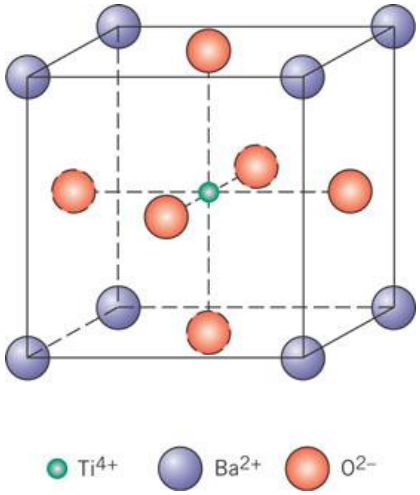
春意盎然、喜迎两会之材料科学基础作业 8

Fundamentals of Materials Science

Homework 8, SS 2017

Point Coordinates

1. List the point coordinates of the titanium, barium, and oxygen ions for a unit cell of the perovskite crystal structure (Figure shown below).



Solution:

the point coordinates of the **titanium** :

$$\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$$

the point coordinates of the **barium** :

$$(0,0,0);(1,0,0);(0,1,0);(1,1,0);(0,0,1);(1,0,1);(0,1,1);(1,1,1)$$

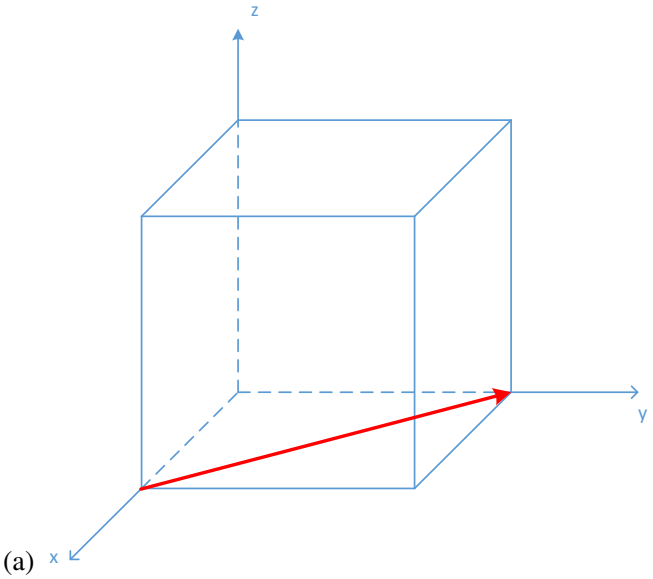
the point coordinates of the **oxygen** :

$$\left(\frac{1}{2},\frac{1}{2},0\right);\left(1,\frac{1}{2},0\right);\left(\frac{1}{2},0,\frac{1}{2}\right);\left(0,\frac{1}{2},\frac{1}{2}\right);\left(\frac{1}{2},1,\frac{1}{2}\right);\left(\frac{1}{2},\frac{1}{2},1\right)$$

