Assignment 2: Solution

1. Diamond belongs to the $Fd\bar{3}m$ with atoms in the $8a$ positions. The relevant pages for this space group taken from the international table of crystallography have been uploaded.

   a) What is the underlying crystal system? **Cubic**

   b) What is the underlying Bravais lattice? **Face centered**

   c) Draw clinographic projection showing all 8 atoms inside the unit cell. This projection can be drawn by looking down the z (or the c)-axis. Identify the 8 atoms by suitable labels and mark the fractional elevation of atoms (if $z > 0$).

   Solution:

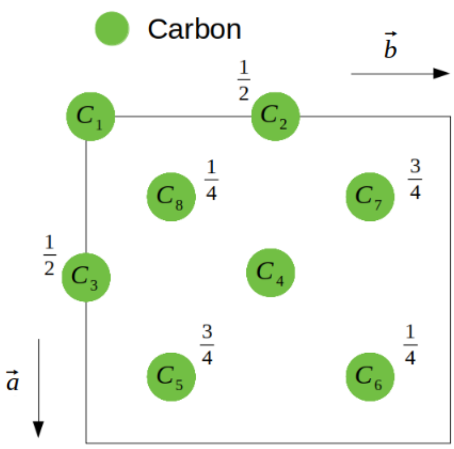

Figure 1: Diamond projection along $\vec{c}$

Coordinates of these atoms are:

$$C_1 \equiv (0, 0, 0),$$

$$C_2 \equiv (0, \tfrac{1}{2}, \tfrac{1}{2}),$$

$$\mathrm{C}_3 \equiv (\tfrac{1}{2}, 0, \tfrac{1}{2}),$$
$$\mathrm{C}_4 \equiv (\tfrac{1}{2}, \tfrac{1}{2}, 0),$$
$$\mathrm{C}_5 \equiv (\tfrac{3}{4}, \tfrac{1}{4}, \tfrac{3}{4}),$$
$$\mathrm{C}_6 \equiv (\tfrac{3}{4}, \tfrac{3}{4}, \tfrac{1}{4}),$$
$$\mathrm{C}_7 \equiv (\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}),$$
$$\mathrm{C}_8 \equiv (\tfrac{1}{4}, \tfrac{3}{4}, \tfrac{3}{4}).$$

d) A four fold screw axis exists at $(\frac{1}{2}, \frac{1}{4}, 0)$. Mark its position and demonstrate the action of $\mathbf{4}_1, \mathbf{4}_2, \mathbf{4}_3$ screw operations on any atom of your choice. Clarify your working. **Solution:**

