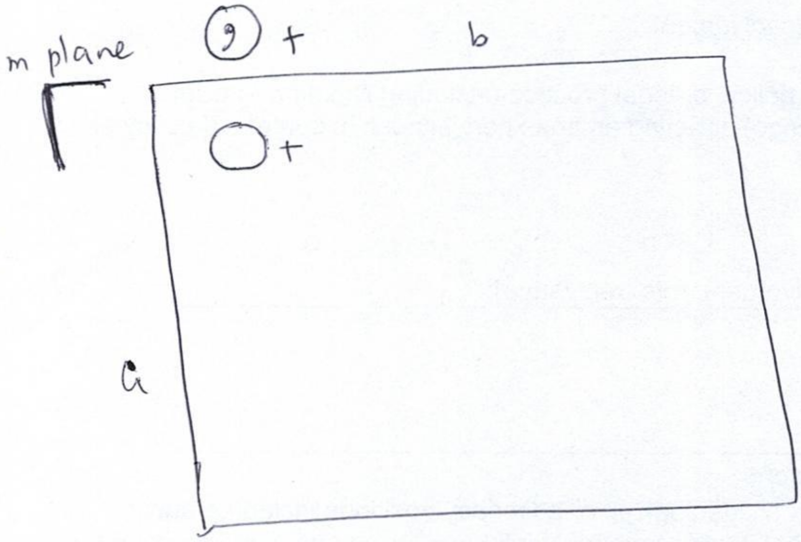
CMP 2026 — HW2 Solution by Sabieh Anwar

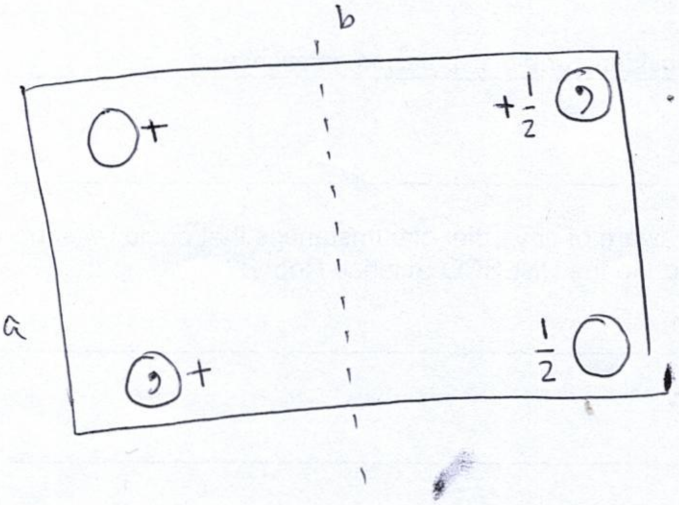
Q1. Sol

(a)



Action of $m \perp c$

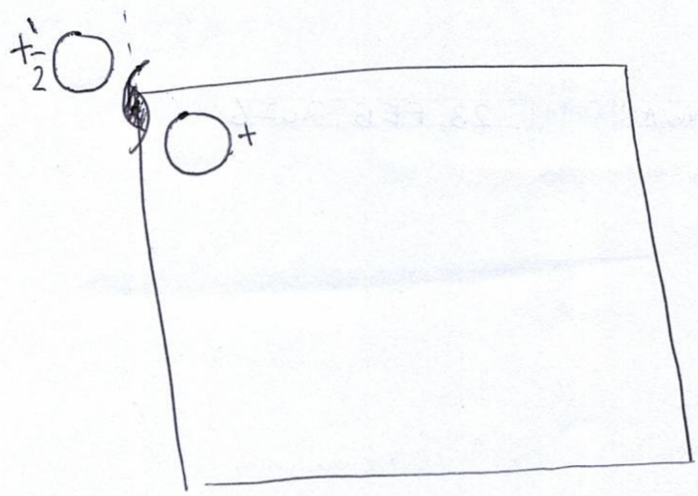
(b)



. The glide plane reflects the point x, y, z and elevates it along c by a distance $z = +\frac{1}{2}$.

I have also drawn the point $\bar{x}, y, z$ in Fig (a) inside the unit cell - Fig (b).

