MSE160 Problem Set 4

James Li

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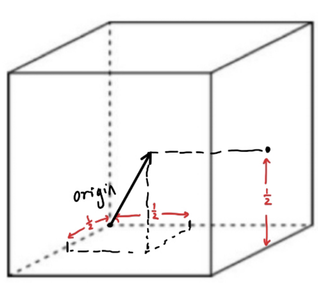
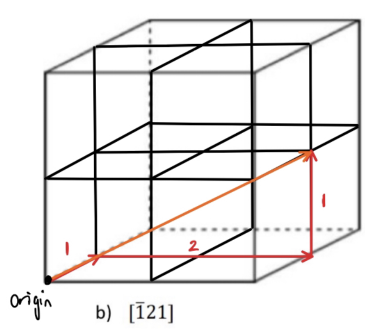
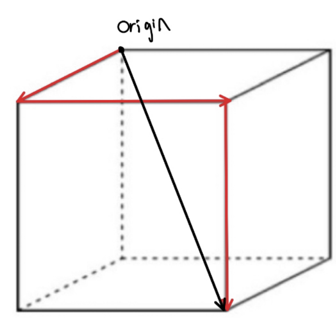
1 Question 1: [5 pts.]



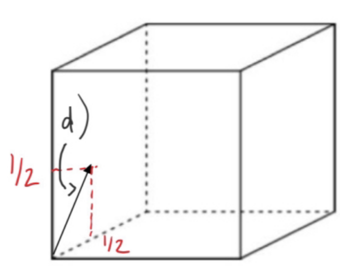
a) ½ ½ ½



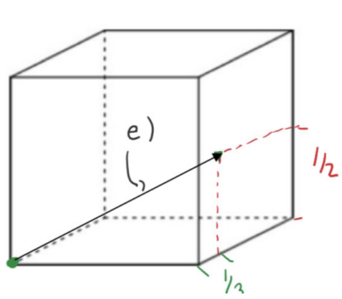
b) [$\bar{1}$21]



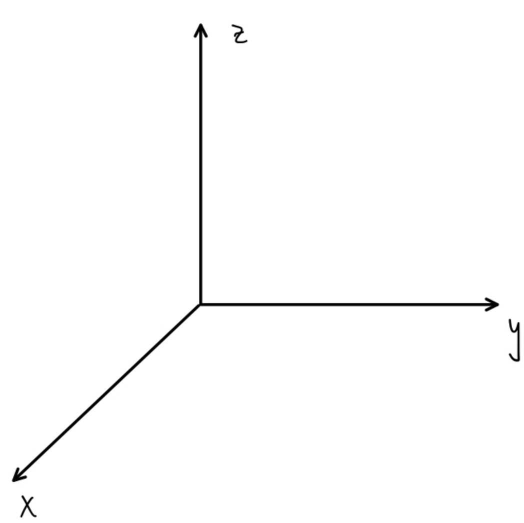
c) [11$\bar{1}$]



$$\left.\begin{array}{l} x = -\frac{1}{2} \\ y = 0 \\ z = +\frac{1}{2} \end{array}\right\} \times 2 \quad [\bar{1}01]$$



$$\left.\begin{array}{l} x = -\frac{1}{3} \\ y = 1 \\ z = \frac{1}{2} \end{array}\right\} \times 6 \quad [\bar{2}63]$$



2 Question 2: [4 pts.]

The method of determining linear density is given as:

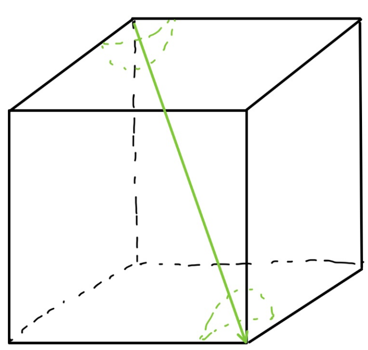
$$\text{Linear Density of Atoms} \equiv \text{LD} = \frac{\text{Number of atoms}}{\text{Unit length of direction vector}} \tag{1}$$

2.a Direction [11$\bar{1}$] in FCC:

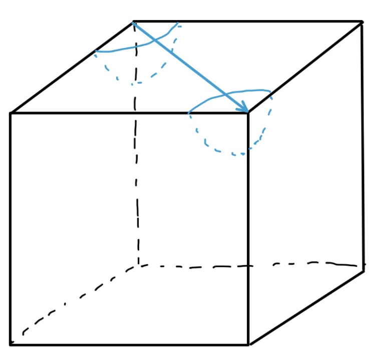
In a FCC structure, there are 4 atoms present per unit cell (8 eighths of an atom and 6 halves of 6 central atoms). However, the unit vector only passes through 2 halves of diameters since there is no central atom. The unit length of the direction vector can be found using the Pythagorean Theorem:

$$\text{Unit length} = \sqrt{a^2+b^2+c^2} = \sqrt{1^2+1^2+(-1)^2} = \sqrt{3} \tag{2}$$

$$\text{LD}_{[11\bar{1}]} = \frac{1 \text{ (Number of diameters crossed)}}{\sqrt{3}a \text{ (Unit length)}} = \frac{1}{\sqrt{3}a} \tag{3}$$



Unit cell structure for 2a).



Unit cell structure for 2b).