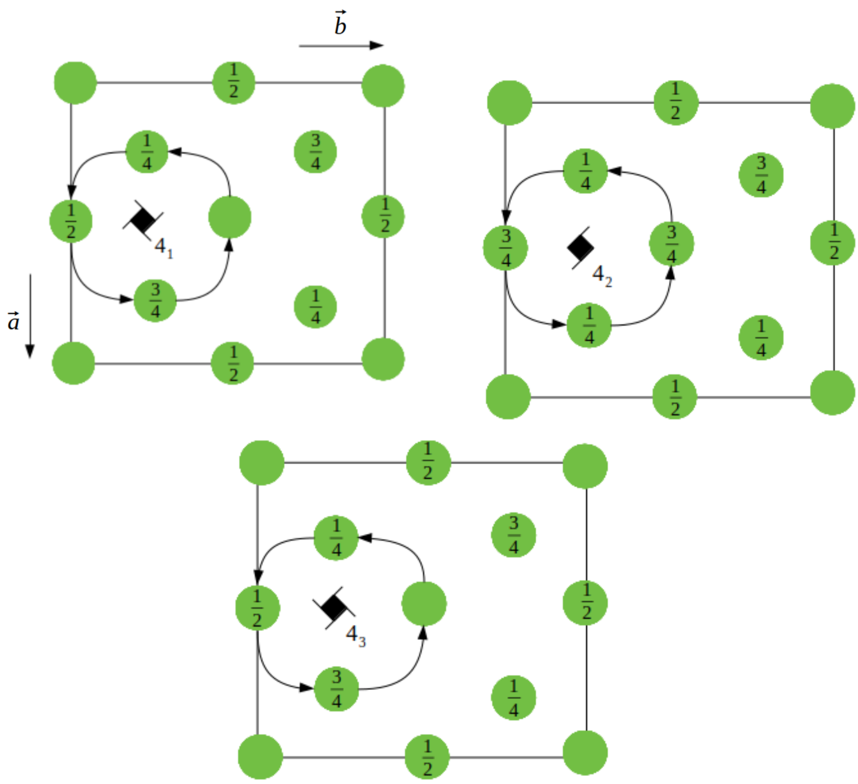

Figure 2

Let's take representative atom, say C_8 , at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ and apply the screw operation successively resulting in the following sequence of points

$$(\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}) \xrightarrow{4_1} (\tfrac{1}{2}, 0, \tfrac{1}{2}) \xrightarrow{4_1} (\tfrac{3}{4}, \tfrac{1}{4}, \tfrac{3}{4}) \xrightarrow{4_1} (\tfrac{1}{2}, \tfrac{1}{2}, 0).$$

$$(\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}) \xrightarrow{4_2} (\tfrac{1}{2}, 0, \tfrac{3}{4}) \xrightarrow{4_2} (\tfrac{3}{4}, \tfrac{1}{4}, \tfrac{1}{4}) \xrightarrow{4_2} (\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{3}{4}).$$

$$(\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4}) \xrightarrow{4_3} (\tfrac{1}{2},0,\tfrac{1}{2}) \xrightarrow{4_3} (\tfrac{3}{4},\tfrac{1}{4},\tfrac{3}{4}) \xrightarrow{4_3} (\tfrac{1}{2},\tfrac{1}{2},0).$$

e) A diamond glide plane also exists at the height $z = \frac{1}{8}$ following by the translation of $\frac{\vec{a}}{4} + \frac{\vec{b}}{4}$. Show by its action on any atom of your choice that this is indeed a symmetry operation.

Solution:

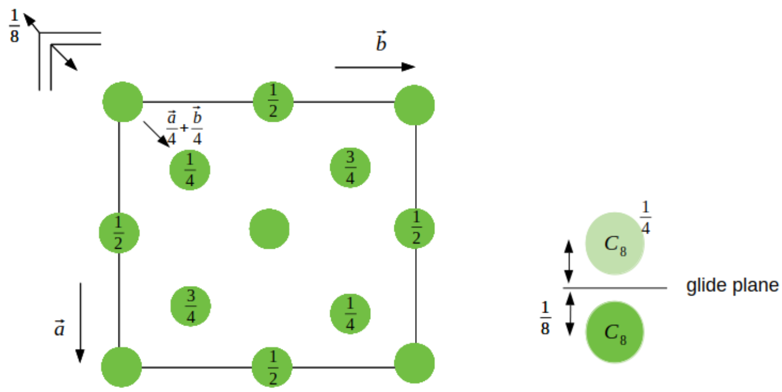

Figure 3: Glide Plane and side view

The glide plane takes $C_1 \equiv (0,0,0)$ to $C_8 \equiv (\frac{1}{4},\frac{1}{4},\frac{1}{4})$ and so on. See figure 3.

f) The m in the $Fd\bar{3}m$ space group symbol denotes a mirror plane along the face diagonal. Verify that it indeed exists in this structure.

Solution:

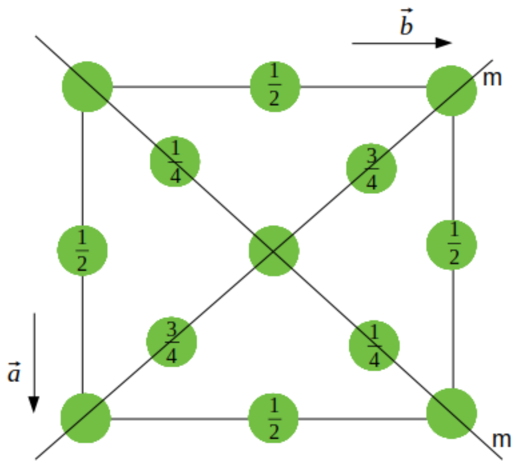

Figure 4: Face Diagonal Mirrors

Figure 4 showing that these face diagonal mirrors exist in this structure because each point has its mirror image e.g C_3 has its mirror image on C_2, $C_5 \Longleftrightarrow$C$_7$ etc.

g) The diamond structure has a centre of inversion at $(\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$. Verify this statement.