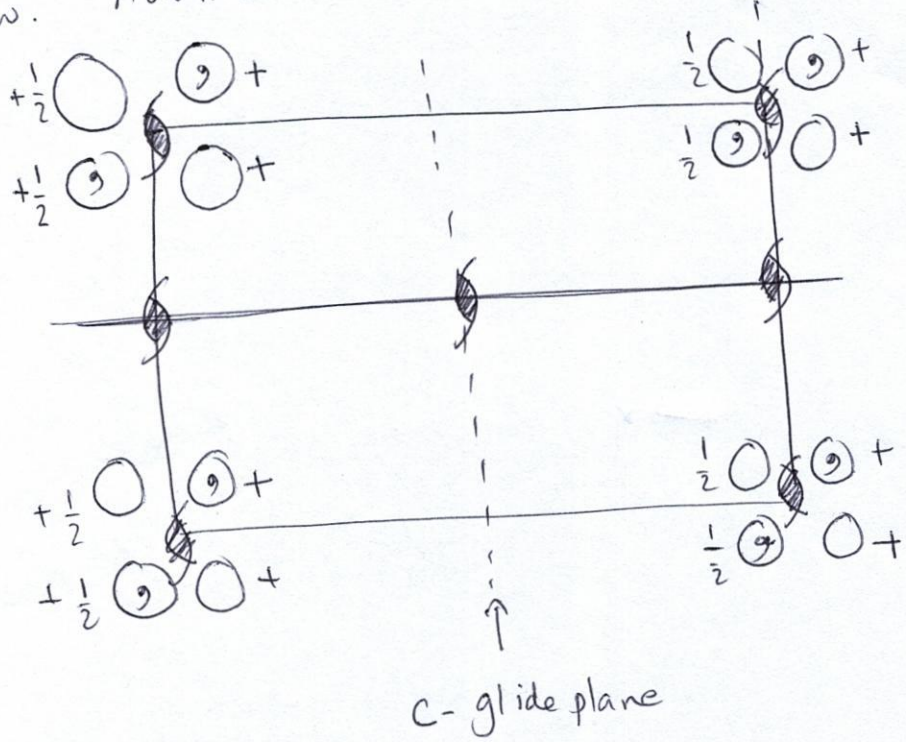
(c)



Action of 2_1 axis is shown.

Q1 sol. cont'd

Overall the 4 general positions are represented below. Additional screw axes, & mirror planes are also shown.



Q2

(a) Cubic

(b) face-centred cubic

(c) The 8a locations are given below.

For the set $(0,0,0)+$ ① $0,0,0$ ② $\frac{3}{4},\frac{1}{4},\frac{3}{4}$

For the set $(0,\frac{1}{2},\frac{1}{2})+$

③ $0,\frac{1}{2},\frac{1}{2}$ ④ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$

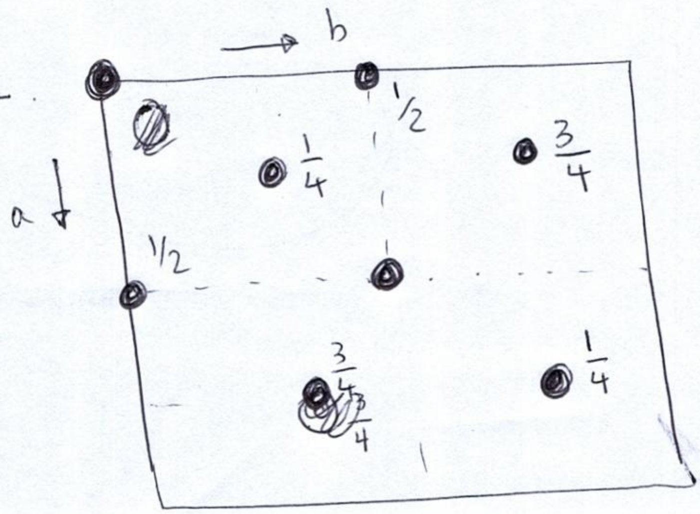
For the set $(\frac{1}{2},0,\frac{1}{2})+$

⑤ $\frac{1}{2},0,\frac{1}{2}$ ⑥ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

For the set $(\frac{1}{2},\frac{1}{2},0)+$

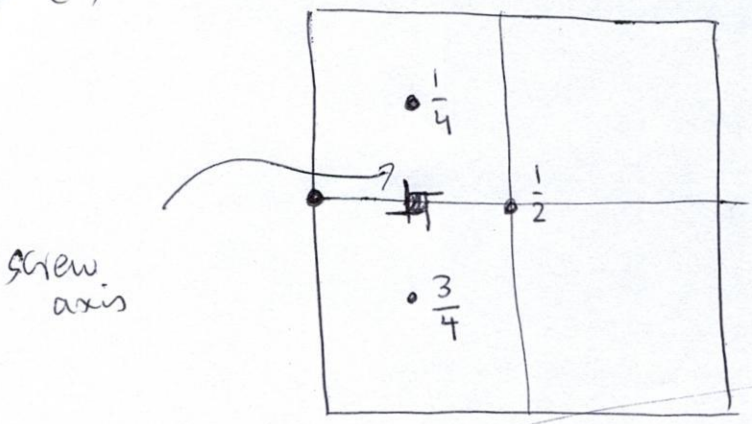
⑦ $\frac{1}{2},\frac{1}{2},0$ ⑧ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$

On a clinographic projection.



