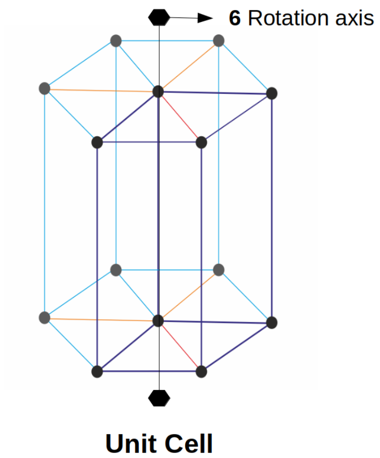
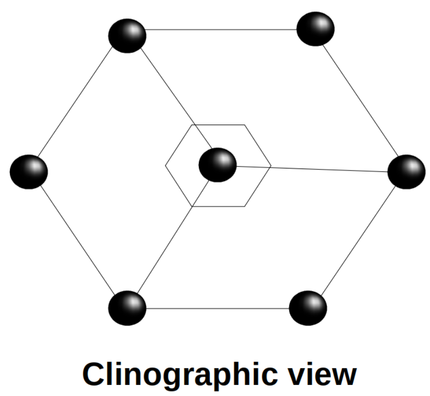
Assignment 1: Lattice and Symmetry

February 8, 2021

1. Show the location of the **6** rotation axis on the hexagonal unit cell.

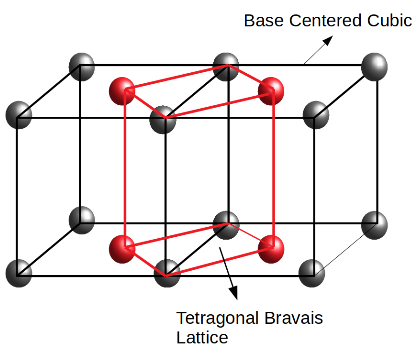
   Solution:
   The six fold rotation axis of hexagonal unit cell lies parallel to the c translation of the unit cell. This means any lattice point of the unit cell can be labeled as a six fold rotation axis.





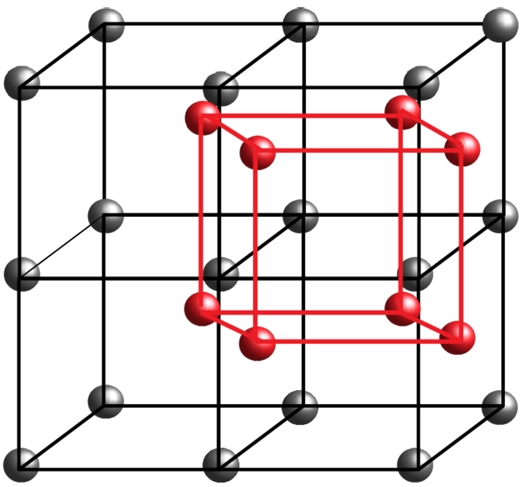
2. Why is there no base-centred (C-centred) cubic lattice? Describe your answer using appropriate geometrical drawings.

   Solution:
   As we know centering is only possible if each point in the resulting lattice has the same environment and furthermore, does not result in going out of the existing crystal system. For base-centered cubic, as we can see in the figure, a new symmetry crystal class tetragonal results. So, base-centered cubic is not a unique lattice type and not considered.

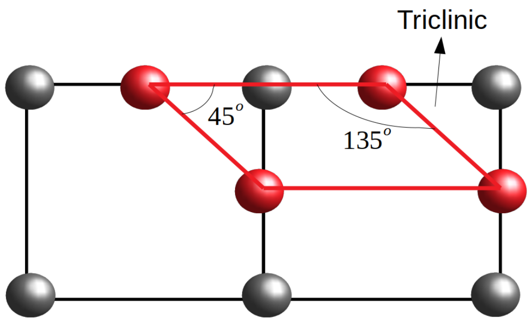


3. Similarly, show that attempting to center two perpendicular faces of a cubic crystal class, does not result in a new Bravais lattice.

   Solution:
   When two points added to two perpendicular faces of a cubic crystal class, we land into the triclinic crystal system which is not a new Bravais lattice. The reasoning from the previous question applies.



