(\alpha + k)Be^{-i(\alpha+k)b} = i(\beta - k)Ce^{-i(\beta-k)c} - i(\beta + k)De^{i(\beta+k)c}$$

- For meaningful solutions to exist, the determinant must be zero:

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

9

9

Dispersion Relation

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

$\beta^2 > 0 \rightarrow \beta$ is real.

$$-\frac{\alpha^2 + \beta^2}{2\alpha\beta} \sin \alpha b \sin \beta c + \cos \alpha b \cos \beta c = \cos ka$$

$\beta^2 < 0 \rightarrow \beta$ is imaginary.

$$\frac{\gamma^2 - \alpha^2}{2\alpha\gamma} \sin \alpha b \sinh \gamma c + \cos \alpha b \cosh \gamma c = \cos ka$$

$$\beta = i\gamma$$

10

10

Dispersion Relation

- Using trigonometry

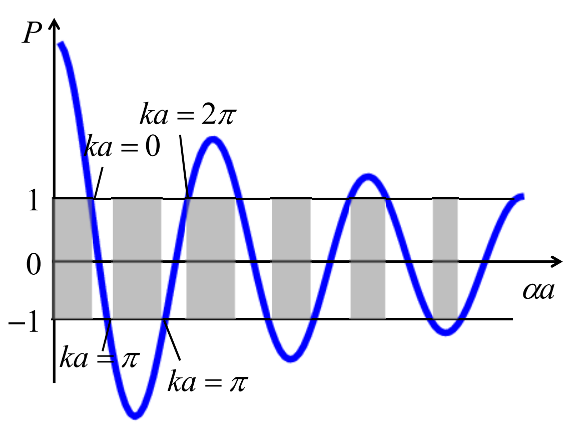
$$\left[1+\frac{V_0^2}{4\varepsilon\left(\varepsilon-V_0\right)}\sin^2\beta c\right]^{1/2}\cos(\alpha b-\delta)=\cos ka, \qquad (\varepsilon > V_0)$$

$$\left[1+\frac{V_0^2}{4\varepsilon\left(V_0-\varepsilon\right)}\sinh^2\gamma c\right]^{1/2}\cos(\alpha b-\delta')=\cos ka, \qquad (0<\varepsilon < V_0)$$

where

$$\tan\delta=-\frac{\alpha^2+\beta^2}{2\alpha\beta}\tan\beta c \quad \text{and} \quad \tan\delta'=\frac{\gamma^2-\alpha^2}{2\alpha\gamma}\tanh\gamma c$$

Energy Bands

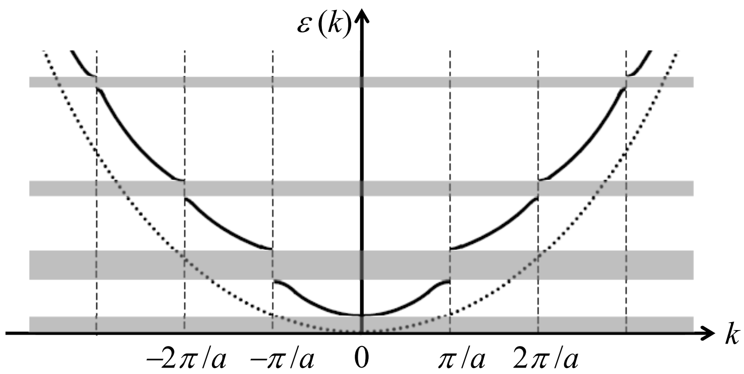


Forbidden energy range

$$\alpha^2=\frac{2m\varepsilon}{\hbar^2}$$

- In an infinite lattice, the states within any allowed band would form a continuum.
- For a lattice of N atoms, there are N discrete states, however, there are $2N$ states for spin degeneracy.
- The energy gaps decrease as electron energy increases → free electron behavior at high energies.

Dispersion Relation



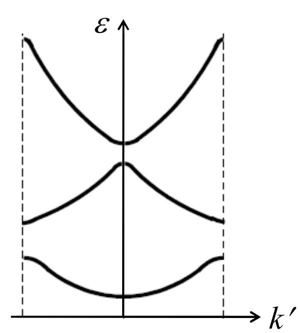
- Energies close to zero are forbidden.
- At $k = n\pi/a$, there are two possible values of energies.
- Bragg reflection at $k = \pm n\pi/a$

13

13

Reduced Zone Representation

- Energy band diagram is plotted in the first Brillouin zone.

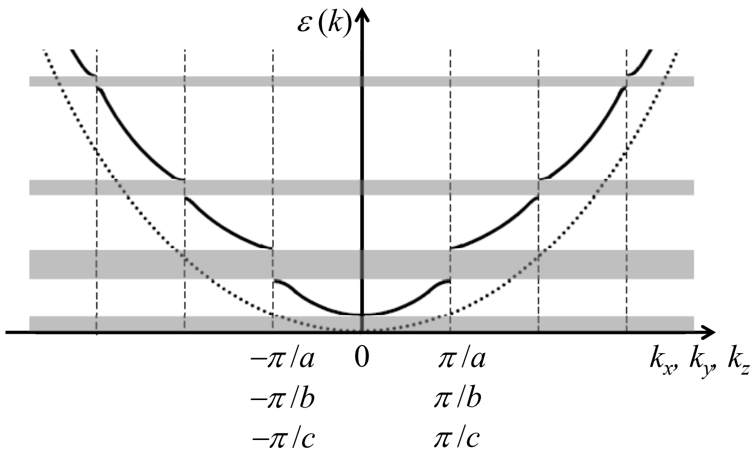


- ***How the energy bands (E-k relation) will change for a 3-D case?***

14

14

Dispersion Relation: 3D



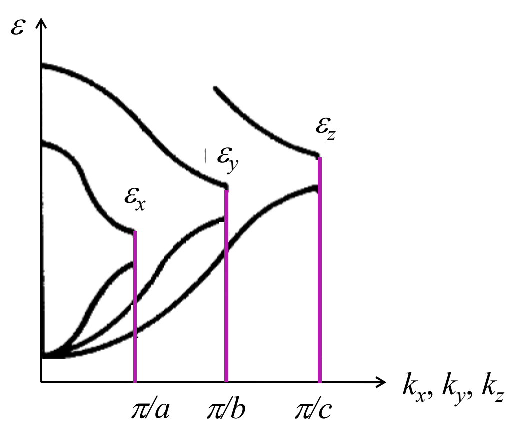
$a = b = c$

15

15

Dispersion Relation: 3-D

- k-values at the zone boundaries along different crystal orientations may be different → overlap of energy states at zone boundaries.



16

16