(d)

Our arbitray point is $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

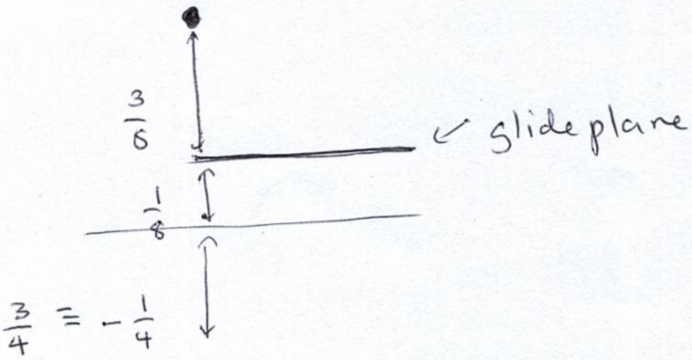


$$\frac{1}{4}, \frac{1}{4}, \frac{1}{4} \xrightarrow{4_1} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \xrightarrow{4_1} \frac{3}{4}, \frac{1}{4}, \frac{3}{4} \xrightarrow{4_1} \frac{1}{2}, 0, 0 \xrightarrow{4_1} \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$$

$$\frac{1}{4}, \frac{1}{4}, \frac{1}{4} \xrightarrow{4_2} \frac{3}{4}, \frac{1}{4}, \frac{3}{4} \qquad \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \xrightarrow{4_3} \frac{1}{2}, 0, 0$$

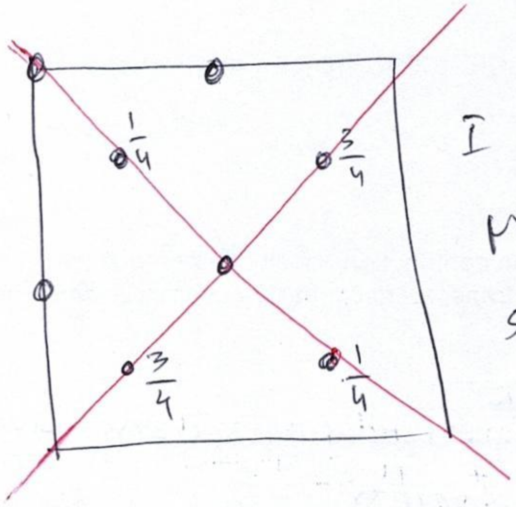
(e) I take the atom $0,0,0$. Under the action of the diamond glide plane, it goes to $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$. The same glide plane, then takes $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ to $\frac{1}{2}, \frac{1}{2}, 0$.

~~The~~ Now consider the point $0, \frac{1}{2}, \frac{1}{2}$. Under the



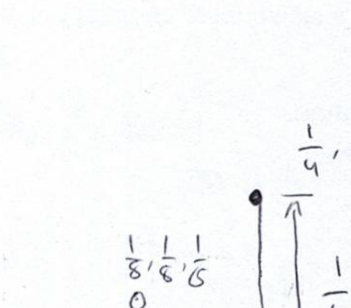
action of the glide plane, $0, \frac{1}{2}, \frac{1}{2}$ is first reflected to $0, \frac{1}{2}, \frac{\overline{1}}{4} = 0, \frac{1}{2}, \frac{3}{4}$ which is then translated by $\frac{\vec{a}}{4} + \frac{\vec{b}}{4}$ making it go to $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$. Hence all points given in part (c) are connected by the $z = 8$ glide plane of the diamond kind.

(f)



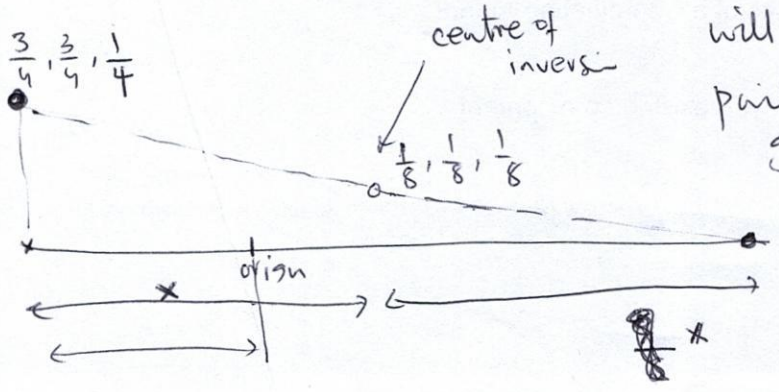
I redraw the projection shown in part (c) and superpose the diagonal mirror planes. Indeed, it can be seen that mirror planes are indeed symmetry planes for the 8a position. This is also reflected by the "m" in the site symmetry "$\bar{4}3m$" for the third position of the 8a Wyckoff positions.

(g)



The points $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ and $0,0,0$ are related through the centre of inversion.

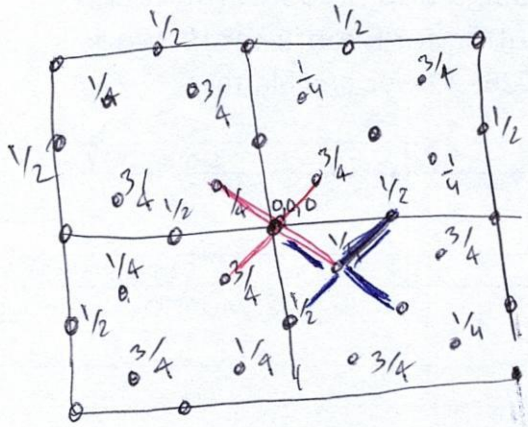
Let's check this for another point. Consider ~~[illegible]~~ $\frac{1}{2},\frac{1}{2},0$. Under the centre of inversion, it will be mapped to the $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ point as one check through geometric arguments.



