ECE 407 Homework # 2 Solutions (Farhan Rana).

2.1

$$2\times\int\frac{d^3\vec{k}}{(2\pi)^3}\longrightarrow\sqrt{\frac{m_x m_y m_z}{m^3}}\;2\times\int\frac{d^3\vec{q}}{(2\pi)^3}$$

Now since $E(\vec{q})=\frac{\hbar^2 q^2}{2m}=\frac{\hbar^2}{2m}(q_x^2+q_y^2+q_z^2)$

$$\Rightarrow\quad\sqrt{\frac{m_x m_y m_z}{m^3}}\;2\times\int\frac{d^3\vec{q}}{(2\pi)^3}\longrightarrow\sqrt{\frac{m_x m_y m_z}{m^3}}\int_0^\infty\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}\;dE$$

$$\Rightarrow\quad g(E)=\frac{1}{2\pi^2}\left(\frac{2m_d}{\hbar^2}\right)^{3/2}\sqrt{E}$$

where $m_d=(m_x m_y m_z)^{1/3}$ = is called the density of states effective mass.

2.2

$$2\times\int\frac{d^2\vec{k}}{(2\pi)^2}\longrightarrow\sqrt{\frac{m_x m_y}{m^2}}\;2\times\int\frac{d^2\vec{q}}{(2\pi)^2}$$

and $E(\vec{q})=\frac{\hbar^2 q^2}{2m}$

$$\Rightarrow \sqrt{\frac{m_x m_y}{m^2}}\; 2 \times \int \frac{d^2 \vec{q}}{(2\pi)^2} \longrightarrow \sqrt{\frac{m_x m_y}{m^2}} \int_0^E \frac{m}{\pi \hbar^2}\, dE$$

$$\Rightarrow g_{2D}(E) = \frac{m_d}{\pi \hbar^2}$$

where $m_d = \sqrt{m_x m_y}$

= density of states effective mass.

2.3

a) $\vec{a}_1 = a\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right)$ b) $\Omega_2 = |\vec{a}_1 \times \vec{a}_2| = \frac{\sqrt{3}}{2}a^2$

$\vec{a}_2 = a\left(\frac{\sqrt{3}}{2}\hat{x} - \frac{1}{2}\hat{y}\right)$ c) See attached figure.

d) $\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \hat{z}}{\Omega_2} = \frac{4\pi}{\sqrt{3}a}\left(-\frac{1}{2}\hat{x} - \frac{\sqrt{3}}{2}\hat{y}\right)$

$\vec{b}_2 = 2\pi \frac{\hat{z} \times \vec{a}_1}{\Omega_2} = \frac{4\pi}{\sqrt{3}a}\left(-\frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}\right)$

e) $\Pi_2 = |\vec{b}_1 \times \vec{b}_2| = \frac{(2\pi)^2}{\Omega_2} = \frac{4\pi^2}{\frac{\sqrt{3}}{2}a^2} = \frac{8\pi^2}{\sqrt{3}a^2}$

f) see attached plot. lattice is hexagonal. g+h+i) See attached plots

2.4

a) For FCC lattice: $\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z})$ $\vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{z})$ $\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y})$

$\Omega_3 = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)| = \frac{a^3}{4}$

$\vec{b}_1 = \frac{2\pi}{\Omega_3}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{a}(\hat{z}+\hat{y}-\hat{x})$ $\vec{b}_2 = \frac{2\pi}{\Omega_3}(\vec{a}_3 \times \vec{a}_1) = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z})$

