Assignment 1: SOLID STATE PHYSICS – CRYSTAL STRUCTURE

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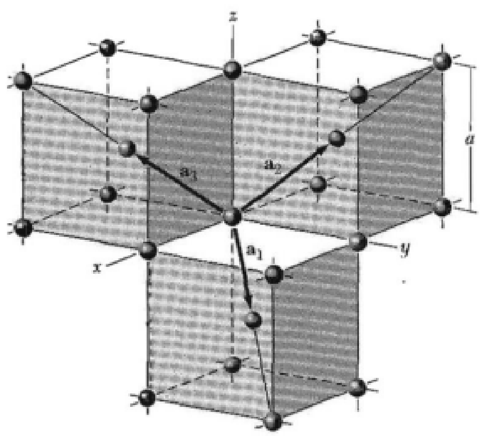
Problem 1

Tetrahedral angles. The angles between the tetrahedral bonds of diamond are the same as the angles between the body diagonals of a cube, as shown in the figure below. Use elementary vector analysis to find the value of the angle.



Answer 1: From the given figure, we can conclude that

$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z}), \;\; \vec{a}_2 = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z}), \;\; \text{and} \;\; \vec{a}_3 = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z}) \tag{1}$$

Using scalar product property

$$\vec{a} \cdot \vec{b} = |\vec{a}||\vec{b}|cos\theta \tag{2}$$

$$\theta = cos^{-1}\frac{\vec{a} \cdot \vec{b}}{|\vec{a}||\vec{b}|} \tag{3}$$

we get

$$cos\theta_{1,2} = \frac{\vec{a}_1 \cdot \vec{a}_2}{|\vec{a}_1||\vec{a}_2|} = \frac{\frac{a}{2}(\hat{x}+\hat{y}-\hat{z}) \cdot \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z})}{(\frac{a}{2}\sqrt{3})(\frac{a}{2}\sqrt{3})} = \frac{(-1+1-1)}{3} = \frac{-1}{3} \tag{4}$$

$$\theta_{1,2} = cos^{-1}(-\frac{1}{3}) \approx 109.47^\circ \tag{5}$$

$$cos\theta_{2,3} = \frac{\vec{a}_2 \cdot \vec{a}_3}{|\vec{a}_2||\vec{a}_3|} = \frac{\frac{a}{2}(-\hat{x}+\hat{y}+\hat{z}) \cdot \frac{a}{2}(\hat{x}-\hat{y}+\hat{z})}{(\frac{a}{2}\sqrt{3})(\frac{a}{2}\sqrt{3})} = \frac{(-1-1+1)}{3} = \frac{-1}{3} \tag{6}$$

$$\theta_{2,3} = cos^{-1}(-\frac{1}{3}) \approx 109.47^\circ \tag{7}$$

$$cos\theta_{3,2} = \frac{\vec{a}_3 \cdot \vec{a}_1}{|\vec{a}_3||\vec{a}_1|} = \frac{\frac{a}{2}(\hat{x}-\hat{y}+\hat{z}) \cdot \frac{a}{2}(\hat{x}+\hat{y}-\hat{z})}{(\frac{a}{2}\sqrt{3})(\frac{a}{2}\sqrt{3})} = \frac{(1-1-1)}{3} = \frac{-1}{3} \tag{8}$$

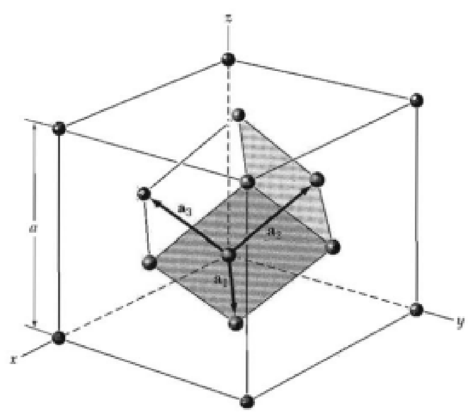
$$\theta_{3,1} = cos^{-1}(-\frac{1}{3}) \approx 109.47^\circ \tag{9}$$

To conclude,

$$\therefore \theta_{1,2} = \theta_{2,3} = \theta_{3,1} \approx 109.47^\circ \tag{10}$$

Problem 2

Indices of planes. Consider the planes with indices (100) and (001); the lattice is fcc, and the indices refer to the conventional cubic cell. What are the indices of these planes when referred to the primitive axes of the figure below.