$\frac{1}{2},\frac{1}{2},0 \Rightarrow$ along face diagonal

(h)

Lets redraw the plan view shown in part (c) with 4 cells drawn together.



The point at $0,0,0$ has 4 nearest neighbors:

① $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

② $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$

③ $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$

④ $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$

which are shown by the red "tentacles" which are actually pointing towards apices of a tetrahedron. The directions of these atoms from $0,0,0$ are

① $[111]$

② $[\bar{1}\bar{1}1]$

③ $[\bar{1}1\bar{1}]$

④ $[1\bar{1}\bar{1}]$.

For $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$, the 4 nearest neigbors are:

⑤ $0,0,0$

⑥ $0, \frac{1}{2}, \frac{1}{2}$

⑦ $\frac{1}{2}, 0, \frac{1}{2}$

⑧ $\frac{1}{2}, \frac{1}{2}, 0$

with direction shown in blue:

⑤ $[\bar{1}\bar{1}\bar{1}]$

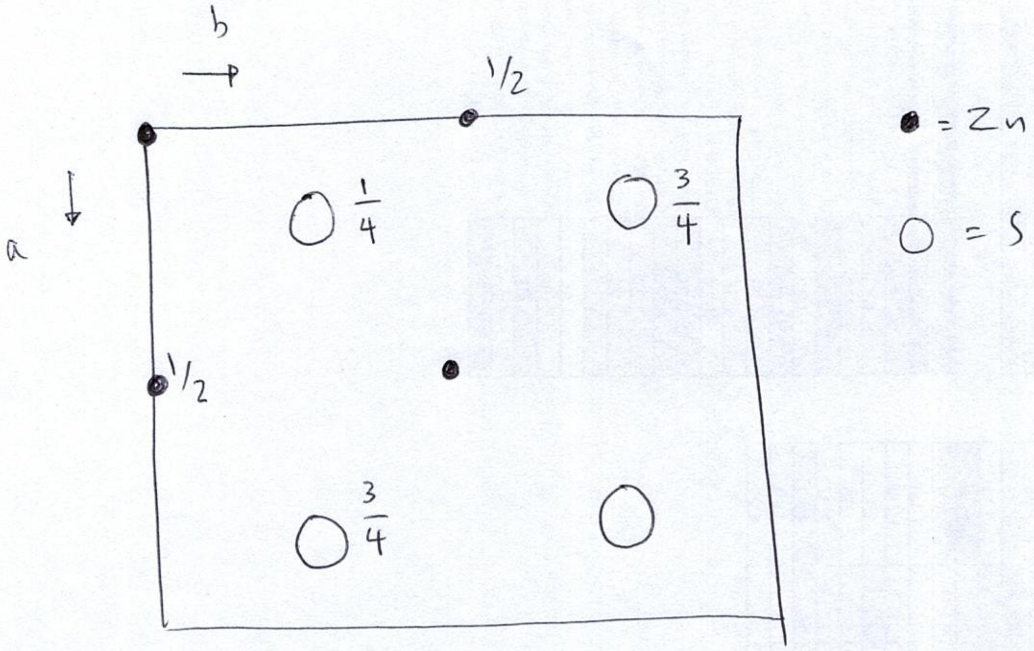
⑥ $[\bar{1}11]$

⑦ $[1\bar{1}1]$

⑧ $[11\bar{1}]$.

The two sets of vectors indeed form tetrahedrons @ $\mathcal{O}$ but the sets are different, which means that the tetrahedrons have different orientations. Hence we have two distinct sets of general position in diamond.

(i)



4c locations are

~~0, 0~~ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

$\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$

$\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$ and

$\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$.

4a locations are

$0, 0, 0$

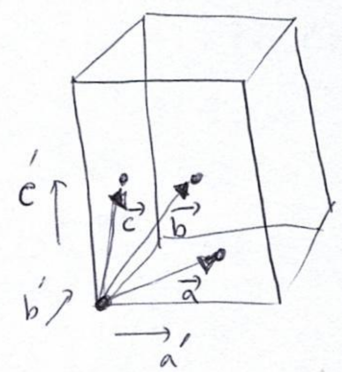
$0, \frac{1}{2}, \frac{1}{2}$

$\frac{1}{2}, 0, \frac{1}{2}$

$\frac{1}{2}, \frac{1}{2}, 0$.

(j) No longer.

Q5



Make a primitive lattice on a FCC.

$$\vec{a} = a\left(\tfrac{1}{2}\vec{a}' + \tfrac{1}{2}\vec{b}'\right) = \tfrac{a}{2}[1,1,0]$$

$$\vec{b} = a\left(\tfrac{1}{2}\vec{a}' + \tfrac{1}{2}\vec{c}'\right) = \tfrac{a}{2}[1,0,1]$$

$$\vec{c} = a\left(\tfrac{1}{2}\vec{b}' + \tfrac{1}{2}\vec{c}'\right) = \tfrac{a}{2}[0,1,1]$$