2.b Direction [110] in BCC:

In a BCC structure, there are 2 atoms present per unit cell (8 eighths of an atom and 1 central atom). The unit vector only passes through the 2 corner atoms which is equivalent to 1 diameter. The unit length of the direction vector can be found using the Pythagorean Theorem:

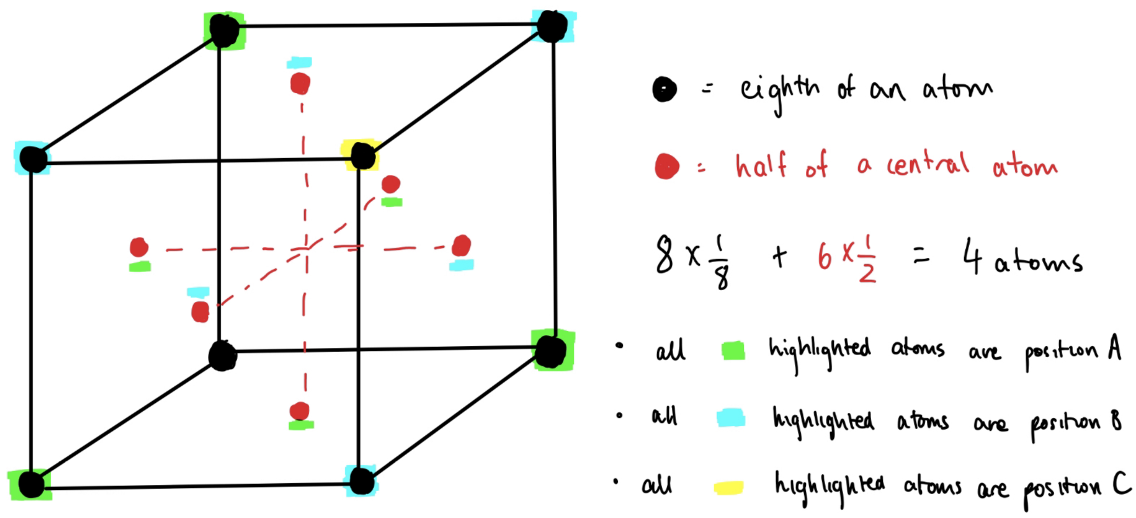
$$\text{Unit length} = \sqrt{a^2+b^2+c^2} = \sqrt{(1^2+1^2+0^2)} = \sqrt{2} \tag{4}$$

$$\text{LD}_{[110]} = \frac{1 \text{ (Number of diameters crossed)}}{\sqrt{2}a \text{ (Unit length)}} = \frac{1}{\sqrt{2}a} \tag{5}$$

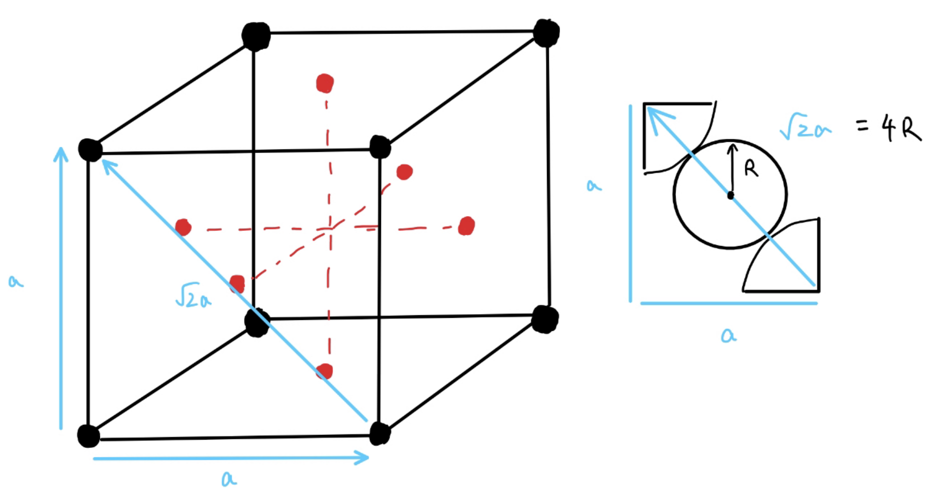
3 Question 3: [6 pts.]

Copper: atomic radius = 0.128 nm, FCC crystal structure, atomic weight = 63.5g/mol

3.a :



3.b :



$$a = \frac{4R}{\sqrt{2}} \tag{6}$$

3.c :

The theoretical density of an atom is defined as:

$$\rho = \frac{nA}{V_C N_A} \tag{7}$$

where n is the number of atoms per unit cell, A is the atomic weight, V_C is the volume of the unit cell, and N_A is Avogadro's Number (6.022×10^{23} atoms per mole).

- n = 4 atoms per unit cell (FCC crystal structure)

- A = 63.5 grams per mole

V_C requires the length of the unit cell, represented by a. The relationship between unit cell length, a, and atomic radius, as seen previously is:

$$a = \frac{4R}{\sqrt{2}} = \frac{4 \cdot 0.128 \text{ nm}}{\sqrt{2}} = 0.362 \text{ nm} \tag{8}$$

Now, the volume of the unit cell can be calculated since the unit cell is cubic (V = a^3).

$$V_C = a^3 = (0.362 \text{ nm})^3 = 0.0475 \text{ nm}^3 \tag{9}$$

Since we have all values needed to calculate for theoretical density:

$$\rho = \frac{nA}{V_C N_A} = \frac{4 \text{ atoms} \times 63.5 \frac{\text{g}}{\text{mol}}}{0.0475 \text{ nm}^3 \times 6.022 \times 10^{23} \frac{\text{atoms}}{\text{mol}}} = 8.888 \times 10^{-21} \frac{\text{g}}{\text{nm}^3} = 8.888 \frac{\text{g}}{\text{cm}^3} \tag{10}$$

The theoretical density is nearly the same as the known density:

$$\% \text{ Error} = \frac{8.94 - 8.888}{8.94} = 0.0058 = 0.6\% \tag{11}$$

There is a 0.6% error when calculating the theoretical value versus the known value, presumably due to lack of precision of significant digits.