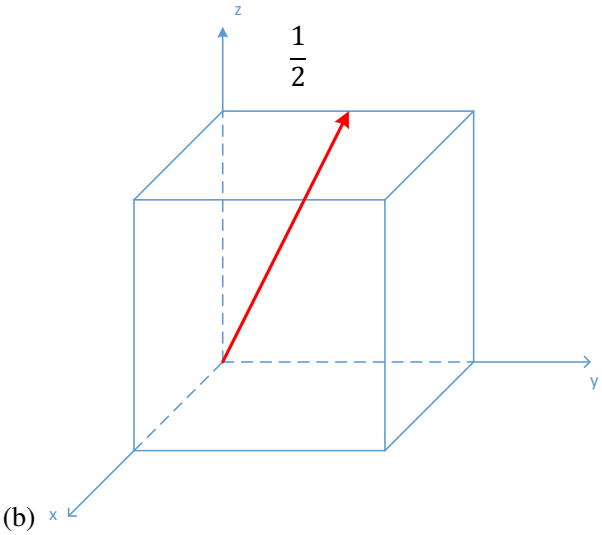
Crystallographic directions

2. Sketch the following directions in unit cells. One unit cell for one direction!

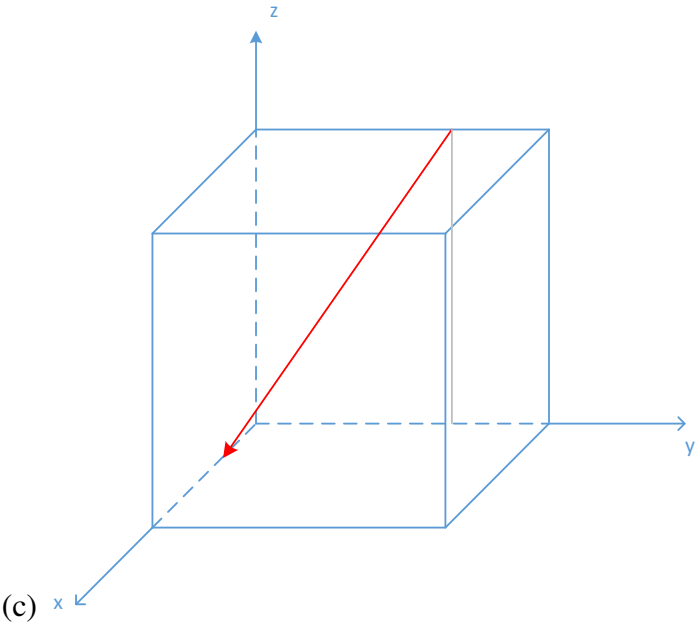
(a) $[\bar{1}10]$; **(b)** $[0\bar{1}2]$; **(c)** $[1\bar{2}\bar{3}]$



(a)

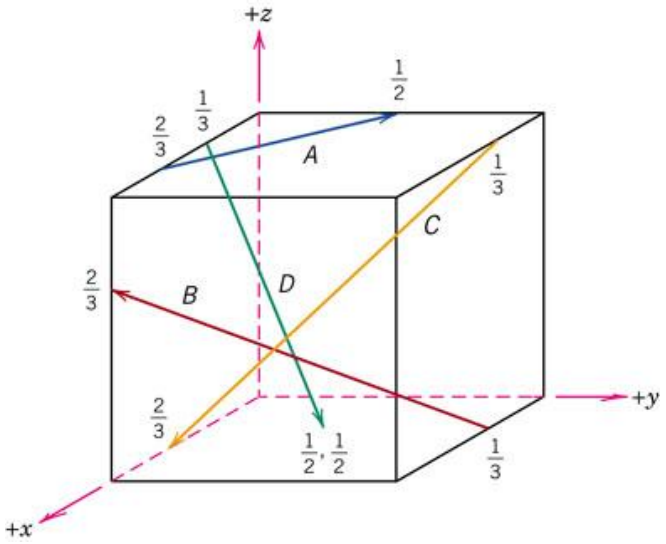


(b)



(c)

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



Solution:

Direction A

	x	***y***	***z***
Projections	-2a/3	b/2	0
Projections in terms of a, b, and c	-2/3	1/2	0
Reductions to integers	-4	3	0
Enclosure	[$\bar{4}$ 3 0]		

Direction B

	x	***y***	***z***
Projections	2a/3	-b	2c/3
Projections in terms of a, b, and c	2/3	-1	2/3
Reductions to integers	2	-3	2
Enclosure	[2 $\bar{3}$ 2]		

Direction C

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

Direction D

	x	***y***	***z***
Projections	a/6	b/2	-c

Projections in terms of a, b, and c	1/6	1/2	-1
Reductions to integers	1	3	-6
Enclosure	[1 3 $\bar{6}$]		

4. Convert the [100] and [111] directions into the four-index Miller–Bravais scheme for hexagonal unit cells.

Solution

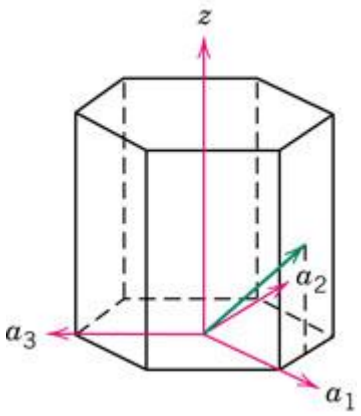
[100]

$$u = \frac{1}{3}(2u' - v') = \frac{2}{3}$$
$$v = \frac{1}{3}(2v' - u') = -\frac{1}{3}$$
$$t = -(u + v) = -\frac{1}{3}$$
$$w = w' = 0$$
$$\therefore [2\bar{1}\bar{1}0]$$