Here $\vec{a}', \vec{b}', \vec{c}'$ are unit translation vectors on the edges of the FCC lattice, while $\vec{a}, \vec{b}, \vec{c}$ are unit vectors along the primitive unit cell. Let $V = \vec{a}\cdot\vec{b}\times\vec{c}$. Now

$$\vec{a}^* = \frac{2\pi}{V}\vec{b}\times\vec{c}, \quad \vec{b}^* = \frac{2\pi}{V}\vec{c}\times\vec{a}, \quad \vec{c}^* = \frac{2\pi}{V}\vec{a}\times\vec{b}.$$

$$\vec{b}\times\vec{c} = \frac{a^2}{4}\begin{vmatrix} \hat{a}' & \hat{b}' & \hat{c}' \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{vmatrix} = \cancel{\hat{a}'\left(-\tfrac{1}{4}\right) \hat{b}'\left(\tfrac{1}{4}\right) \ldots + \hat{b}' - \tfrac{1}{4}}$$

$$= \left(\frac{a^2}{4}\right)[-1,-1,1]$$

$$\vec{c}\times\vec{a} = \frac{a^2}{4}\begin{vmatrix} \hat{a}' & \hat{b}' & \hat{c}' \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{vmatrix} = \frac{a^2}{4}[-1,1,-1]$$

$$\vec{a}\times\vec{b} = \frac{a^2}{4}\begin{vmatrix} \hat{a}' & \hat{b}' & \hat{c}' \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{vmatrix} = \frac{a^2}{4}[1,-1,-1]$$

$$\frac{2\pi}{V} = ?$$

$$V = \vec{a} \cdot \vec{b} \times \vec{c}$$

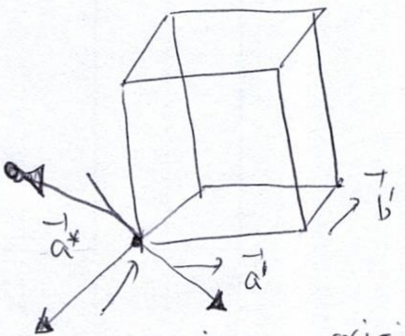
$$= \frac{a}{2}[1,1,0] \cdot \frac{a^2}{4}[-1,-1,1]$$

$$= \frac{a^3}{8}\left|[-1,-1,0]\right|^2 = \frac{a^3}{8}(2) = \frac{a^3}{4}.$$

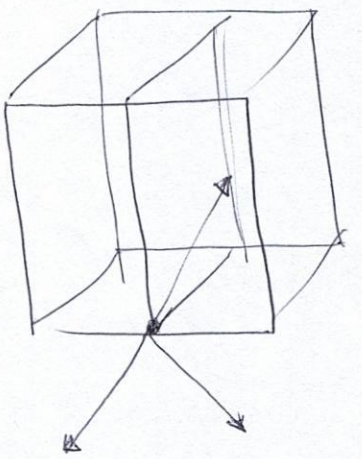
$$\vec{a}^* = \frac{8\pi}{a^3} \cdot \frac{a^2}{4}[-1,-1,1] = \left(\frac{2\pi}{a}\right)[-1,-1,1]$$

$$\vec{b}^* = \frac{2\pi}{a}[-1,1,-1]$$

$$\vec{c}^* = \frac{2\pi}{a}[1,-1,-1]$$



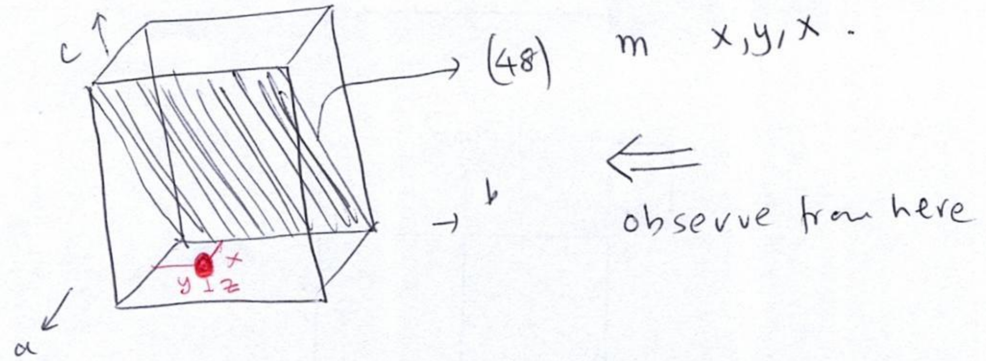
using this as origin for convenience

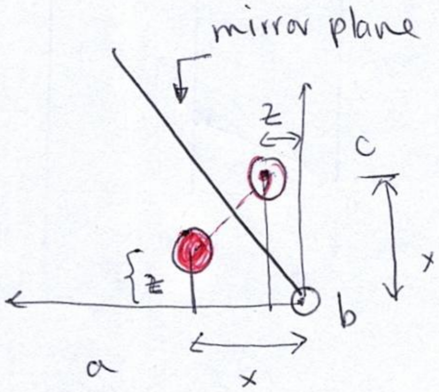


$\vec{a}^*$, $\vec{b}^*$ and $\vec{c}^*$ are vectors pointing towards body centres of adjacent unit cells. Hence reciprocal to FCC we have a BCC arrangement of points.

