

1. Tantalum has a BCC crystal structure with an atomic weight of 180.948 g/mol. If the density of Tantalum is 16.6826 g/cm³, calculate the radius of its atom in nanometer?

Solution:

$$\begin{aligned} &>> \text{density} = n \cdot A / (V_c \cdot N_a) \\ &\rightarrow V_c = n \cdot A / (\text{density} \cdot N_a) \end{aligned}$$

$$\begin{aligned} &>> n = 2; \\ &>> \text{density} = 16.6826 \text{ g/cm}^3; \\ &>> A = 180.948 \text{ g/mol}; \\ &>> N_a = 6.023 \times 10^{23}; \end{aligned}$$

$$V_c = n \cdot A / (\text{density} \cdot N_a) = 3.6017 \times 10^{-23} \text{ cm}^3$$

$$\text{The lattice parameter is } a = V_c^{(1/3)} = 3.3024 \times 10^{-8} \text{ cm}$$

For BCC, $a = 4R / \sqrt{3}$

$$\rightarrow \text{The radius of V is } R = a \cdot \sqrt{3} / 4 = 1.43 \times 10^{-8} \text{ cm} = \underline{0.1430 \text{ nm}}$$

2. Determine whether Rhodium has an FCC or BCC crystal structure if it has an atomic radius of 0.1345 nm, a density of 12.41 g/cm³, and an atomic weight of 102.9055 g/mol.

Solution:

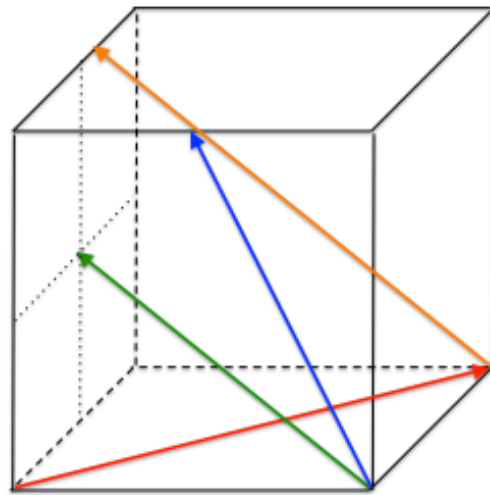
Let us assume that Rhodium has a BCC crystal structure, then $n=2$ & $a=4R/\sqrt{3}$ \rightarrow $\text{density} = n \cdot A / (V_c \cdot N_a) = 11.4023 \text{ g/cm}^3$ which is not equal to the value given in the problem.

Thus, Rhodium should have an FCC crystal structure. To check that, for FCC: $n=4$ & $a=4R/\sqrt{2}$ \rightarrow $\text{density} = n \cdot A / (V_c \cdot N_a) = 12.4132 \text{ g/cm}^3$ which is the value given in the problem.

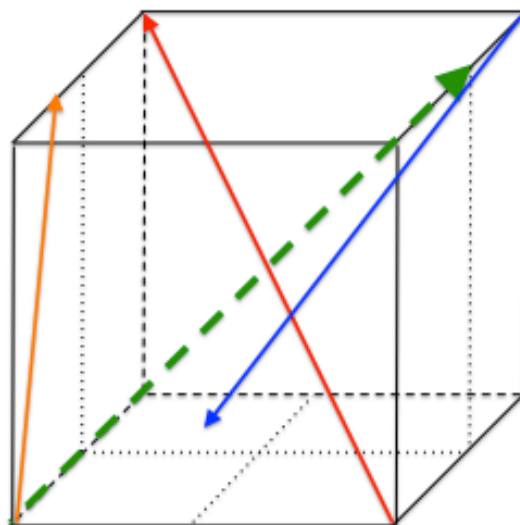
3. Sketch the following directions within a cubic unit cell (you can draw more than one unit cell to indicate the directions):

- | | |
|---------------------|---------------------------|
| (a) $[\bar{1}10]$, | (e) $[\bar{1}\bar{1}1]$, |
| (b) $[\bar{1}21]$, | (f) $[\bar{1}22]$, |
| (c) $[0\bar{1}2]$, | (g) $[\bar{1}2\bar{3}]$, |
| (d) $[1\bar{3}3]$, | (h) $[\bar{1}03]$ |

Solution:

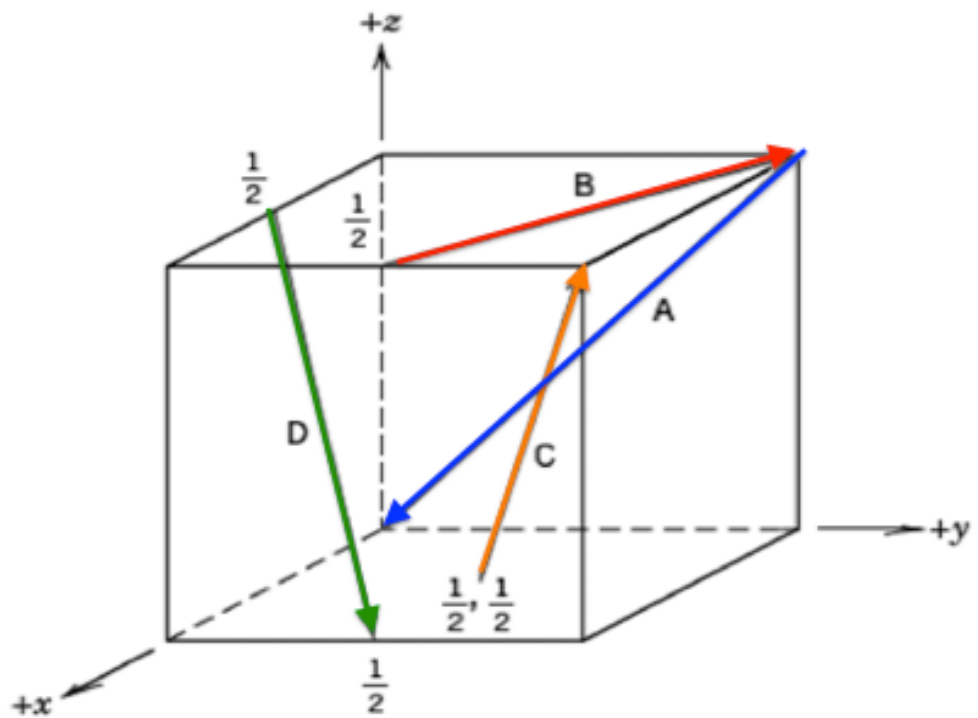


- (a) $[-1\ 1\ 0]$ Red
- (b) $[-1\ -2\ 1]$ Green
- (c) $[0\ -1\ 2]$ Blue
- (d) $[1\ -3\ 3]$ Orange



- e) $[-1\ -1\ 1]$ Red
- f) $[-1\ 2\ 2]$ Green
- g) $[1\ -2\ -3]$ Blue
- h) $[-1\ 0\ 3]$ Orange

4. Determine the indices for the following directions shown in the cubic unit cell:



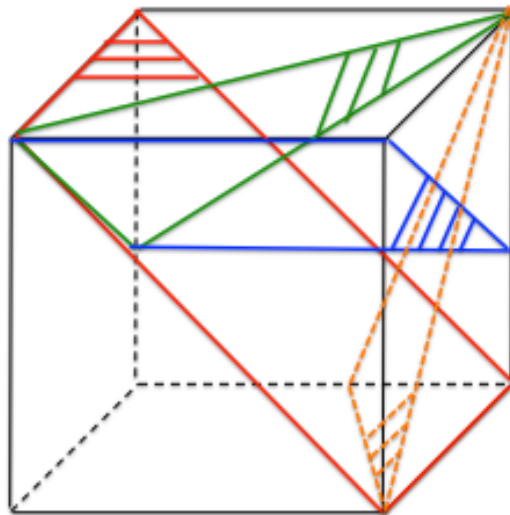
Solution:

A.	B.	C.	D.
$[0\bar{1}\bar{1}]$	$[\bar{2}10]$	$[112]$	$[11\bar{2}]$

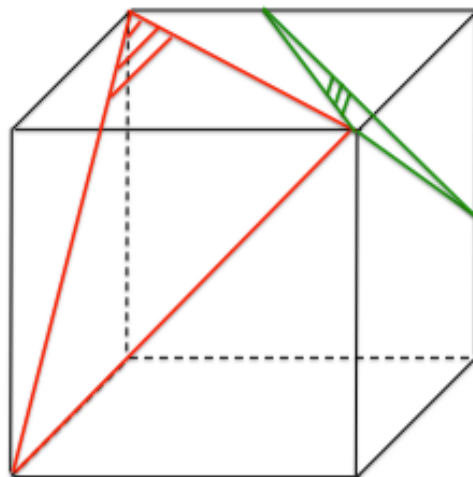
5. Sketch within a cubic unit cell the following planes:

- | | |
|---------------------------|---------------------------|
| (a) $(0\bar{1}\bar{1})$, | (e) $(\bar{1}1\bar{1})$, |
| (b) $(11\bar{2})$, | (f) $(1\bar{2}\bar{2})$, |
| (c) $(10\bar{2})$, | (g) $(\bar{1}2\bar{3})$, |
| (d) $(1\bar{3}1)$, | (h) $(0\bar{1}\bar{3})$ |

Solution:

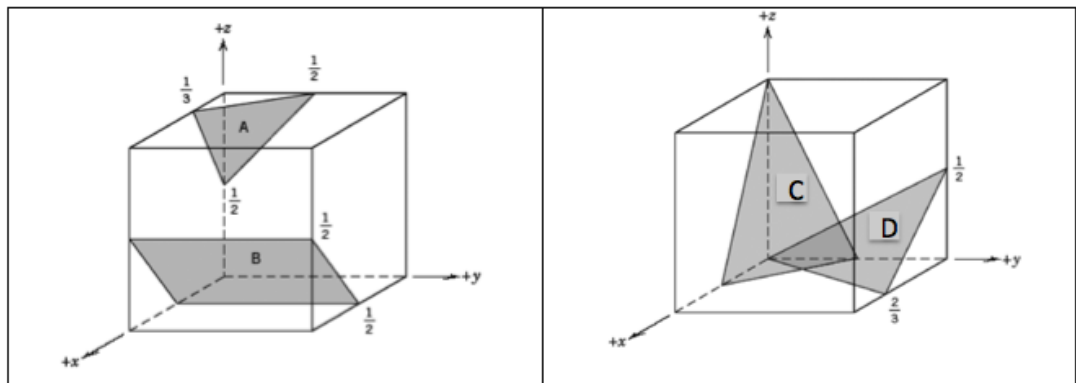


- (a) $(0 -1 -1)$ Red
- (b) $(1 1 -2)$ Green
- (c) $(1 0 -2)$ Blue
- (d) $(1 -3 1)$ Orange



- e) $(-1 1 -1)$ Red
- f) $(1 -2 -2)$ Green
- g) $(-1 2 -3)$ Not shown
- h) $(0 -1 -3)$ Not shown

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

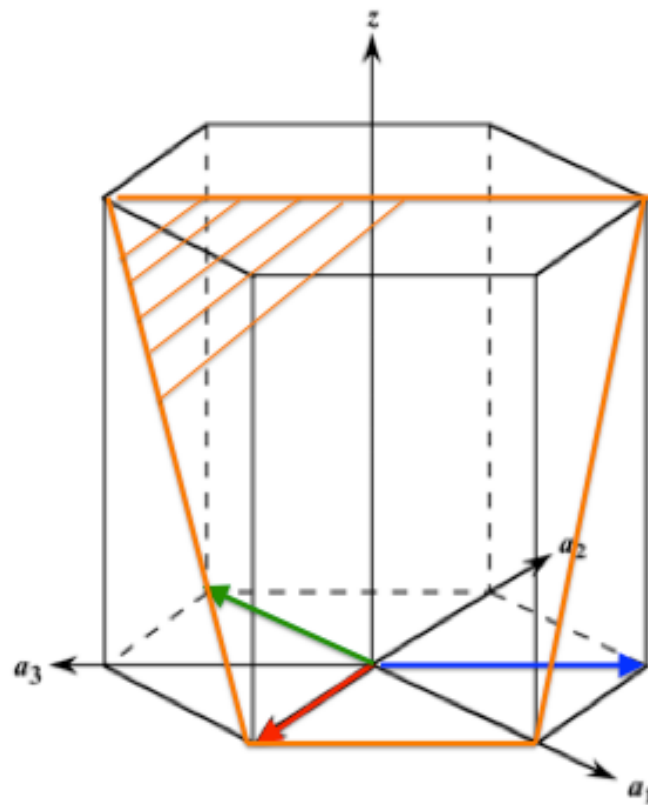


Solution:

A.	B.	C.	D.
$(3\bar{2}\bar{2})$	$(\bar{1}01)$	(221)	$(3\bar{2}4)$

7. Sketch the following planes and directions in HCP unit cell:
 $(1\bar{1}01)$, $[11\bar{2}0]$, (0001) , $[\bar{2}110]$, and $[1\bar{2}10]$.

Solution:



- $[1 -2 1 0]$ Red
- $[1 1 -2 0]$ Blue
- $[-2 1 1 0]$ Green
- $(1 -1 0 1)$ Orange
- (0001) Basal plane

8. Calculate the atomic radius for aluminum given that Al has an FCC crystal structure and a planar density of $1.412 \times 10^{17} \text{ m}^{-2}$ for the (111) plane. What are the values of the linear density for the [100], [110], and [111] directions.

The planar density for the (111) plane in FCC crystal is given by

$$\begin{aligned} PD_{(111)\text{FCC}} &= 4 / (\sqrt{3} * a^2) \quad (\text{See Ch.3}) \\ \rightarrow a &= \sqrt{4 / (\sqrt{3} * PD_{(111)\text{FCC}})} \\ &= \sqrt{4 / (\sqrt{3} * 1.412 \times 10^{17})} \\ &= 4.0442 \times 10^{-9} \text{ m} = 0.404 \text{ nm} \end{aligned}$$

For FCC, the relation between a and R:

$$\begin{aligned} \sqrt{2} a &= 4 R \\ \rightarrow R &= \sqrt{2} * 0.404 / 4 \\ &= \underline{1.4298 \text{ nm}} \end{aligned}$$

The values of the linear density for the [100], [110], and [111] directions are:

$$\begin{aligned} LD_{[100]\text{FCC}} &= 1 / a = 2.4727 \times 10^8 \text{ atom/m} \\ LD_{[110]\text{FCC}} &= 2 / (\sqrt{2} * a) = \mathbf{3.4969 \times 10^8 \text{ atom/m}} \\ LD_{[111]\text{FCC}} &= 1 / (\sqrt{3} * a) = 1.4276 \times 10^8 \text{ atom/m} \end{aligned}$$

Please note that the highest linear density in FCC is along [110], which is the closed-packed direction.