Solutions for Homework 1

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1 Tetrahedral angles

Referring to Fig10, the angles between the tetrahedral bonds of diamond are equal to those between $\overrightarrow{a_1}$ and $\overrightarrow{a_2}$,$\overrightarrow{a_2}$ and $\overrightarrow{a_3}$, or $\overrightarrow{a_3}$ and $\overrightarrow{a_1}$.

So

$$cos\theta = \frac{a_1 \times a_2}{\|a_1\|\|a_2\|} = \frac{\frac{1}{4}a^2(-1-1+1)}{\frac{1}{4}a^2(1^2+1^2+1^2)} = -\frac{1}{3}$$

$$\theta = cos^{-}1(-\frac{1}{3}) \approx 109.47^0$$

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2 Indices of Planes

Referring to Fig 11, the plane with index (100) is the plane which parallel to y-z plane abd cuts x-axis at x=a. and this plane intercepts $\overrightarrow{a_1}$, $\overrightarrow{a_2}$, $\overrightarrow{a_3}$ axes at $2\overrightarrow{a_1}$,$\infty\overrightarrow{a_2}$ (does not intercept $\overrightarrow{a_2}$axis) and $2\overrightarrow{a_3}$ respectively. $\frac{1}{2}$:0:$\frac{1}{2}$=1:0:1. The index referred to the primitive axes $\overrightarrow{a_1}$,$\overrightarrow{a_2}$,$\overrightarrow{a_3}$ is then (1,0,1).

Similarly, the plan with index (0,0,1) referred to cubic cell. The plane is parallel to x-y plane and cuts z-axis at z=a. And this plane intercepts $\overrightarrow{a_1}$,$\overrightarrow{a_2}$,$\overrightarrow{a_3}$ axes at $\infty\overrightarrow{a_1}$,$2\overrightarrow{a_2}$,$2\overrightarrow{a_3}$.Hence the index referred to the primitive axes is (0,1,1).

3 Hcp Structure

Suppose the radius of an atom is r. Since it's an ideal hexagonal close-packed structure, see Fig 21, c=2r (the two atoms touch) and $a_1 or a_2 = 2r$(the two atoms touch). Also, from the geometry the distance between the center layer atom and top atom is $\sqrt{(\frac{a}{\sqrt{3}})^2 + (\frac{c}{2})^2}$=2r (the two atoms touch)=a, so we obtain

$$\frac{a^2}{3} + \frac{c^2}{4} = a^2$$

$\Rightarrow$

$$(\frac{c}{a})^2 = \frac{8}{3} or \frac{c}{a} = \sqrt{\frac{8}{3}} \cong 1.633$$

If $\frac{c}{a} \gg \sqrt{\frac{8}{3}}$, the atoms on the top do not touch the atoms on the center layer. And this means, the crystal structure is composed of planes of closely packed atoms (atoms on the each layer still touch each other), the plane being loosely stacked.

4 Problem 4

- For ideal close packed hcp,

$$r = \frac{a}{2}, c = \sqrt{\frac{8}{3}}a$$

The volume of conventional unit cell=$[(\frac{\sqrt{3}}{4}a^2) \times 6] \times \sqrt{\frac{8}{3}}a = 3\sqrt{2}a^3$.

Since there are 6 atoms in a unit cell, the volume occupied by those 6 atoms= $6 \times \frac{4}{3}\pi(\frac{a}{2})^3 = \pi a^3$.

Therefore packing fraction= $\frac{\pi a^3}{3\sqrt{2}a^3} = \frac{\sqrt{2}\pi}{6} \cong 0.74$

- For close packed fcc,

$$4r = \sqrt{2}a \Rightarrow r = \frac{\sqrt{2}}{4}a$$

and there are 4 atoms per conventional cell, therefore packing fraction= $\frac{4\times\frac{4}{3}\pi r^3}{a^3} = \frac{\frac{16}{3}\pi(\frac{\sqrt{2}}{4})^3 a^3}{a^3} = \frac{\sqrt{2}}{6}\pi \cong 0.74$

- For 'close packed' bcc, $4r = \sqrt{3}a$ (body diagonal), and there are only two atoms per unit cell. Therefore packing fraction=$\frac{2\times\frac{4}{3}\pi r^3}{a^3} = \frac{\sqrt{3}}{8}\pi \cong 0.68$

5 Problem 5

Suppose the plane intercepts x,y,z axes at $x_1\overrightarrow{a_1}, x_2\overrightarrow{a_2}, x_3\overrightarrow{a_3}$ respectively.Then $x_1 : x_2 : x_3 = \frac{1}{h} : \frac{1}{k} : \frac{1}{l}$.

(a) Prove that the reciprocal lattice vector $\overrightarrow{G} = h\overrightarrow{b_1} + k\overrightarrow{b_2} + l\overrightarrow{b_3}$ is perpendicular to this plane.

The normal vector to the plane is

$$(-x_1\overrightarrow{a_1} + x_2\overrightarrow{a_2}) \times (-x_1\overrightarrow{a_1} + x_3\overrightarrow{a_3})$$

$$= x_1x_3\overrightarrow{a_3} \times \overrightarrow{a_1} + x_1x_2\overrightarrow{a_1} \times \overrightarrow{a_2} + x_2x_3\overrightarrow{a_2} \times \overrightarrow{a_3}$$

$$= x_1x_2x_3(\frac{1}{x_1}\overrightarrow{a_2} \times \overrightarrow{a_3} + \frac{1}{x_2}\overrightarrow{a_3} \times \overrightarrow{a_1} + \frac{1}{x_3}\overrightarrow{a_1} \times \overrightarrow{a_2})$$

$$\sim h\overrightarrow{b_1} + k\overrightarrow{b_2} + l\overrightarrow{b_3}$$

Therefore $\overrightarrow{G} = h\overrightarrow{b_1} + k\overrightarrow{b_2} + l\overrightarrow{b_3}$ is perpendicular to this plane.