حل

Q7 (a) Look at the positions table for the general coordinates (96 l 1). At number (48), we have the coordinates z, y, x which comes from x, y, z by application of the symmetry operation number (48) which reads m, x, y, x which is a mirror plane along the body diagonal:





The geometry shows that x and z are interchanged by the mirror plane and the y coordinate remains unchanged

(b) With the same approach, we find that the relevant symmetry operation is (48) in the $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$ set which reads as

(48) $\quad n\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) \quad x, y, x$

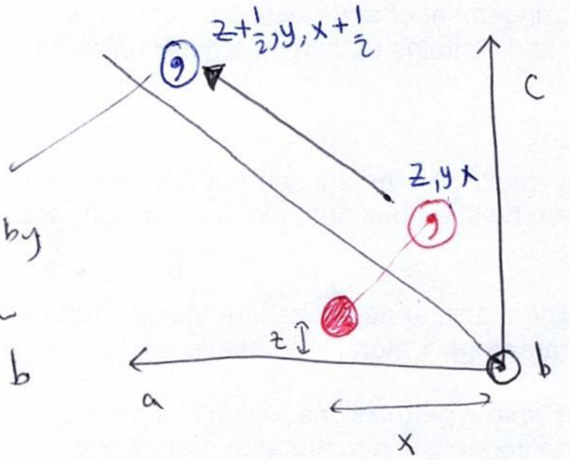
which is an n glide plane along x, y, x followed by the translation $\frac{\vec{a}}{2} + \frac{\vec{b}}{2} + \frac{\vec{c}}{2}$.

This a bit hard to visualize in 2D [illegible]

but essentially it starts by taking an image

about the x, y, x mirror plane as in the previous

part. This is followed by a translation.



Follow by translation along b to

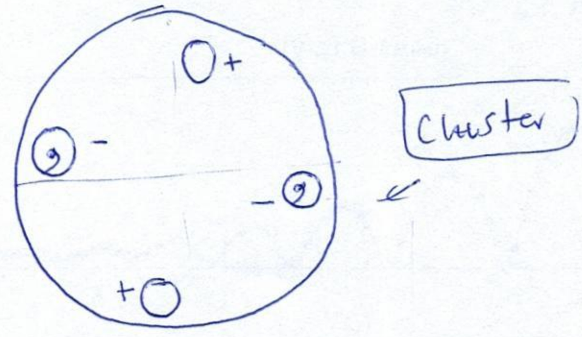
achieve $z+\frac{1}{2}, y+\frac{1}{2}, x+\frac{1}{2}$. Unfortunately, I cannot display

this on this diagram. My pen and paper work -

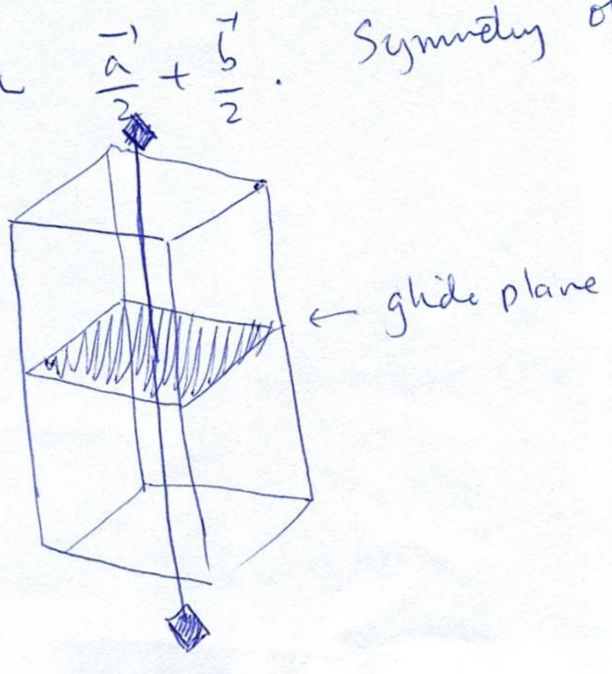
2D, the mind doesn't!

Q8

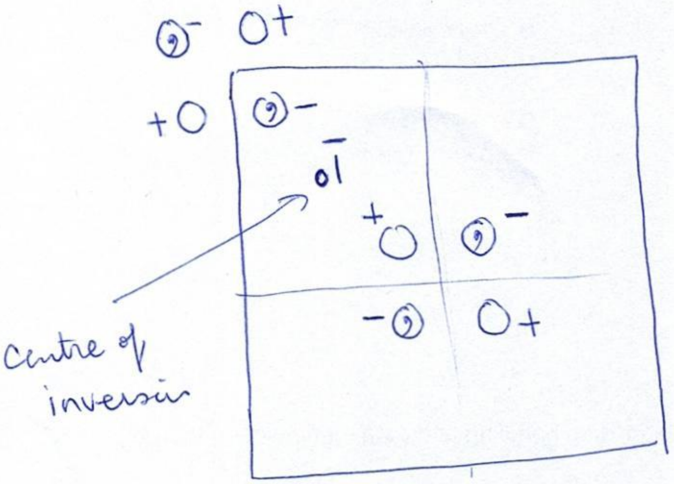
(a) The symbol C_{4h}^3 shows that this space group is derived from the point group C_{4h} whose atomic distribution is first drawn.