Answer 2: The points $(\vec{a}_1, \vec{a}_2, \vec{a}_3)$ can be expressed in terms of unit vectors $(\vec{x}, \vec{y}.\vec{z})$ such that

$$\vec{a}_1 = \frac{a}{2}(\vec{x}+\vec{y}), \;\; \vec{a}_2 = \frac{a}{2}(\vec{y}+\vec{z}), \;\text{ and }\; \vec{a}_3 = \frac{a}{2}(\vec{x}+\vec{z}), \tag{11}$$

The only points that intersects the plane with indices (100) at $2\vec{a}_1$ and $2\vec{a}_3$ are the point a_1 and a_3. Given the magnitude of the vectors along primitive axis, i.e., $|\vec{a}_1| = |\vec{a}_2| = |\vec{a}_3| = \frac{a\sqrt{2}}{2}$, we get

$$(\frac{1}{a\sqrt{2}} \;\; \frac{1}{\infty} \;\; \frac{1}{a\sqrt{2}}) = (\frac{1}{a\sqrt{2}} \;\; 0 \;\; \frac{1}{a\sqrt{2}}) = \frac{1}{a\sqrt{2}}(1 \;\; 0 \;\; 1) \tag{12}$$

In addition, the only points that intersects the plane ith indices (001) are the points a_2 and a_3, resulting to

$$(\frac{1}{\infty} \;\; \frac{1}{a\sqrt{2}} \;\; \frac{1}{a\sqrt{2}}) = (0 \;\; \frac{1}{a\sqrt{2}} \;\; \frac{1}{a\sqrt{2}}) = \frac{1}{a\sqrt{2}}(0 \;\; 1 \;\; 1) \tag{13}$$

To conclude,

$\therefore$ when referred to the primitive axes, planes with indices (100) and (001) have (101) and (011) indices respectively.

Problem 3

Hcp structure. Show that the c/a ratio for an ideal hexagonal closed-packed structure $(\frac{8}{3})^{\frac{1}{2}} =$ 1.633. If c/a is significantly larger than this value, the crystal structure may be thought of as composed of planes of closely packed atoms, the planes being loosely stacked.

Answer 3: Using the perpendicular bisector

$$|\overline{AO}| = |\overline{BO}| = |\overline{CO}| = d \tag{14}$$

and pythagorean theorem, we get

$$d = \frac{\frac{a}{2}}{\frac{\sqrt{3}}{2}} = \frac{a}{2}\cdot\frac{2\sqrt{3}}{3} = \frac{a}{\sqrt{3}} \tag{15}$$

If the unprojected lattice points are at the center of spheres, we have

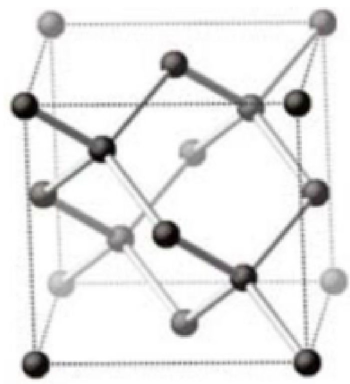
$$a^2 = (\frac{a}{\sqrt{3}})^2 + (\frac{c}{2})^2 \tag{16}$$

$$\frac{2}{3}a^2 = \frac{1}{4}c^2 \tag{17}$$

$$\frac{c}{d} = \frac{\sqrt{8}}{3} \approx 1.633 \tag{18}$$

Problem 4

The figure below illustrates the unit cell of a diamond crystal structure. (a) How many carbon atoms are there per unit cell? (b) What is the coordination number for each carbon atom? (C.N. is the number of equidistant nearest neighbors to an atom in a crystal structure).



Answer 4:
a. The center of the sub-cubic body are the atoms in diagonals. Therefore, we have

$$\text{corner: } \frac{1}{8} \times 8 = 1 \tag{19}$$

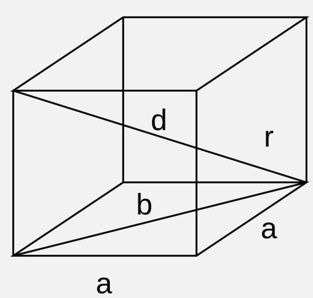
$$\text{face: } \frac{1}{2} \times 6 = 3 \tag{20}$$

$$\text{body: } 1 \times 4 = 4 \tag{21}$$

Therefore,

$$TOTAL\ \ Carbon\ \ Atoms = 8 \tag{22}$$

b. The carbon atom at the center of the tetrahedron is surrounded by 4 carbon atoms present at 4 corners which can be seen on the figure below as connected bonds. Therefore, **C.N. = 4**.