(b) Prove that the distance between two adjacent parallel planes of the lattice is $d(hkl) = \frac{2\pi}{\|G\|}$.

For any $\overrightarrow{R} = x_1\overrightarrow{a_1} + x_2\overrightarrow{a_2} + x_3\overrightarrow{a_3}$, the expression $e^{i\overrightarrow{G}\,\overrightarrow{R}} = const.$ Since the lattice contain $0\overrightarrow{a_1}+0\overrightarrow{a_2}+0\overrightarrow{a_3}$, we obtain that $e^{i\overrightarrow{G}\,\overrightarrow{R}} = const = 1$. Therefore $\overrightarrow{G}\,\overrightarrow{R} = 2\pi n \Rightarrow \overrightarrow{G}\Delta\overrightarrow{R} = 2\pi\Delta n$.

The distance between two adjacent parallel plane ($\Delta n = 1$) is

$$d = \frac{\overrightarrow{G}}{\|\overrightarrow{G}\|}\Delta\overrightarrow{R} = \frac{2\pi}{\|\overrightarrow{G}\|}$$

(c) For a simple cubic lattice,

$$\overrightarrow{G} = h\overrightarrow{b_1} + k\overrightarrow{b_2} + l\overrightarrow{b_3}$$

$$\|\overrightarrow{G}\| = \sqrt{h^2 + k^2 + l^2} \times (\frac{2\pi}{a})$$

Thus

$$d = \frac{2\pi}{\|G\|} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

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6 Problem 6

There is a very useful relation about the density of atoms in a lattice plane. The density of atoms

$$(\frac{number\ of\ atoms}{unit\ area}) = \frac{d}{c}$$

, where d is the distance between adjacent lattice planes and v is the volume of a primitive cell.

Proof:

Suppose there are N atoms in the lattice, N_1 atoms in a lattice plane. Then the number N_2 of such lattice planes is $N_2 = \frac{N}{N_1}$. The total volume $V = Nv = N_2(dA)$, where A is the area of the lattice plane. Therefore

$$density = \frac{N_1}{A} = \frac{N/N_2}{Nv/N_2 d} = \frac{d}{v}$$

Since the volume of a primitive cell v is constant for a lattice, we see that the density of atoms per area is proportional to the distance between adjacent lattice planes. Also $d = \frac{2\pi}{\|\overrightarrow{G}\|}$, where $\overrightarrow{G} = h\overrightarrow{b_1} + k\overrightarrow{b_2} + l\overrightarrow{b_3}$.

For fcc,

$$\overrightarrow{b_1} = \frac{2\pi}{a}(-\overrightarrow{x} + \overrightarrow{y} + \overrightarrow{z}), \overrightarrow{b_3} = \frac{2\pi}{a}(\overrightarrow{x} + \overrightarrow{y} - \overrightarrow{z}), \overrightarrow{b_1} = \frac{2\pi}{a}(\overrightarrow{x} + \overrightarrow{y} + \overrightarrow{z})$$

In order to get largest densities, we need to find the smallest reciprocal lattice vector $\overrightarrow{G}$ associated with the lattice plane.

$$\overrightarrow{G} = \frac{2\pi}{a}[(-h+k+l)\overrightarrow{x} + (h-k+l)\overrightarrow{y} + (h+k-l)\overrightarrow{z}]$$

$$\|\overrightarrow{G}\|^2 = (\frac{2\pi}{a})^2[(-h+k+l)^2 + (h-k+l)^2 + (h+k-l)^2]$$

Hence$\|\overrightarrow{G}\|^2$ may have values$(\frac{2\pi}{a})^2 \times 1$,$(\frac{2\pi}{a})^2 \times (1^2+1^2)$,$(\frac{2\pi}{a})^2 \times (1^2+1^2+1^2)$,...

- When$\|\overrightarrow{G}\|^2 = (\frac{2\pi}{a})^2 \times 1$, we can obtain that $-h+k+l = \pm 1$,$h-k+l =$ 0,$h+k-l$=0, they give the solution

  $$h = 0, k = l, 2l = \pm 1$$

  Since h,k,l are integers,$\|\overrightarrow{G}\|^2$cannot be $(\frac{2\pi}{a})^2 \times 1$ in fcc.

- when $\|\overrightarrow{G}\|^2 = (\frac{2\pi}{a})^2 \times (1^2+1^2)$, we obtain $-h+k+l = \pm 1$,$h-k+l =$ ± 1,$h+k-l = 0$, they give the solution

  $$2h = \pm 1$$

  . Same reason as above, this can not happen in fcc.

- When $\|\overrightarrow{G}\|^2 = (\frac{2\pi}{a})^2 \times (1^2+1^2+1^2)$, we obtain $-h+k+l = \pm 1$,$h-k+l =$ ± 1,$h+k-l = \pm 1$, they give many solutions, eg. (h,k,l)=($\pm$1,0,0), which means $\overrightarrow{G} = \frac{2\pi}{a}[\pm\overrightarrow{x} \pm \overrightarrow{y} \pm \overrightarrow{z}]$ and $\|\overrightarrow{G}\| = \frac{2\pi}{a}\sqrt{1^2+1^2+1^2}$.

So the smallest $\|\overrightarrow{G}\| = \frac{2\pi}{a}\sqrt{1^2+1^2+1^2}$, and$\overrightarrow{G} = \frac{2\pi}{a}[\pm\overrightarrow{x} \pm \overrightarrow{y} \pm \overrightarrow{z}]$ which (referred to cubic cell) represents family of lattice planes(1,1,1).

So (1,1,1) has largest density of atoms per unit area.