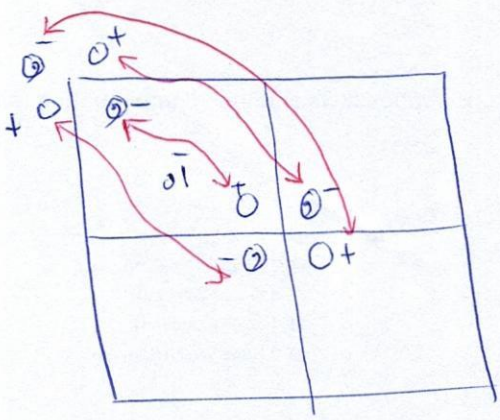
The "P" in the symbol P4/n indicates a primitive space group. So this $\boxed{\text{Cluster}}$ is placed at each lattice point (1 per u.c.). The "4" in P4/n shows that the space group is of the tetragonal class and that a glide plane exists $\perp$ to the 4-fold axis. The 4-fold axis is obviously along the unique (c) axis. The glide plane is at location $z = 1/2$ (see operation (6) in the International Tables entry). The diagonal glide n includes a translation $\frac{\vec{a}}{2} + \frac{\vec{b}}{2}$. Symmetry operations are shown here.



As a result of the glide plane, the motif will be reflected across the glide plane and translated, resulting in the plan shown below. See this very carefully.



(b) Yes, there is a $\bar{1}$ centre at $\frac{1}{4}, \frac{1}{4}, 0$, e.g. it connects the points shown below.



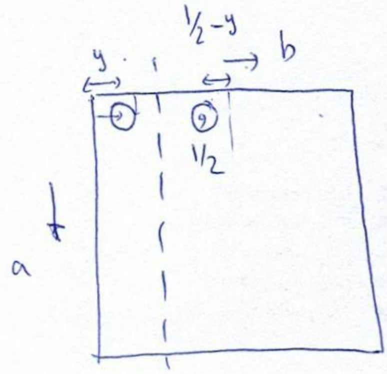
(c) Yes. Operation number (6) in the Tables. It takes x, y, z to $x+\frac{1}{2}, y+\frac{1}{2}, \bar{z}$ which can be seen both by the diagram I've drawn in part (a) as well as entry # 6 in the Wyckoff position 8g.

Q9. This question was aimed to tingle your minds.

$\frac{1}{4} - y$

$\frac{1}{4} + \frac{1}{4} - y$

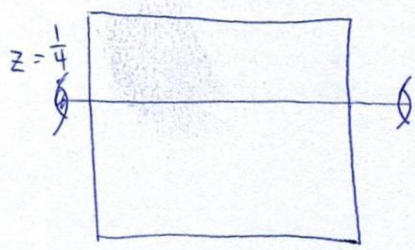
(a)

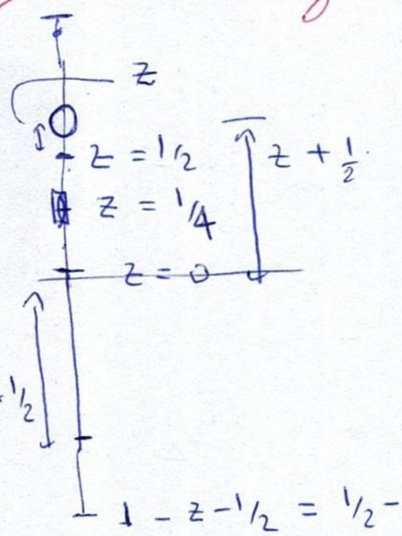


c glide plane

- $x, y, z \xrightarrow{\text{c glide}} x, \frac{1}{2} - y, z + \frac{1}{2}$

rough





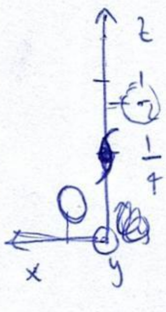
- $x, \frac{1}{2} - y, z + \frac{1}{2} \xrightarrow{2_1 \text{ at } [0, y, \frac{1}{4}]} x, y, \frac{1}{2} - z$

$1 - z - \frac{1}{2} = \frac{1}{2} - z$

(c) If I reverse the order

$\frac{1}{2} + y + \frac{1}{2} = y$

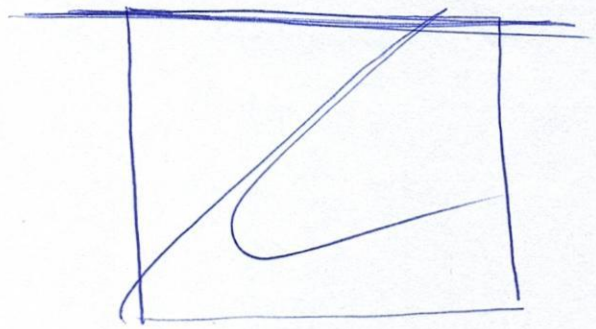
- $x, y, z \xrightarrow{2_1 \text{ at } [0, y, \frac{1}{4}]} \bar{x}, y + \frac{1}{2}, \frac{1}{2} - z$