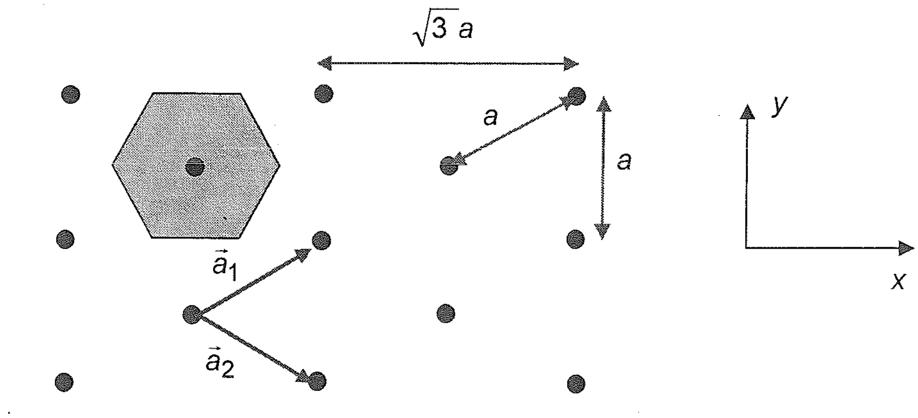
$\vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z}) \Rightarrow \vec{b}_1, \vec{b}_2$ and $\vec{b}_3$ correspond to a BCC lattice with a unit cell dimension of $\frac{4\pi}{a}$.

b) For BCC lattice: $\vec{a}_1 = \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z})$ $\vec{a}_2 = \frac{a}{2}(\hat{x}-\hat{y}+\hat{z})$

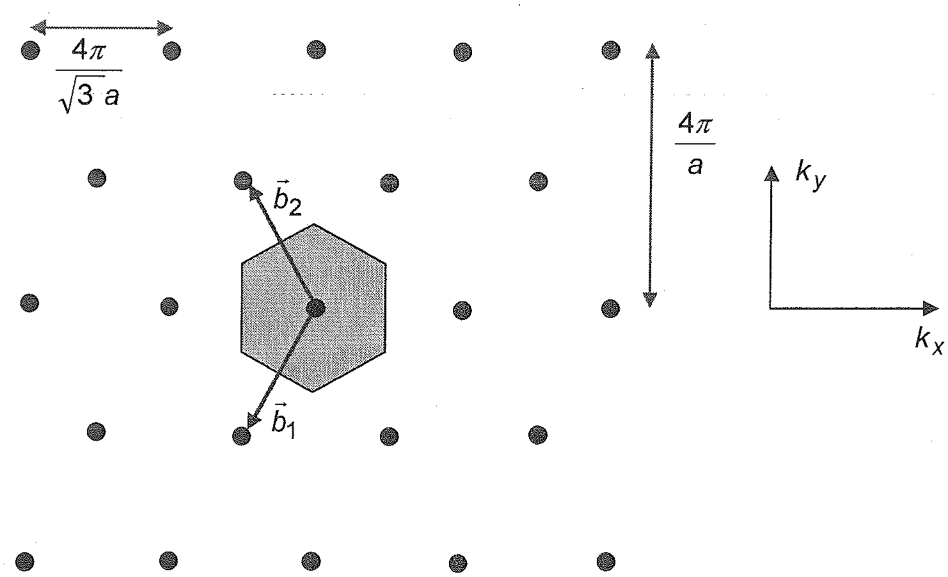
$\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z})$

Problem 2.3 plots

Direct Lattice:

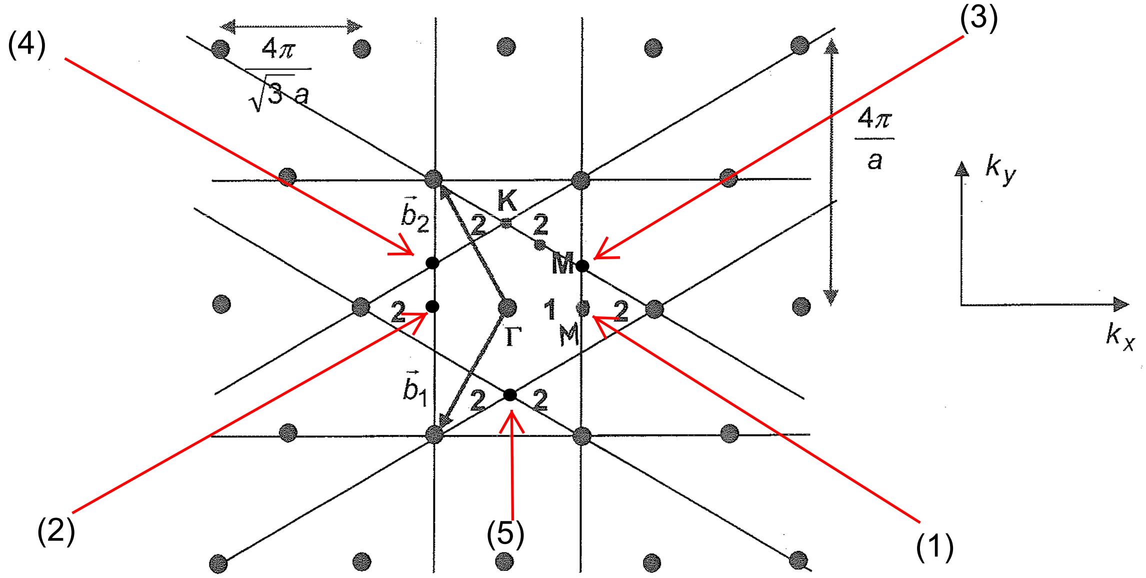


Reciprocal Lattice:



Bragg Planes and Higher BZs

g)



h) The electron wavevector is at the point indicated as (1) above. (1) lies on a Brag plane. This is one of the many equivalent M points in the FBZ. Bragg scattering will take it to the point marked (2) above. (2) is also an M point in the FBZ.

i) The electron wavevector is at the point indicated as (3) above. This is one of the many equivalent K' points in the FBZ and lies at the intersection of two Bragg planes. Bragg scattering can take it to the points marked (4) or (5) above. (4) and (5) are also K' points in the FBZ.

(2.4(b)...contd)

$$\Omega_3 = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)| = \frac{a^3}{2}$$

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{y}+\hat{z}) \quad \vec{b}_2 = \frac{2\pi}{a}(\hat{x}+\hat{z}) \quad \vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y})$$

$\Rightarrow$ $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$ correspond to a FCC lattice with unit cell size equal to $\frac{4\pi}{a}$.

2.4(c)

There are 8 Si atoms in a unit cell of volume a x a x a. Each Si atom has a mass of 28 amu. One amu is approximately the mass of a proton (or a neutron). So the density is 2335 Kg/cubic-meter.

2.5

a) $\vec{a}_1 = \sqrt{3}a\,\hat{x} \quad \hat{a}_2 = a\,\hat{y}$

b) $\Omega_2 = |\vec{a}_1 \times \vec{a}_2| = \sqrt{3}a^2$.

c) See attached. There are two atoms per primitive cell: one black and one red.

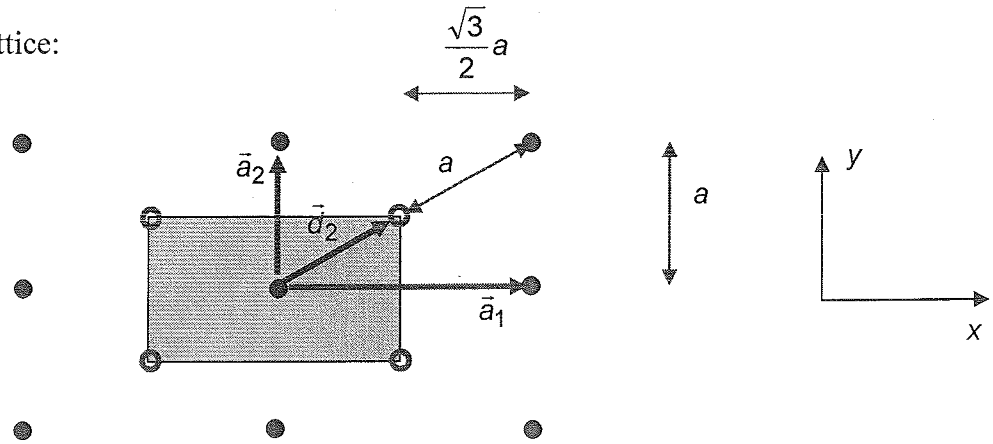
d) $\vec{b}_1 = \frac{2\pi}{\sqrt{3}a}\hat{x} \quad \vec{b}_2 = \frac{2\pi}{a}\hat{y}$.

e) $\Pi_2 = |\vec{b}_1 \times \vec{b}_2| = \frac{(2\pi)^2}{\Omega_2}$.

f) See attached

Problem 3.3 (f)

Direct lattice:



Reciprocal lattice: