ENGG*2120 Materials Science
Assignments: Chapter 3 with Answers

1. Describe the difference between atomic structure and crystal structure.

Ans:

Atomic structure relates to the number of protons and neutrons in the nucleus of an atom, as well as the number and probability distributions of the constituent electrons. On the other hand, crystal structure pertains to the arrangement of atoms in the crystalline solid material.

2. a) Explain what is meant by atomic packing factor and coordination number.

b) Find atomic packing factor and co-ordination number of body-centered cubic crystal structure.

Ans:

a) Atomic packing factor is defined as sum of the sphere volumes of all atoms within a unit cell divided by the unit cell volume.

Number of closest neighbours to which an atom is bonded is called co-ordinate number.

b) The atomic packing factor is defined as the ratio of sphere volume (*Vs*) to the total unit cell volume (*Vc*), or

$$\text{APF} = \frac{V_S}{V_C}$$

Since there are two spheres associated with each unit cell for BCC

$$V_S = 2(\text{sphere volume}) = 2\left(\frac{4\pi R^3}{3}\right) = \frac{8\pi R^3}{3}$$

Also, the unit cell has cubic symmetry, that is $V_C = a^3$. But a depends on R

$$a = \frac{4R}{\sqrt{3}}$$

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

Thus,

$$\text{APF} = \frac{V_S}{V_C} = \frac{8\pi R^3/3}{64R^3/3\sqrt{3}} = 0.68$$

The atomic packing factor for BCC is 0.68.

Co-ordination number of BCC is 8

3. Niobium, Nb (Atomic weight is 92.90638 gm/mol) has atomic radius of 0.143 nm and density of 8.57 gm/cc. Determine whether it has an FCC or BCC crystal structure.

Ans:

In order to determine whether Nb has an FCC or a BCC crystal structure, we need to compute its density for each of the crystal structures. For FCC, $n = 4$, and $a = 2R\sqrt{2}$. Also, its atomic weight is 92.91 g/mol. Thus, for FCC

$$\rho = \frac{nA_{\text{Nb}}}{a^3 N_A} = \frac{nA_{\text{Nb}}}{(2R\sqrt{2})^3 N_A}$$

$$= \frac{(4 \text{ atoms/unit cell})(92.91 \text{ g/mol})}{\left\{\left[(2)(1.43 \times 10^{-8} \text{ cm})(\sqrt{2})\right]^3 /(\text{unit cell})\right\}(6.023 \times 10^{23} \text{ atoms/mol})}$$

$$= 9.33 \text{ g/cm}^3$$

$$\text{For BCC, } n = 2\text{, and } a = \frac{4R}{\sqrt{3}}$$

$$\rho = \frac{nA_{\text{Nb}}}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_A}$$

$$\rho = \frac{(2 \text{ atoms/unit cell})(92.91 \text{ g/mol})}{\left\{\left[\frac{(4)(1.43 \times 10^{-8} \text{ cm})}{\sqrt{3}}\right]^3 /(\text{unit cell})\right\}(6.023 \times 10^{23} \text{ atoms/mol})}$$

$$= 8.57 \text{ g/cm}^3$$

which is the value provided in the problem statement. Therefore, Nb has a BCC crystal structure.

4. Calculate the radius of a palladium atom, given that Pd has an FCC crystal structure, a density of 12.0 gm/cm^3 and atomic weight of 106.4 g/mol.

Ans:

For FCC, n = 4 atoms/unit cell, and $V_C = 16R^3\sqrt{2}$

Now,

$$\rho = \frac{nA_{\text{Pd}}}{V_C N_A}$$

$$= \frac{nA_{\text{Pd}}}{(16R^3\sqrt{2})N_A}$$

And solving for R from the above expression yields

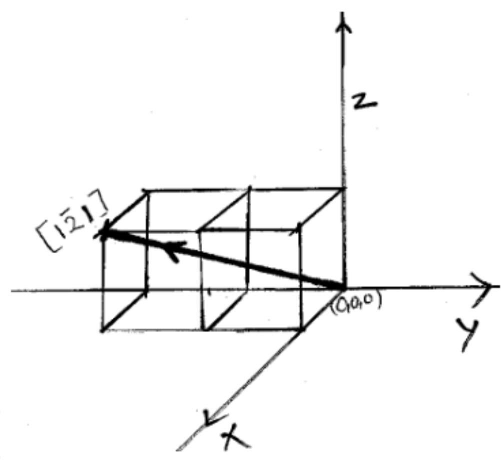
$$R = \left(\frac{nA_{Pd}}{16\rho N_A \sqrt{2}} \right)^{1/3}$$

$$= \left[\frac{(4 \text{ atoms/unit cell})(106.4 \text{ g/mol})}{(16)(12.0 \text{ g/cm}^3)(6.02 \times 10^{23} \text{ atoms/mol})(\sqrt{2})} \right]^{1/3}$$

$= 1.36 \times 10^{-8}$ cm = 0.136 nm

5. Draw [1 $\bar{2}$ 1] direction in a cubic unit cell.

Ans:



6. Draw ($\bar{2}$ 1 0) plane in a cubic unit cell.

Ans:

Given miller indices ($\bar{2}$ 1 0)

Take reciprocal $\frac{1}{-2}$, $\frac{1}{1}$, $\frac{1}{0}$

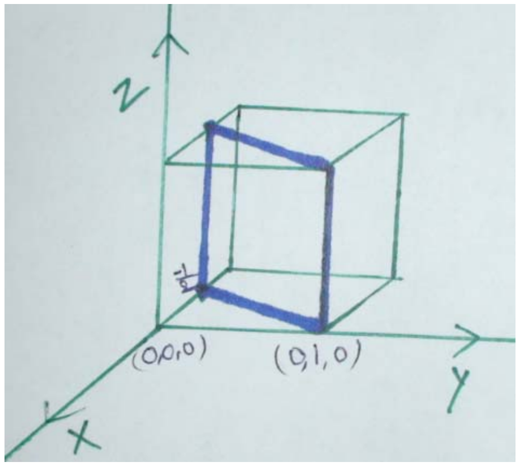
$\frac{1}{-2}$, 1, ∞

Intercept on X-axis = - ½

Intercept on Y-axis = 1

Plane is parallel to Z-axis.

The plane (2 1 0) in a cubic unit cell is as shown in figure.



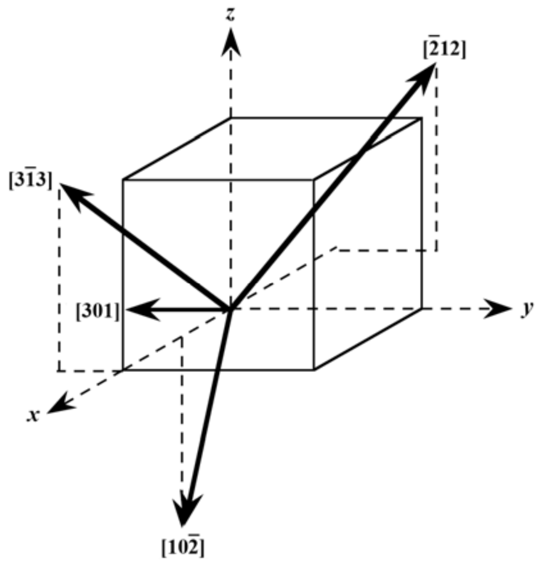
7. Within a cubic unit cell, sketch the following directions:

(a) $[10\bar{2}]$, (c) $[\bar{2}12]$,

(b) $[3\bar{1}3]$, (d) $[301]$.

Ans:

The directions asked for are indicated in the cubic unit cell shown below.