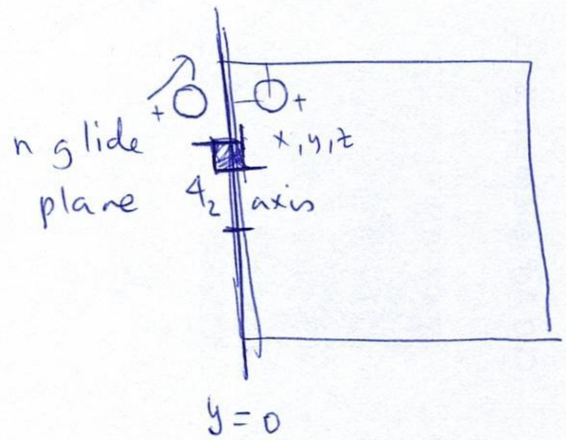


- $\bar{x}, y + \frac{1}{2}, \frac{1}{2} - z \xrightarrow{\text{c glide}} \bar{x}, \bar{y}, \bar{z}$

$\frac{1}{2} - z + \frac{1}{2} =$

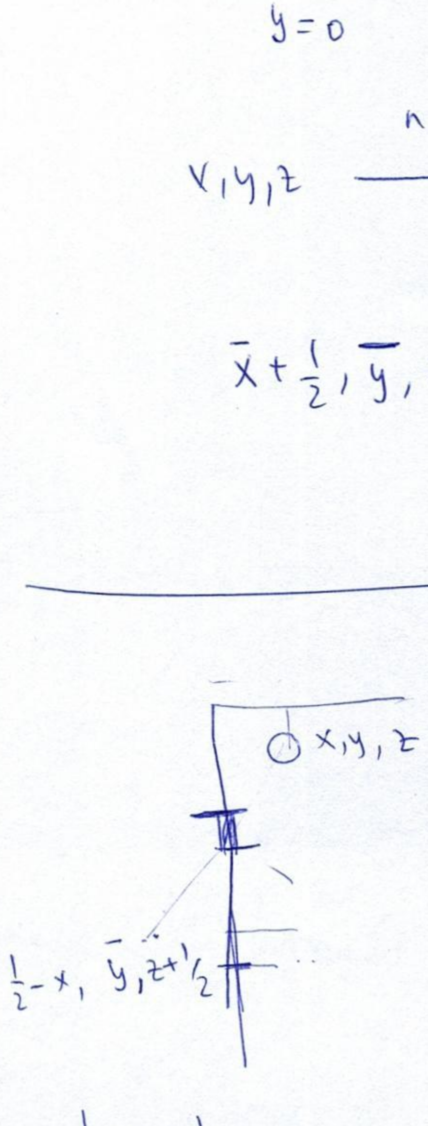
(b)

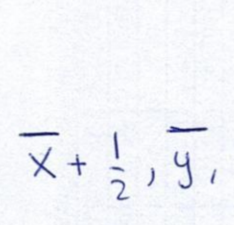




$$x, y, z \xrightarrow{\text{n glide plane}} \bar{x}+\tfrac{1}{2}, \bar{y}, z+\tfrac{1}{2}$$

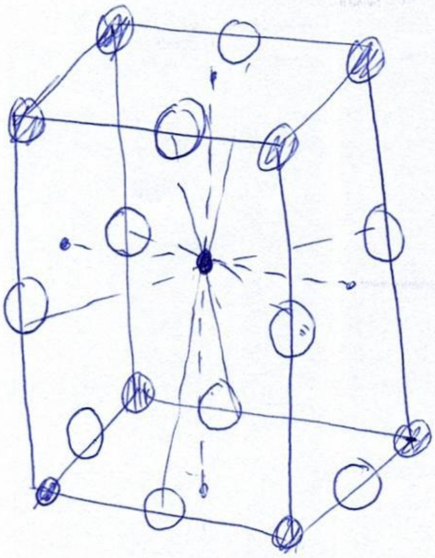
$$\bar{x}+\tfrac{1}{2}, \bar{y}, z+\tfrac{1}{2} \xrightarrow{4_2 \equiv \text{axis}} x,\ y\ ,z$$





Q10

(a)

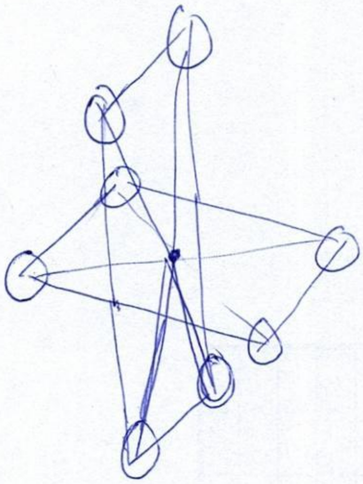


Pb at 1a

Zr at 1b

O at 3d

(b)



Each Zr atom is coordinated with 8 O atoms as shown.

Directions of interatomic Zr – O vectors are:

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

and $[101]$, $[10\bar{1}]$, $[\bar{1}01]$, $[\bar{1}0\bar{1}]$.