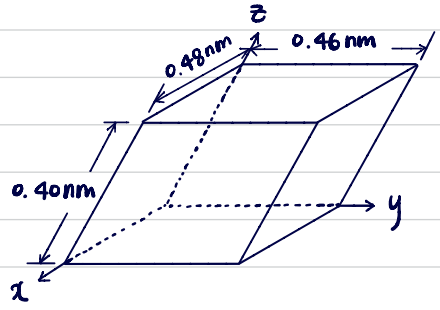
Example Problem 3.1

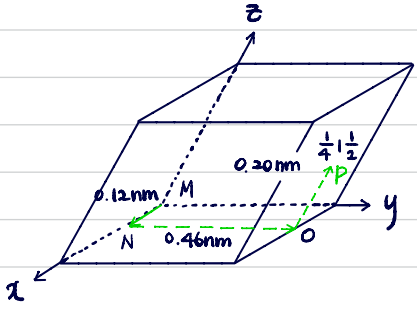


$\frac{1}{4}$ 1 $\frac{1}{2}$

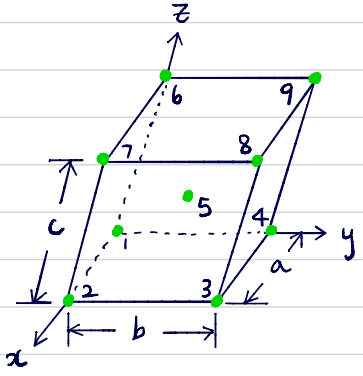
x : $qa = \frac{1}{4} \times 0.48nm = 0.12nm.$

y : $rb = 1 \times 0.46nm = 0.46nm.$

z : $sc = \frac{1}{2} \times 0.40nm = 0.20nm.$



Example Problem 3.2



point 1 : $qa = 0$, $rb = 0$, $sc = 0$. $\Rightarrow$ $q = r = s = 0$.

point 2 : $qa = a$, $rb = 0$, $sc = 0$. $\Rightarrow$ $q = 1$, $r = s = 0$.

point 3 : $qa = a$, $rb = b$, $sc = 0$. $\Rightarrow$ $q = r = 1$, $s = 0$.

point 4 : $qa = a$, $rb = 0$, $sc = c$. $\Rightarrow$ $q = s = 1$, $r = 0$.

point 5 : $qa = \frac{1}{2}a$, $rb = \frac{1}{2}b$, $sc = \frac{1}{2}c$. $\Rightarrow$ $q = r = s = \frac{1}{2}$.

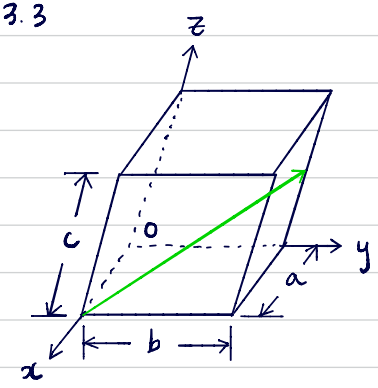
point 6 : $qa = 0$, $rb = 0$, $sc = c$. $\Rightarrow$ $q = r = 0$, $s = 1$.

point 7 : $qa = a$, $rb = 0$, $sc = c$. $\Rightarrow$ $q = s = 1$, $r = 0$.

point 8 : $qa = a$, $rb = b$, $sc = c$. $\Rightarrow$ $q = r = s = 1$.

point 9 : $qa = 0$, $rb = b$, $sc = c$. $\Rightarrow$ $q = 0$, $r = s = 1$.

Example Problem 3.3



tail
$\begin{cases} x_1 = a \\ y_1 = 0 \\ z_1 = 0 \end{cases}$

head
$\begin{cases} x_2 = 0 \\ y_2 = b \\ z_2 = \frac{1}{2}c \end{cases}$

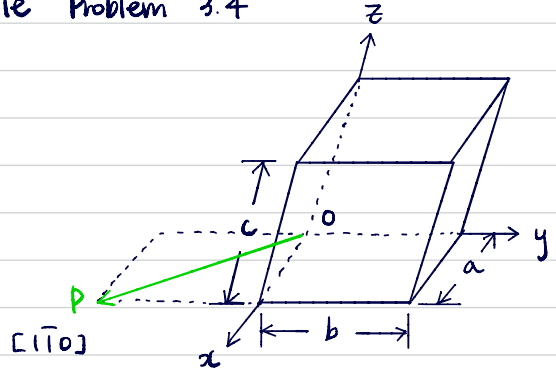
$u = 2 \cdot \frac{0-a}{a} = -2.$

$v = 2 \cdot \frac{b-0}{b} = 2.$

$w = 2 \cdot \frac{\frac{1}{2}c - 0}{c} = 1.$

$\therefore [\bar{2}21].$

Example Problem 3.4



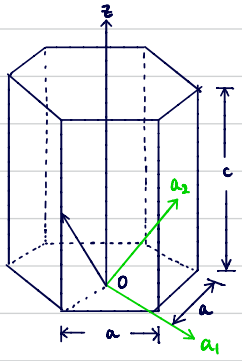
$[1\bar{1}0] \rightarrow u = 1 = \frac{x_2 - 0}{a}$

$v = -1 = \frac{-y_2 - 0}{b}$

$w = 0 = \frac{z_2 - 0}{c}.$

$\therefore x_2 = a, \quad y_2 = -b, \quad z_2 = 0c.$

Example Problem 3.5



$[\ 0 \quad -1 \quad \frac{1}{2}\ ]$

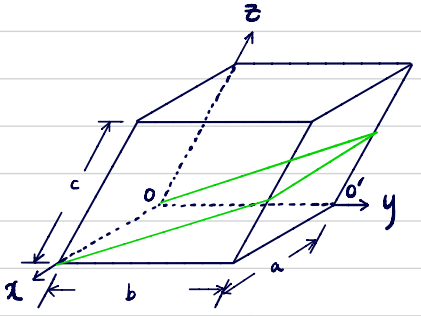
$[\ 0 \quad -2 \quad 1\ ]$

$[\ \frac{2}{3} \quad -\frac{4}{3} \quad \frac{2}{3} \quad 1\ ]$

$[\ 2 \quad -4 \quad 2 \quad 3\ ]$

$\therefore [2\bar{4}23]$

Example Problem 3.6



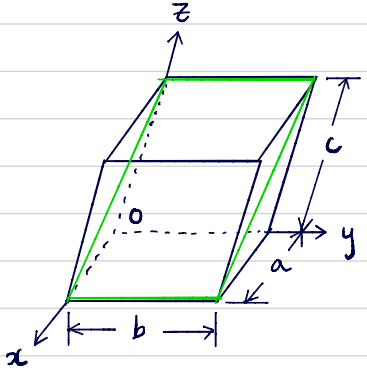
$h = \frac{1a}{\infty} = 0$

$k = \frac{1b}{-b} = -1.$

$l = \frac{1c}{\frac{1}{2}c} = 2$

$\therefore (0\bar{1}2)$

Example Problem 3.7



(101) plane.

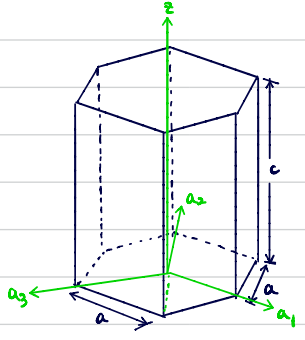
$h = \frac{1a}{A} = 1.$

$k = \frac{1b}{B} = 0.$

$l = \frac{1c}{C} = 1.$

$\therefore A = a,\ B = \infty b,\ C = c.$

Example Problem 3.8



1 −1 ∞ 1

1 −1 0 1

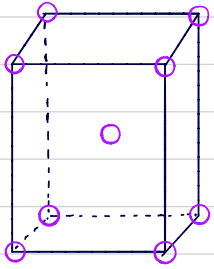
$\therefore (1\bar{1}01)$

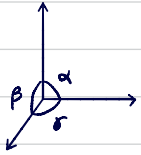
Problem 3.1

- Atomic Structure : number of neutrons & protons in the nucleus of an atom.
  probability distribution of the constituent atoms.
- Crystal Structure : arrangement of atoms in the crystalline solid material.

Problem 3.3

body-centered orthorhombic crystal structure.



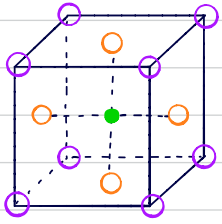


$\alpha = \beta = \delta = 90^\circ$

$a \neq b \neq c$.

Problem 3.5

perovskite crystal structure.

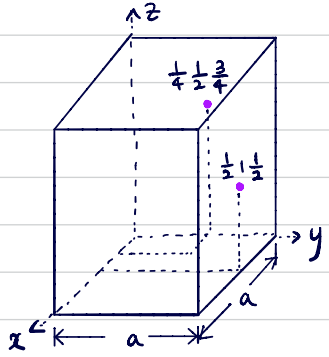


point coordinates of atoms :

- ○ barium ions (corners) — 000, 001, 010, 011, 100, 101, 110, 111
- ○ oxygen ions (face-centered positions) — $0\frac{1}{2}\frac{1}{2}$, $\frac{1}{2}0\frac{1}{2}$, $\frac{1}{2}\frac{1}{2}0$, $\frac{1}{2}\frac{1}{2}1$, $\frac{1}{2}1\frac{1}{2}$, $1\frac{1}{2}\frac{1}{2}$
- ○ titanium ion (center of cubic unit cell) — $\frac{1}{2}\frac{1}{2}\frac{1}{2}$

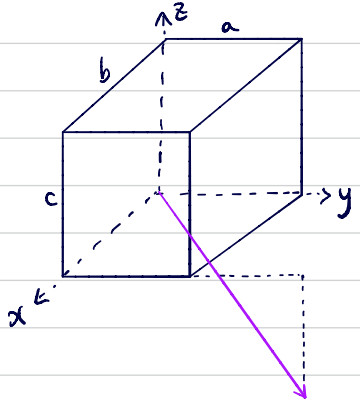
Problem 3.7

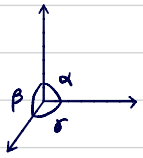
tetrigonal structure.



Problem 3.9

orthorhombic unit cell, [12$\bar{1}$] direction.

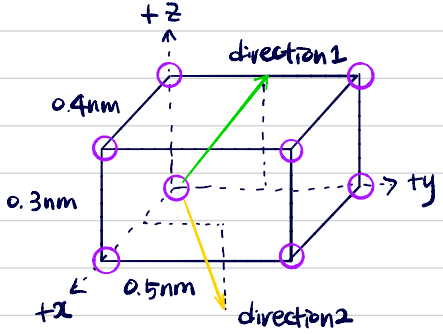




$\alpha = \beta = \gamma = 90°$

$a \neq b \neq c$.

Problem 3.11



direction 1

	a	b	c
	0	$\frac{1}{2}$	1
	0	1	2

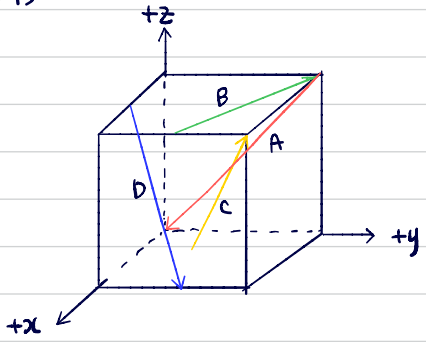
$\therefore$ [012]

direction 2

	a	b	$-c$
	$\frac{1}{2}$	$\frac{1}{2}$	-1
	1	1	-2

$\therefore$ [11$\bar{2}$]

Problem 3.13



A) $0a \quad -b \quad -c$

$0 \quad -1 \quad -1$

$\therefore [0\bar{1}\bar{1}]$

B) $-a \quad \frac{1}{2}b \quad 0c$

$-1 \quad \frac{1}{2} \quad 0$

$-2 \quad 1 \quad 0$

$\therefore [\bar{2}10]$

C) $\frac{1}{2}a \quad \frac{1}{2}b \quad c$

$\frac{1}{2} \quad \frac{1}{2} \quad 1$

$1 \quad 1 \quad 2$

$\therefore [112]$

D) $\frac{1}{2}a \quad \frac{1}{2}b \quad -c$

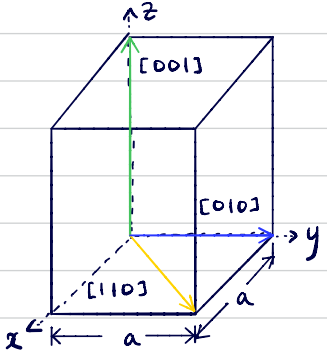
$\frac{1}{2} \quad \frac{1}{2} \quad -1$

$1 \quad 1 \quad -2$

$\therefore [11\bar{2}]$

Problem 3.15

tetrigonal structure.



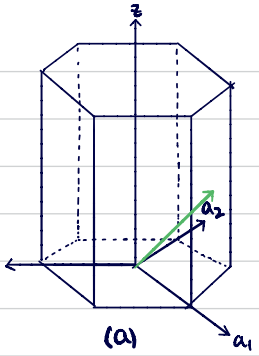
equivalent directions of

$[001]$: $[00\bar{1}]$

$[110]$: $[\bar{1}10]$ $[1\bar{1}0]$ $[\bar{1}\bar{1}0]$

$[010]$: $[0\bar{1}0]$ $[100]$ $[\bar{1}00]$

Problem 3.17



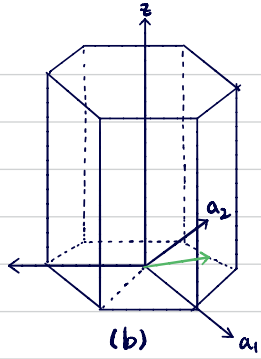
(a)

$[1\ \frac{1}{2}\ \frac{1}{2}]$

$[2\ 1\ 1]$

$[1\ 0\ -1\ 1]$

$\therefore [1\ 0\ \bar{1}\ 1]$



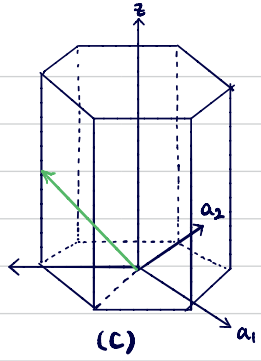
(b)

$[\frac{1}{2}\ 1\ 0]$

$[1\ 2\ 0]$

$[0\ 1\ -1\ 0]$

$\therefore [0\ 1\ \bar{1}\ 0]$



(c)

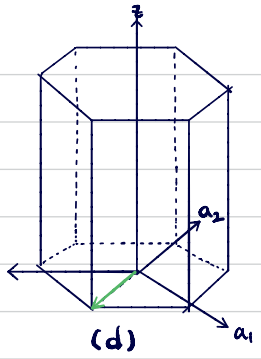
$[-1\ -1\ \frac{1}{2}]$

$[-2\ -2\ 1]$

$[\frac{2}{3}\ -\frac{2}{3}\ \frac{4}{3}\ 1]$

$[2\ -2\ 4\ 3]$

$\therefore [2\ \bar{2}\ 4\ 3]$



(d)

$[0\ -1\ 0]$

$[\frac{1}{3}\ -\frac{2}{3}\ \frac{1}{3}\ 0]$

$[1\ -2\ 1\ 0]$

$\therefore [1\ \bar{2}\ 1\ 0]$

Problem 3.19

$[UVW] \rightarrow [uvtw]$ $\quad u = \frac{1}{3}(2U-V)$ $\quad v = \frac{1}{3}(2V-U)$ $\quad t = -(u+v)$ $\quad w = W$

$V = 2U - 3u$

$u = \frac{2}{3}U - \frac{V}{3}$

$V = 2U - 3u$

$2U - 3u = \frac{2}{3}V - \frac{1}{3}V$

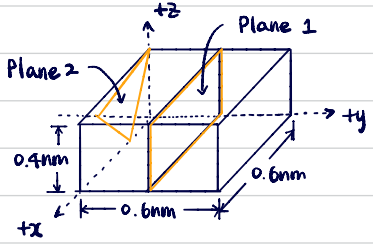
$\frac{2}{3}U = \frac{2}{3}V + 3u$

$U = v + 2u.$

$v = \frac{1}{3}(4U - 3u - U)$

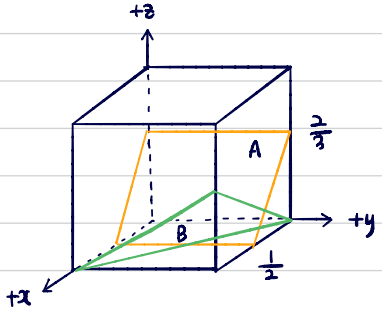
$v = U - u$

Problem 3.21



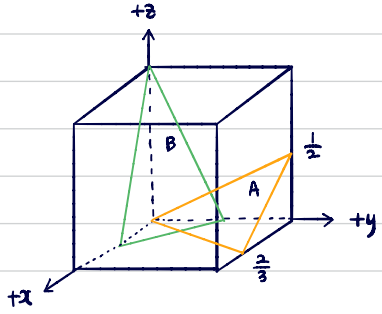
Plane 1			Plane 2		
∞a	$\frac{1}{2}b$	∞c	$\frac{1}{2}a$	$-\frac{1}{2}b$	c
∞	$\frac{1}{2}$	∞	$\frac{1}{2}$	$-\frac{1}{2}$	1
0	2	0	2	-2	1
$\therefore (020)$			$\therefore (2\bar{2}1)$		

Problem 3.23



Plane A			Plane B		
$\frac{1}{2}a$	∞b	$\frac{2}{3}c$	$-a$	$-b$	$\frac{1}{2}c$
$\frac{1}{2}$	∞	$\frac{2}{3}$	-1	-1	$\frac{1}{2}$
2	0	$\frac{3}{2}$	-1	-1	2
4	0	3	$\therefore (\bar{1}\bar{1}2)$		
$\therefore (403)$					

Problem 3.25



Plane A

$\frac{2}{3}a$	$-b$	$\frac{1}{2}c$
$\frac{2}{3}$	-1	$\frac{1}{2}$
$\frac{3}{2}$	-1	2
3	-2	4

$\therefore (3\bar{2}4)$

Plane B

$\frac{1}{2}a$	$\frac{1}{2}b$	c
$\frac{1}{2}$	$\frac{1}{2}$	1
2	2	1

$\therefore (221)$

Problem 3.27

$(UVW) \rightarrow (uvtw)$. $\quad t = -(u+v)$

$(010) \rightarrow (01\bar{1}0)$

$t = -1$

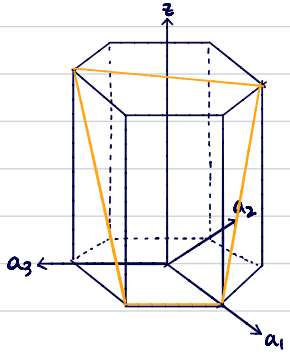
$(101) \rightarrow (10\bar{1}1)$

$t = -1$

Problem 3.29

$(1\ \bar{1}\ 0\ 1)$

$1\ -1\ \infty\ 1$



$(1\ 1\ \bar{2}\ 0)$

$1\ 1\ -\frac{1}{2}\ \infty$