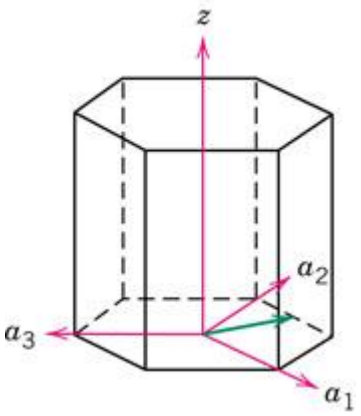
[111]

$$u = \frac{1}{3}(2u' - v') = \frac{1}{3}$$
$$v = \frac{1}{3}(2v' - u') = \frac{1}{3}$$
$$t = -(u + v) = -\frac{2}{3}$$
$$w = w' = 1$$
$$\therefore [11\bar{2}3]$$

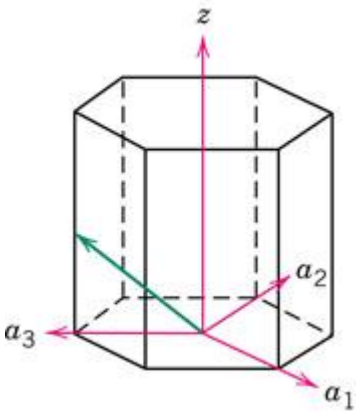
5. Determine indices for the directions shown in the following hexagonal unit cells:



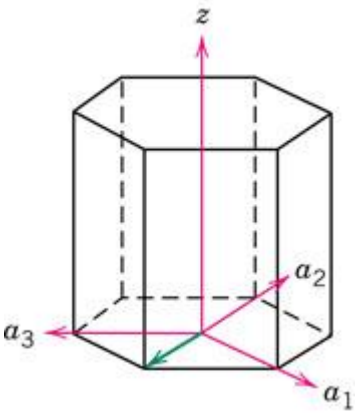
(a)



(b)



(c)



(d)

Solution

(a)

$$u' = 1$$
$$v' = \frac{1}{2}$$
$$u = \frac{1}{3}(2u' - v') = \frac{1}{2}$$
$$v = \frac{1}{3}(2v' - u') = 0$$
$$t = -(u + v) = -\frac{1}{2}$$
$$w = w' = \frac{1}{2}$$
$$[10\bar{1}1]$$

(b)

$$u' = \frac{1}{2}$$
$$v' = 1$$
$$u = \frac{1}{3}(2u' - v') = 0$$
$$v = \frac{1}{3}(2v' - u') = \frac{1}{2}$$
$$t = -(u + v) = -\frac{1}{2}$$
$$w = w' = 0$$
$$[01\bar{1}0]$$

(c)

$$u' = -1$$
$$v' = -1$$
$$u = \frac{1}{3}(2u' - v') = -\frac{1}{3}$$

$$v = \frac{1}{3}(2v' - u') = -\frac{1}{3}$$
$$t = -(u + v) = \frac{2}{3}$$
$$w = w' = 1/2$$
$$[\bar{2}\bar{2}43]$$

(d)

$$u' = 0$$
$$v' = -1$$
$$u = \frac{1}{3}(2u' - v') = \frac{1}{3}$$
$$v = \frac{1}{3}(2v' - u') = -\frac{2}{3}$$
$$t = -(u + v) = \frac{1}{3}$$
$$w = w' = 0$$
$$[1\bar{2}10]$$