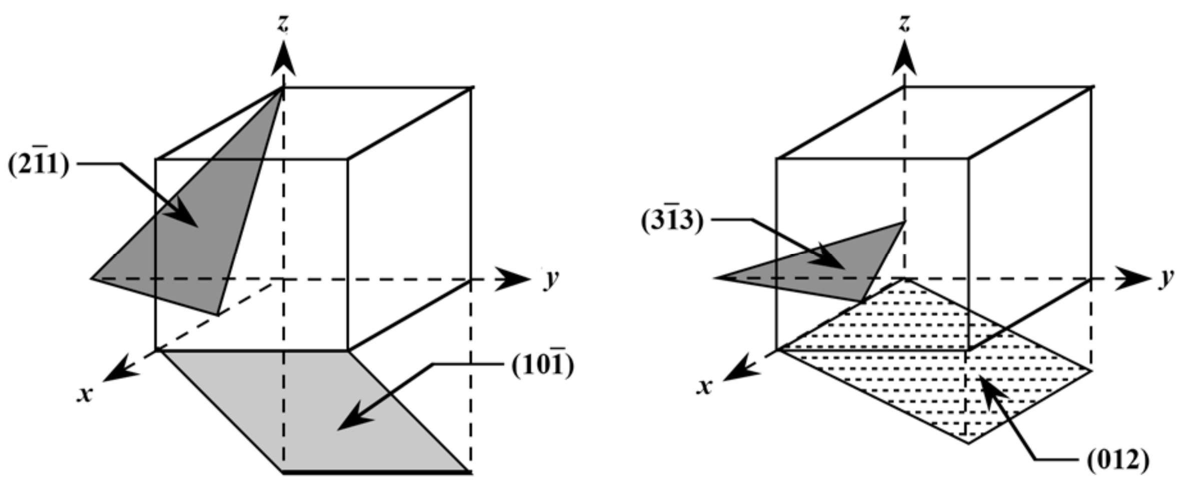


8. Sketch within a cubic unit cell the following planes:

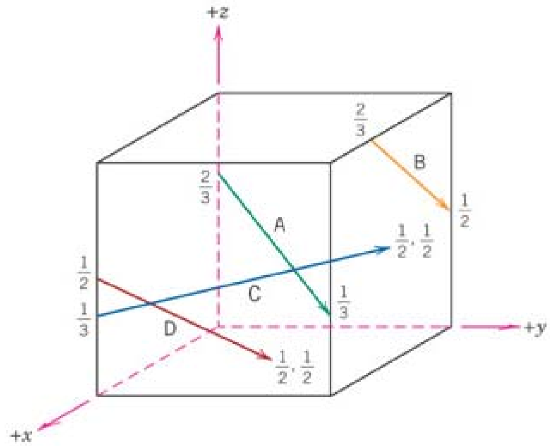
(a) $(2\bar{1}1)$ (b) $(10\bar{1})$, (c) $(3\bar{1}3)$, (d) (012)

Ans:

The planes called for are plotted in the cubic unit cells shown below.



9. Determine the indices of directions shown in following figure.



Ans:

Direction A is a $[33\bar{1}]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	a	b	$-\frac{c}{3}$
Projections in terms of a, b, and c	1	1	$-\frac{1}{3}$
Reduction to integers	3	3	-1
Enclosure		$[33\bar{1}]$	

Direction B is a $[\bar{4}0\bar{3}]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z

Projections	$-\frac{2a}{3}$	$0b$	$-\frac{c}{2}$
Projections in terms of *a*, *b*, and *c*	$-\frac{2}{3}$	0	$-\frac{1}{2}$
Reduction to integers	–4	0	–3
Enclosure		$[\bar{4}0\bar{3}]$	

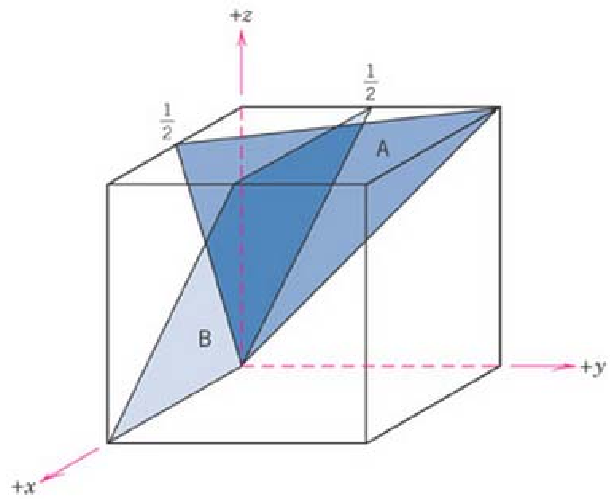
Direction C is a $[\bar{3}61]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$-\frac{a}{2}$	b	$\frac{c}{6}$
Projections in terms of *a*, *b*, and *c*	$-\frac{1}{2}$	1	$\frac{1}{6}$
Reduction to integers	–3	6	1
Enclosure		$[\bar{3}61]$	

Direction D is a $[\bar{1}1\bar{1}]$ direction, which determination is summarized as follows. We first of all position the origin of the coordinate system at the tail of the direction vector; then in terms of this new coordinate system

	x	y	z
Projections	$-\frac{a}{2}$	$\frac{b}{2}$	$-\frac{c}{2}$
Projections in terms of *a*, *b*, and *c*	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$
Reduction to integers	–1	1	–1
Enclosure		$[\bar{1}1\bar{1}]$	

10. Determine the Miller indices for the planes shown in the following unit cell:



Ans:

For plane A since the plane passes through the origin of the coordinate system as shown, we will move the origin of the coordinate system one unit cell distance vertically along the *z* axis; thus, this is a $(21\bar{1})$ plane, as summarized below.

	x	y	z
Intercepts	$\frac{a}{2}$	b	$-c$
Intercepts in terms of *a*, *b*, and *c*	$\frac{1}{2}$	1	– 1
Reciprocals of intercepts	2	1	– 1
Reduction		not necessary	
Enclosure		$(21\bar{1})$	

For plane B, since the plane passes through the origin of the coordinate system as shown, we will move the origin one unit cell distance vertically along the *z* axis; this is a $(02\bar{1})$ plane, as summarized below.

	x	y	z
Intercepts	∞a	$\frac{b}{2}$	$-c$

Intercepts in terms of *a*, *b*, and *c*	∞	$\frac{1}{2}$	– 1
Reciprocals of intercepts	0	2	– 1
Reduction		not necessary	
Enclosure		$(02\bar{1})$	