Centering Two Perpendicular Planes

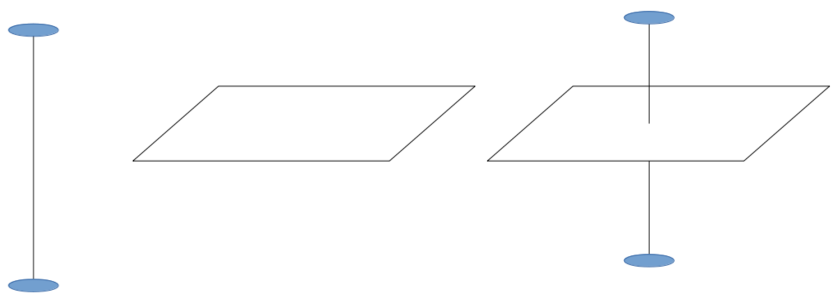


Clinographic view

4. The monoclinic unit cell is compatible with the point group 2, m and 2/m. They are described by the symmetry elements.

2	a lone two rotation axis
m	a single mirror place
2/m	a two fold axis with a perpendicular mirror plane

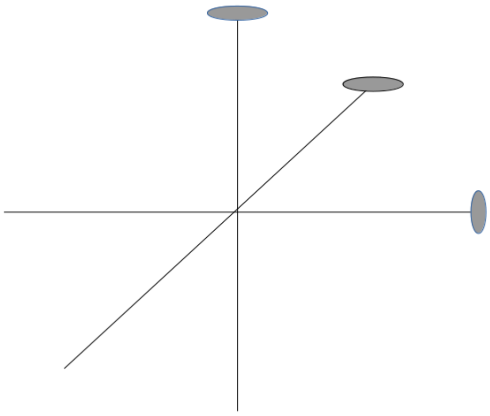
   Diagrammatically, let's represent this as following,



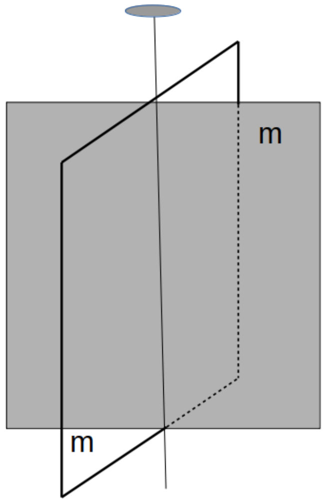
2-fold Rotation **Mirror Plane (m)** **2/m**

   Draw similar diagram for the group **222**, **mm**, and **mmm** compatible with the orthorohmbic system.

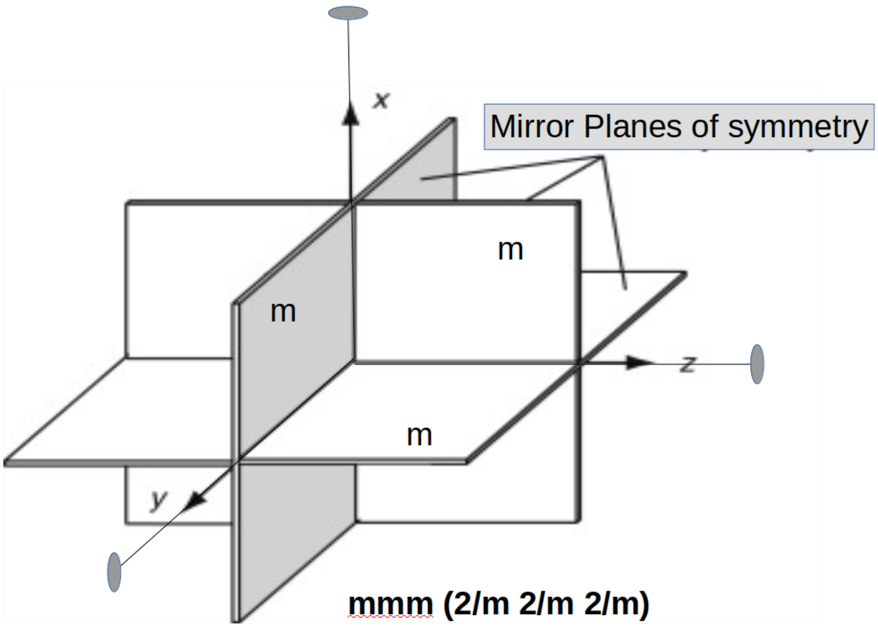
Solution:



222



mm (mm2)



5. The point group D_{4h} or **4/mmm** is developed from the point group C_{4h} or **4/m** by introducing a **2** rotation axis perpendicular to the principal 4 axis of the **4/m** point group. This construction can be written as:

$$D_{4h} = C_{4h} \times \{1, 2'\}.$$

Draw the sterograms of $C_4 \equiv$ **4**, $C_{4h} \equiv$ **4/m**, $D_{4h} \equiv$ **4/mmm** evolving them in a step-by-step fashion.

Solution:

a)

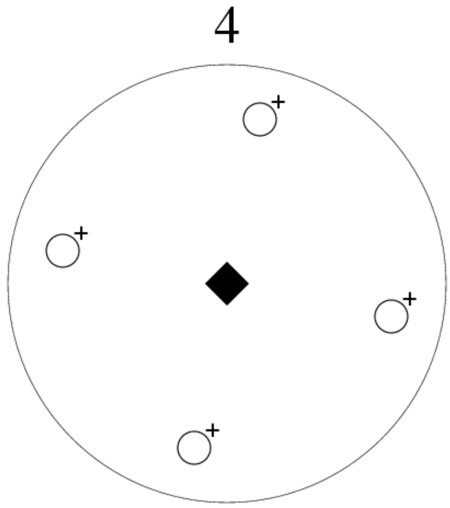


Figure 1

b) Introduce a 2 fold rotation axis $\vec{ab}$ onto the figure (2). This rotation axis is perpendicular to the 4 fold axis of rotation. The impact of the rotation is shown in figure (3).

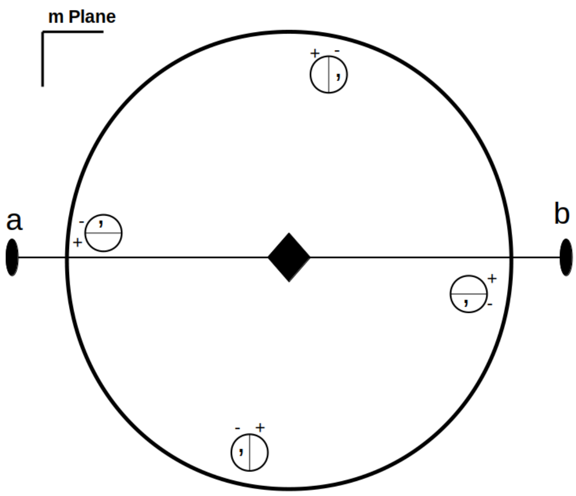


Figure 2

c) This automatically creates additional 2 fold rotation axes and vertical mirror planes m_2, m_3, m_4 and m_5. It is sufficient to mention m_2 and m_3 only as other (m_4 and m_5)

are automatically created.

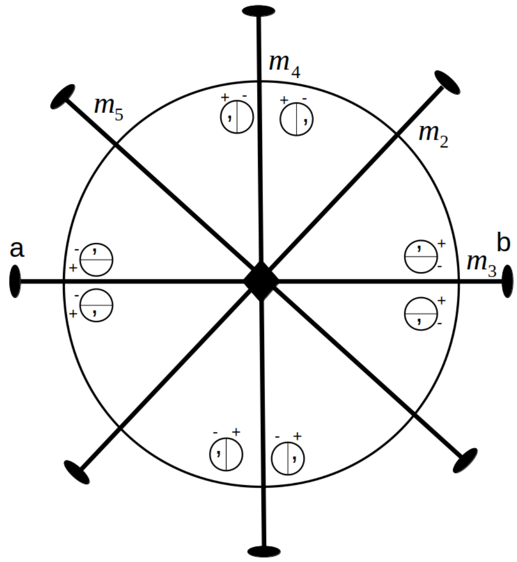


Figure 3