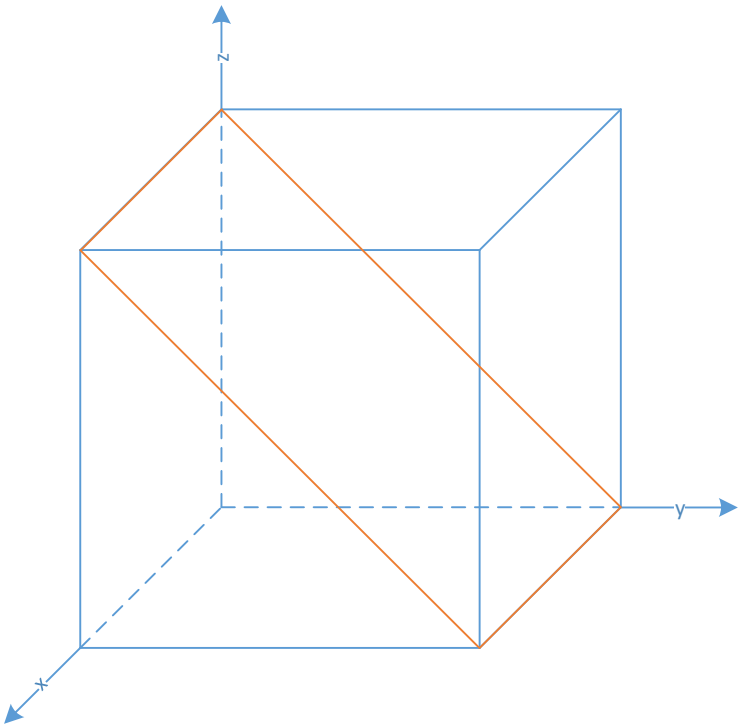
Crystallographic planes

6. Sketch the following planes. One plane in one unit cell.

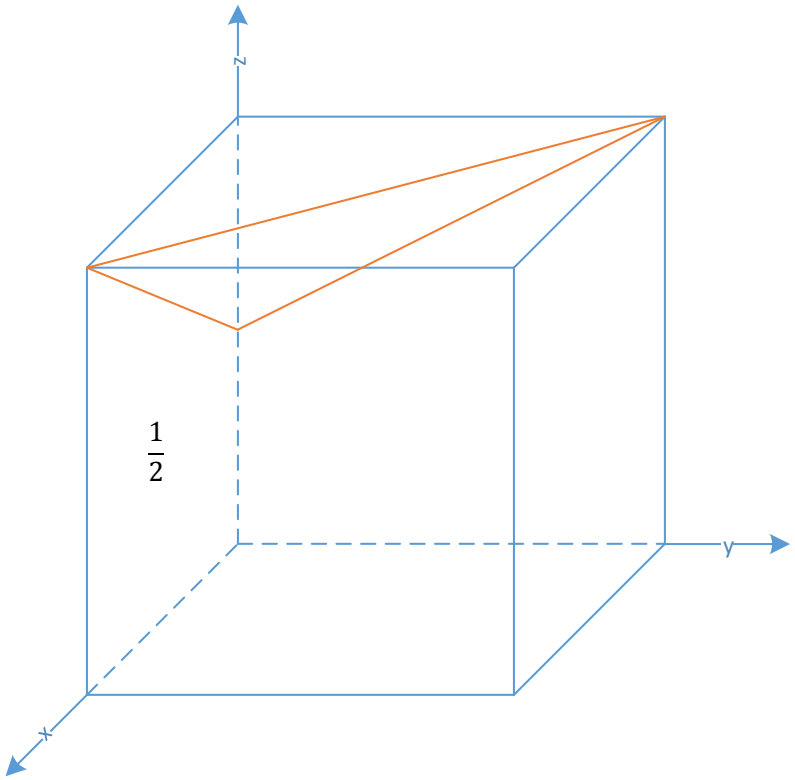
(a) $(0\bar{1}\,\bar{1})$**;** **(b)** $(11\bar{2})$**;** **(c)** $(1\bar{3}1)$

Solution

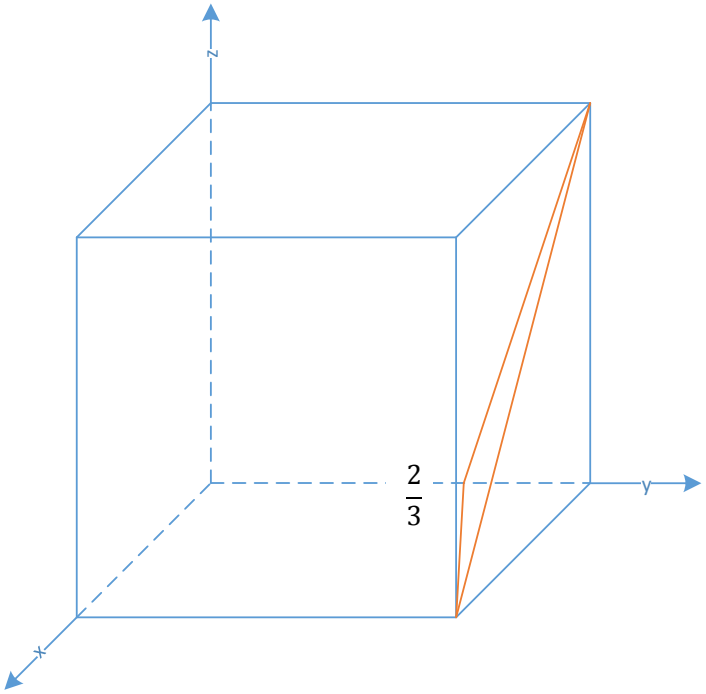
(a)



