Quiz 4

1

Bragg's Law

$$n\lambda = 2d\sin(\theta)$$

where:

d is interplanar spacing, n is order of the diffraction peak, θ is angle of diffraction.

$$d = \frac{n\lambda}{2sin(\theta)}$$

for $2\theta = 42.3degree$: $d1 \approx 1.203$Å;

for $2\theta = 49.2degree$: $d2 \approx 1.070$Å;

for $2\theta 72.2degree$: $d3 \approx 0.851$Å;

for $2\theta = 87.4degree$: $d4 \approx 0.811$Å.

The ratios between these d-spacings: $d1 : d2 : d3 : d4 \approx 2.245 : 1.946 : 1.375 : 1.172 \approx 1 : 0.867 : 0.612 : 0.522$

These ratios suggest that it might be a BCC lattice. Then, we have:

$$\frac{d1}{(a/\sqrt{2})} \approx \frac{d1}{(a/\sqrt{4})} \approx \frac{d1}{(a/\sqrt{6})} \approx \frac{d1}{(a/\sqrt{8})}$$

The lattice constant is $a \approx 3.178$Å

3

In terms of wave vector k and group velocity $v_g(k)$ can express the momentum $p = \hbar k$

The group velocity is thederivative of the energy E with respect to the wave vector k:

$$v_g(k) = \frac{\partial E}{\partial k}$$

where $E = \hbar\omega(k)$.

Applied the Newton's law:

$$F = \frac{\mathrm{d}p}{\mathrm{d}t} = m\frac{\mathrm{d}v}{\mathrm{d}t}$$

and $\mathrm{d}p = \hbar \mathrm{d}k$

We have:

$$m^* \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial E}{\partial k}\right) = \hbar\frac{\mathrm{d}k}{\mathrm{d}t}$$

We arrive the expression for the effective mass:

$$m^* = \hbar^2 \left(\frac{\partial^2 E}{\partial k^2}\right)^{-1}$$

Q.E.D

4

(a)

In a 2-dimensional square lattice, the first Brillouin zone is also a square. The corner points of the first Brillouin zone are at wave vectors $(k_x, k_y) = (\pm\pi/a, \pm\pi/a)$, while the midpoints of the side faces are at $(k_x, k_y) = (0, \pm\pi/a)$ or $(\pm\pi/a, 0)$, where a is the lattice constant.

For a free electron in a 2-dimensional lattice, the dispersion relation is

$$E(kx, ky) = \frac{\hbar^2(k_x^2 + k_y^2)}{2m}$$

The kinetic energy of a free electron at a corner of the first Brillouin zone:

$$E_{corner} = \frac{\hbar^2((\pi/a)^2 + (\pi/a)^2)}{2m} = \frac{\hbar^2(2\pi^2/a^2)}{2m}$$

Next, calculate the kinetic energy of a free electron at the midpoint of a side face of the zone:

$$E_{midpoint} = \frac{\hbar^2(\pi/a)^2}{2m}$$

Then, we arrive the factor b:

$$b = \frac{E_{corner}}{E_{midpoint}} = \frac{2\pi^2}{\pi^2} = 2$$

(b)

Fot the 3-dimensional simple cubic lattice, the first Brillouin zone is also a cube. The corner points of the first Brillouin zone are at wave vectors $(k_x, k_y, k_z) = (\pm\pi/a, \pm\pi/a, \pm\pi/a)$, while the midpoints of the side faces are at $(k_x, k_y, k_z) = (\pm\pi/a, 0, 0)$,$(0, \pm\pi/a, 0)$, or $(0, 0, \pm\pi/a)$.

For a free electron in a three-dimensional lattice, the dispersion relation is given by the equation:

$$E(k_x, k_y, k_z) = \frac{\hbar^2(k_x^2 + k_y^2 + k_z^2)}{2m}$$

The kinetic energy of a free electron at a corner of the first Brillouin zone:

$$E_{corner} = \frac{\hbar^2((\pi/a)^2 + (\pi/a)^2 + (\pi/a)^2)}{2m} = \frac{\hbar^2(3\pi^2/a^2)}{2m}$$

Next, calculate the kinetic energy of a free electron at the midpoint of a side face of the zone:

$$E_{midpoint} = \frac{\hbar^2(\pi/a)^2}{2m}$$

Then, we arrive the factor b:

$$b = \frac{E_{corner}}{E_{midpoint}} = \frac{3\pi^2}{\pi^2} = 3$$

(c)

In a 2D or 3D crystal of a divalent element, the solid can be a metal if the energy bands are partially filled, allowing for free movement of electrons and electrical conduction.

This is possible in the nearly-free electron model, where electrons are weakly bound by a periodic potential.

For a divalent element, there are two valence electrons per unit cell, which can lead to partially filled bands in certain lattice structures.

A partially filled band allows electrons to move freely, making the solid a metal.