MSE160 Problem Set 5

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1 Question 1: [4 pts.]

The origin used is the origin provided by the x, y, z axes.

1.a :

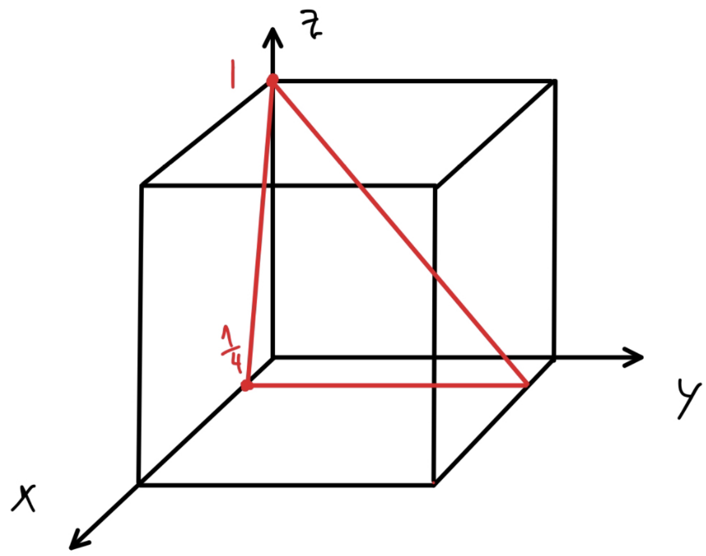
	x	y	z
Intercepts	1	1	-1
Reciprocals	$\frac{1}{1}$	$\frac{1}{1}$	$\frac{1}{-1}$
Reduction	1	1	-1
Miller Indices	$(11\bar{1})$		

	x	y	z
Intercepts	$\frac{1}{2}$	$\frac{1}{3}$	∞
Reciprocals	2	3	$\frac{1}{\infty}$
Reduction	2	3	0
Miller Indices	(230)		

1.b :

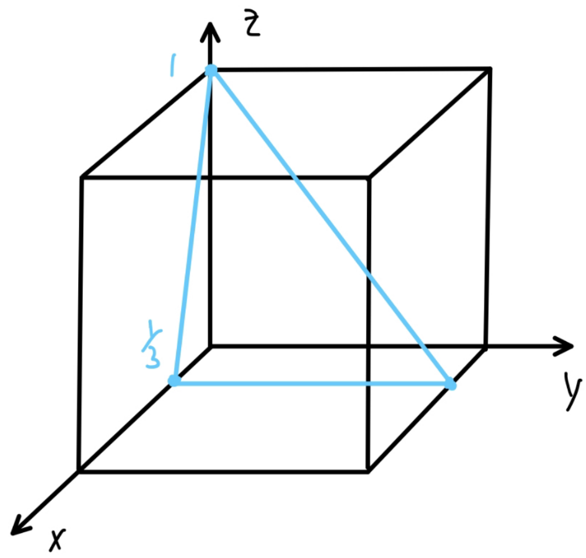
Miller Indices (401)

	x	y	z
Miller Indices	(401)		
Reduction	4	0	1
Reciprocals	4	$\frac{1}{\infty}$	$\frac{1}{1}$
Intercepts	$\frac{1}{4}$	∞	1



Miller Indices (301)

	x	y	z
Miller Indices	(301)		
Reduction	3	0	1
Reciprocals	3	$\frac{1}{\infty}$	$\frac{1}{1}$
Intercepts	$\frac{1}{3}$	∞	1



2 Question 2: [4 pts.]

The equation to measure the spacing between planes, d, is as follows:

$$d = \frac{n\lambda}{2\sin\theta_C} \tag{1}$$

However, the diffraction angle is measured as 2θ since the angle formed between the incident and reflected ray is 2θ.

$$2\theta \rightarrow 75.99^\circ \text{ , therefore } \theta \rightarrow 37.995^\circ \tag{2}$$