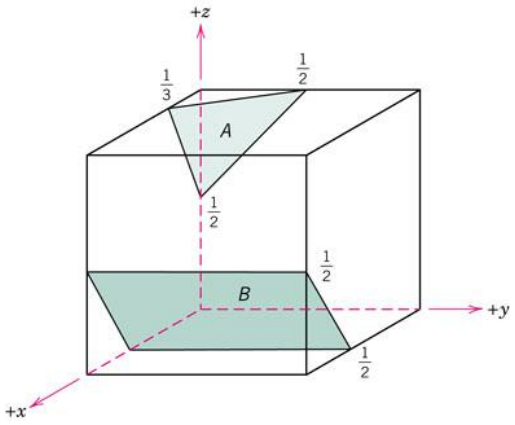
(b)



(c)



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



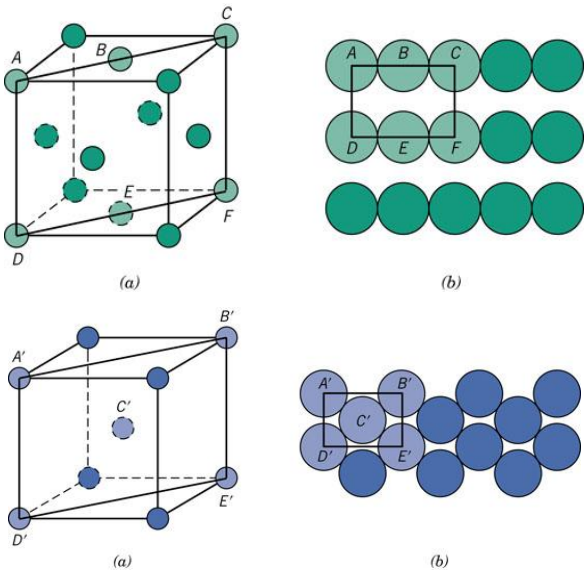
Solution

$$A(32\bar{2})$$
$$B(\bar{2}02)$$

Equivalent Directions and Planes

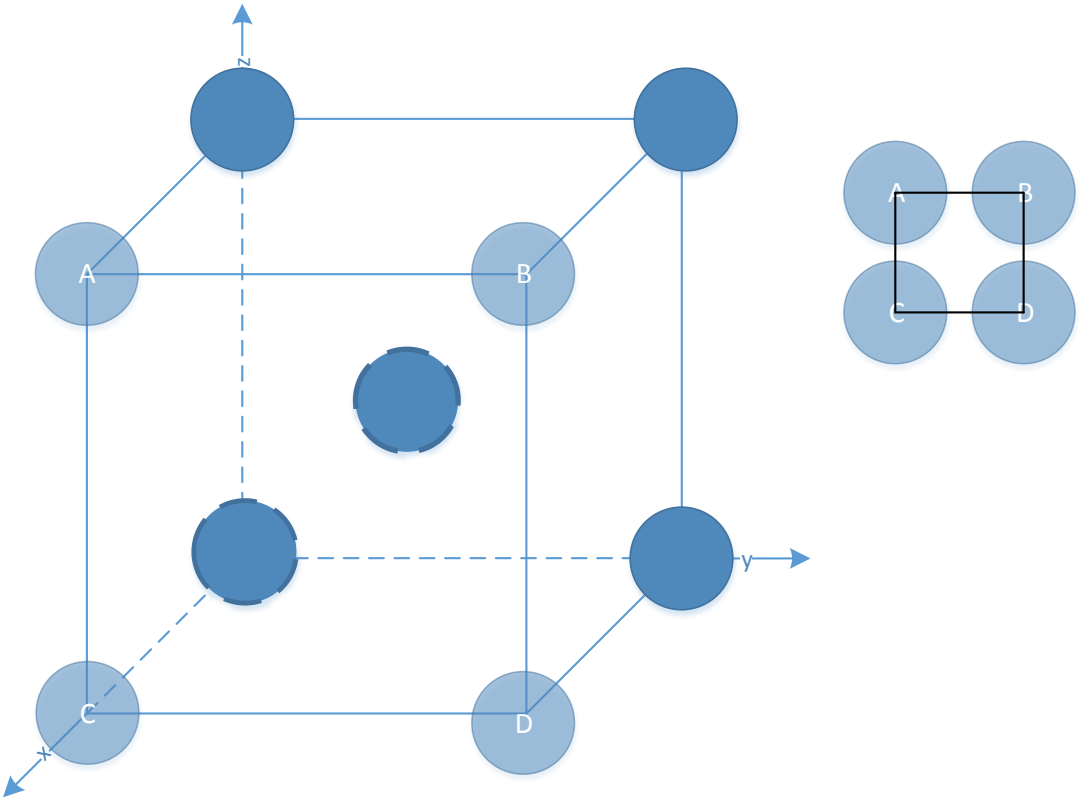
8. Sketch the atomic packing of **(a)** the (100) plane for the BCC crystal structure, and **(b)** the (201) plane for the FCC crystal structure. Examples of such drawings are shown below.

Examples: Atomic packing of (110) plane in FCC and BCC unit cell.

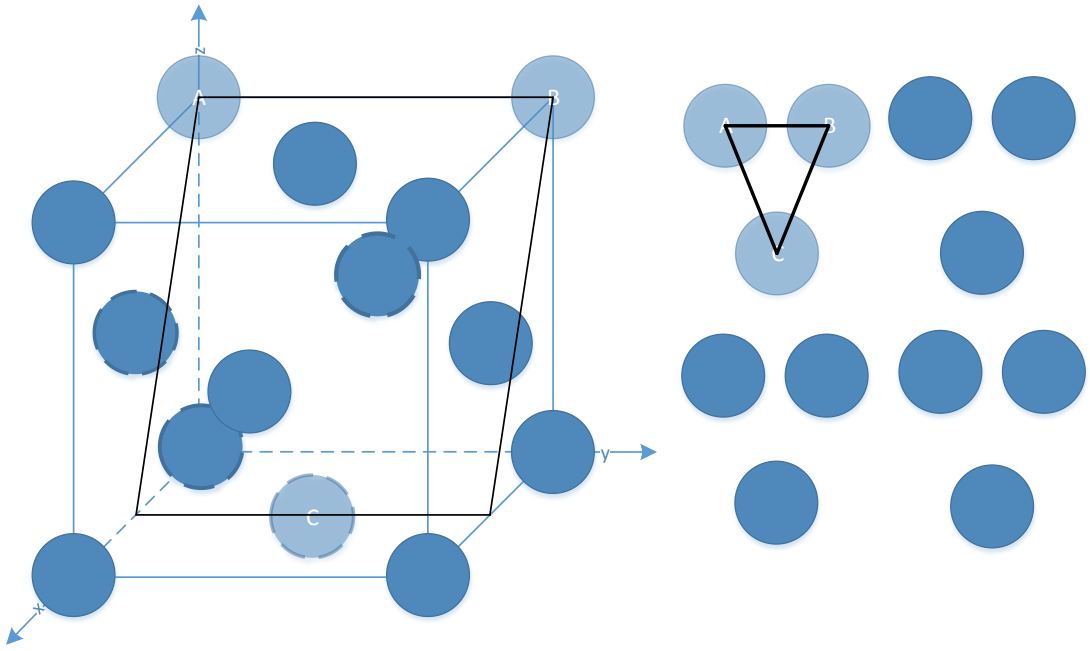


Solution

(a)

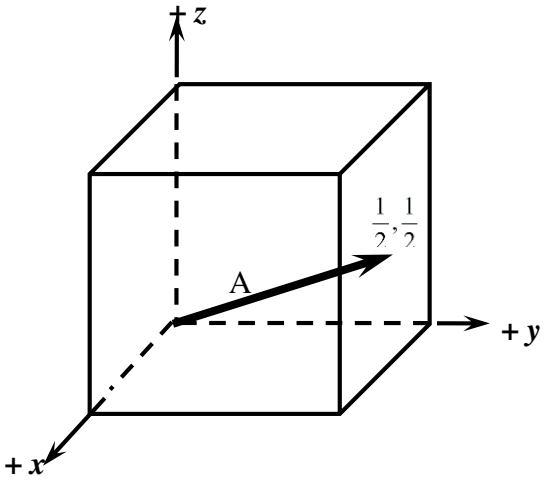


(b)



Template for doing directions or plane indices problems

Example: find the indices for the following crystallographic direction:



Direction A

	x	*y*	*z*
Projections	a/2	b	c/2
Projections in terms of a, b, and c	1/2	1	1/2
Reductions to integers	1	2	1
Enclosure	[1 2 1]		

Please complete the crystallographic direction problems with the above suggested format.