Problem 5

Body-centered cubic structure. **(a)** Show that for BCC the lattice length a in terms of the atomic radius is $4R/\sqrt{3}$. **(b)** Calculate the volume of a BCC unit cell in terms of the atomic radius R. **(c)** Show that the atomic packing factor for the BCC crystal structure is 0.68.

Answer 5:
a. Using the Pythagorean theorem, face diagonal b can be expressed as

$$b^2 = a^2 + a^2 = 2a^2 \tag{23}$$

Using the above expression, the solution for d can be expressed as

$$d^2 = a^2 + b^2 \tag{24}$$

The center point has two atomic radii while each corner has one because the corner atoms of a body-centered cubic cell make up only 1/8 of an atom while the center atom is a whole. As a result, d=4r in a body diagonal of a body centered cube cell. Therefore, we have

$$(4r)^2 = a^2 + (2a^2) \tag{25}$$

$$a = \frac{4r}{\sqrt{3}} \tag{26}$$

b. Defining the result in **a.** in terms of radius, we have

$$r = \frac{\sqrt{3}a}{4} \tag{27}$$

Solving for the total volume inside the body, we have

$$V_s = 2 \times \frac{4}{3}\pi(\frac{\sqrt{3}}{4}a)^3 = \frac{8}{3}\pi(3\frac{\sqrt{3}a^3}{64}) = \frac{\sqrt{3}}{8}\pi a^3 \tag{28}$$

c. Given the formula for atomic packing factor

$$APF = \frac{V_s}{V_c} \tag{29}$$

where $V_c = a^3$, we have

$$APF = \frac{\frac{\sqrt{3}}{8}\pi a^3}{a^3} = \frac{\sqrt{3}\pi}{8} \approx 0.68 \tag{30}$$

Problem 6

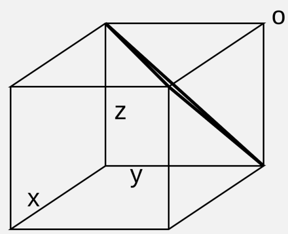
Draw in unit cubes the crystal planes that have the following Miller indices: a.) $(1\bar{1}\bar{1})$; b.) $(10\bar{2})$; c.) $(1\bar{2}1)$; d.) $(11\bar{3})$.

Answer 6:

a. The intercepts for $(1\bar{1}\bar{1})$ can be expressed as

$$(1\bar{1}\bar{1}) = (\frac{1}{1}\ \ \frac{1}{-1}\ \ \frac{1}{-1}) = (1, -1, -1) \tag{31}$$

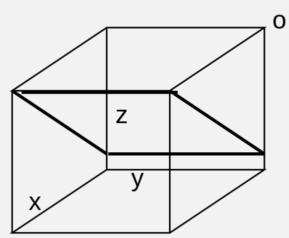
Now,the crystal plane is shown below given that the original point of the unit cube has been shifted.



b. The intercept of $(10\bar{2})$ can be expressed as

$$(10\bar{2}) = (\frac{1}{1}\ \ \frac{1}{0}\ \ \frac{1}{2}) = (1, \infty, -\frac{1}{2}) \tag{32}$$

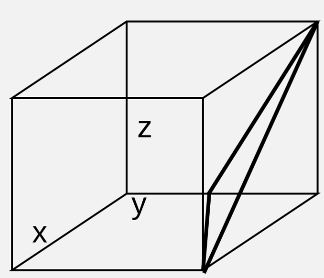
By shifting the original point of the unit cube, we have



c. The intercept for $(1\bar{2}1)$ can be expressed as

$$(1\bar{2}1) = (\frac{1}{1}\ \ \frac{1}{-2}\ \ \frac{1}{1}) = (1, -\frac{1}{2}, 1) \tag{33}$$

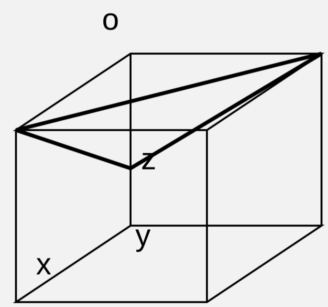
By shifting the origin point of the unit cube so y is negative, we have



d. The intercept for $(11\bar{3})$ can be expressed as

$$(11\bar{3}) = (\frac{1}{1}\ \frac{1}{1}\ \frac{1}{-3}) = (1, 1, -\frac{1}{3}) \tag{34}$$

By shifting the origin point of the unit cube so z is negative, we have



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