Solution:

We can see in the figure that each point has an inverted image, at an equal distance, on the opposite side of the point $(\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$. For example, $C_8 \equiv (\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ has inverted image at $C_1 \equiv (0, 0, 0)$, $C_4 \Longleftrightarrow$C$_6$ etc.

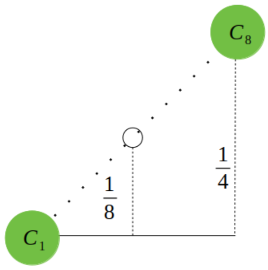

Figure 5: Side view

h) A closely related structure is Zincblende (ZnS) which belongs to the space group $F\bar{4}3m$. By looking up the entry of this space group on my website, draw a clinographic projection by placing Zn at the $4a$ site and S at the $4c$ sites. Where are all the atoms located inside the unit cell?

Solution:

See figure 6.

i) Does this zincblende structure have a center of symmetry?

Solution:

No, the zincblende structure does not have a center of symmetry.

2. The $P2_1/b$ (C_{2h}^5) space group is extremely well-represented in crystal structures. Its symmetry operations are shown in Figure 7.

   a) What is the crystal system and Bravais lattice type?

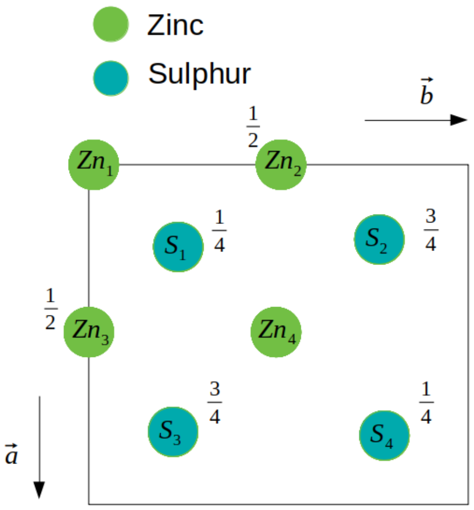

Figure 6: ZnS projection along $\vec{c}$

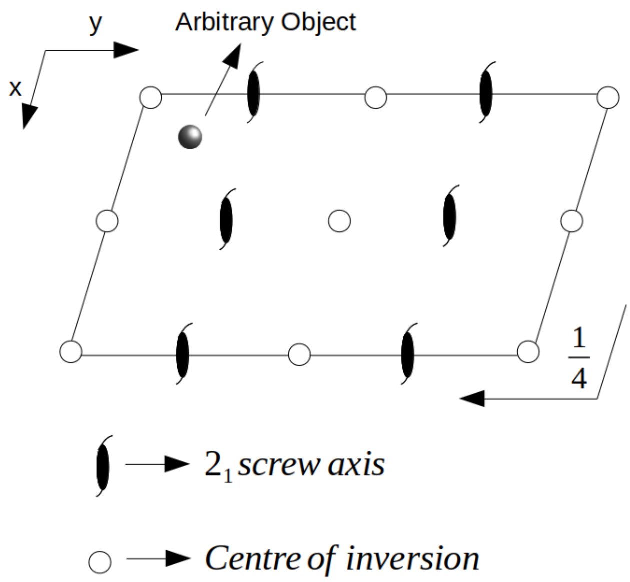

Figure 7

Draw a general position at the top left of the unit cell projected onto the xy plane.