Assume that n = 1, $\lambda = 0.1659$ nm:

$$d = \frac{(1)(0.1659)}{2(\sin(37.995^\circ))} = 0.1347 \text{ nm} \tag{3}$$

In addition, the planar distance can also be represented as the ratio between the length of the unit cell, a, and the length of the unit vector:

$$d(hkl) = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \tag{4}$$

Solving for a (length of unit cell) in a (211) BCC structure:

$$a = d \cdot \sqrt{h^2 + k^2 + l^2} = 0.1347\text{nm} \cdot \sqrt{2^2 + 1^2 + 1^2} = 0.1347\text{nm} \cdot \sqrt{6} = 0.33041\text{nm} \tag{5}$$

In a BCC structure, the relationship between the atomic radius, R, and unit cell length, a, is:

$$4R = \sqrt{3}a \rightarrow R = \frac{\sqrt{3}a}{4} = \frac{\sqrt{3}(0.33041\text{nm})}{4} = 0.14296\text{nm} = 0.143\text{nm} \tag{6}$$

The atomic radius of the niobium (Nb) atom is 0.143 nm.

3 Question 3: [3 pts.]

The temperature of gold (Au) is 900°C, the energy formation is 0.98 eV/atom, the density of the atom is 18.63 $\frac{g}{cm^3}$, and the atomic weight is 196.9 $\frac{g}{mol}$.

To estimate the vacancy concentration, expressed as $\frac{N_V}{N}$, the formula:

$$\frac{N_V}{N} = \exp(\frac{-Q_V}{kT}) \tag{7}$$

where -Q_V is the energy formation, k is the Boltzmann's constant, T is the temperature in Kelvins, and N is expressed as:

$$N = \rho \times \frac{N_A}{A_{Au}} \times 1\text{m}^3 \tag{8}$$

where ρ is the density of the atom, A_Au is the atomic weight of gold (Au), and N_A is Avogadro's constant.

$$N = 18.63\frac{g}{cm^3} \times \frac{6.022 \times 10^{23}\frac{\text{atoms}}{mol}}{196.9\frac{g}{mol}} \times 1\text{m}^3 \times \frac{10^6\ \text{cm}^3}{1\text{m}^3} = 5.7 \times 10^{28}\ \text{Sites} \tag{9}$$

$$N_V = N \cdot \exp(\frac{-Q_V}{kT}) = 5.7 \times 10^{28} \cdot \exp(\frac{-0.98\frac{\text{eV}}{\text{atom}}}{(8.62 \times 10^{-5}\frac{\text{eV}}{\text{Atom-K}})(1173K)}) = 3.52 \times 10^{24}\ \text{Vacancies} \tag{10}$$

At 900°C, the gold atom has 3.52 × 10^{24} vacancies per cubic meter.

4 Question 4: [4 pts.]

4.a :

Interstitial diffusion refers to when an additional atom will diffuse in the crystal lattice structure, whereas substitutional diffusion refers to when an additional atom replaces one of the atoms in the crystal lattice.

4.b :

- One reason why interstitial diffusion is more rapid than vacancy diffusion is because the interstitial bonds between atoms is much weaker.
- In addition, there are many more interstitial sites for the atom to jump to rather than vacancy sites.

5 Question 5: [2 pts.]

If a linear concentration profile is assumed, it can be inferred that:

$$\frac{dC}{dx} \approx \frac{\Delta C}{\Delta x} = \frac{C_2 - C_1}{x_2 - x_1} \tag{11}$$

To calculate for flux, J, the following equation can be implemented:

$$J = -D\frac{dC}{dx} = -D\frac{\Delta C}{\Delta x} = -D\frac{C_2 - C_1}{x_2 - x_1} \tag{12}$$

where D $\equiv$ diffusion coefficient $= 6 \times 10^{-11}\frac{m^2}{s}$, $C_1 = 4\ \frac{kg}{m^3}$, $C_2 = 2\ \frac{kg}{m^3}$, and $J = 1.2\times\ 10^{-7}\frac{kg}{m\cdot s}$. Rearranging for Δx, we obtain:

$$\Delta x = -D\frac{\Delta C}{J} = -(6 \times 10^{-11}\frac{m^2}{s})\frac{2\frac{kg}{m^3} - 4\frac{kg}{m^3}}{1.2 \times 10^{-7}\frac{kg}{m\cdot s}} = 0.001\text{m} = 1\text{mm} \tag{13}$$

Therefore, the sheet will have a concentration of 2 $\frac{kg}{m^3}$ 1.0 millimeter deep into the 1.5 millimeter deep sheet.