What is the impact of:

b) The $\mathbf{2}_1$ axis at $(0, \frac{1}{4}, 0)$?

c) The centre of inversion at $(\frac{1}{2}, \frac{1}{2}, 0)$?

d) There exists a glide plane at height $z = \frac{1}{4}$. It is parallel to the (001) plane and translates a general position by $\frac{\vec{b}}{2}$. What is the impact of this glide plane?

Solution:

The crystal system is monoclinic, while the lattice type is primitive. Let's take a general position at the top left of the unit cell and label this point as P.

The 2_1 screw axis at $(0, \frac{1}{4}, 0)$ takes P to the point Q which is equivalent to the point R. The centre of inversion at $(\frac{1}{2}, \frac{1}{2}, 0)$ transforms P to S. There is also a b-glide plane at height $z = \frac{1}{4}$. The glide plane affects a reflection about the plane $(0, 0, \frac{1}{4})$, i.e., height $z = \frac{1}{4}$, followed by translation $+\frac{1}{2}\vec{b}$. This transforms P to point U.

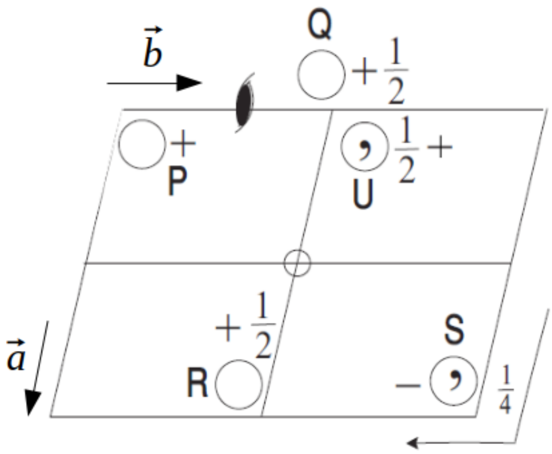

Figure 8: $P2_1/b$ (C_{2h}^5) unit cell and its four general equivalent positions

3. **Pmc2_1: Primitive Orthorhombic**

a) The space group notation shows that in this crystal structure, there is a mirror plane perpendicular to the $\vec{a}$ axis.

b) c is a glide plane perpendicular to the $\vec{b}$ axis. The plane produces a reflection followed by a translation along the $\vec{c}$ axis.

c) Finally, 2_1 is a screw axis along the $\vec{c}$ axis. The equivalent positions generated by the symmetry operations can be seen in accompanying projective diagram.

Solution:

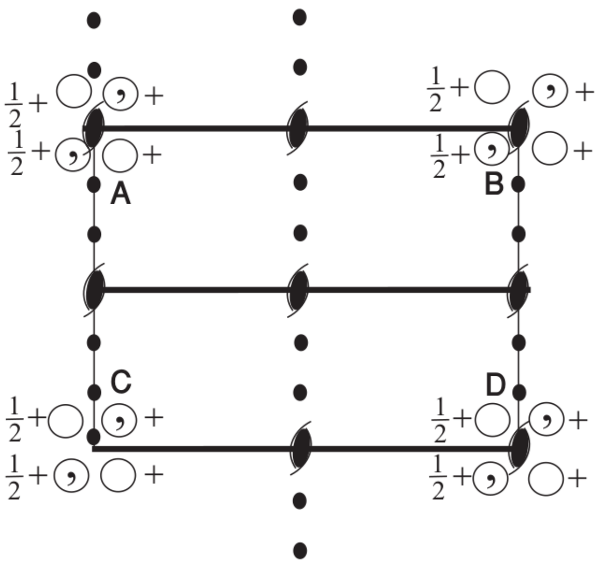

Figure 9: Primitive Orthorhombic

There are four equivalent positions in the unit cell,

$$(x, y, z), (x, \bar{y}, z + \tfrac{1}{2}), (\bar{x}, y, z), (\bar{x}, \bar{y}, z + \tfrac{1}{2}),$$

which are the positions shown by A, B, C, D in the projective diagram. The thick horizontal lines represent mirror planes. The vertical dotted lines are glide planes and the dgadic symbols are screw axes.