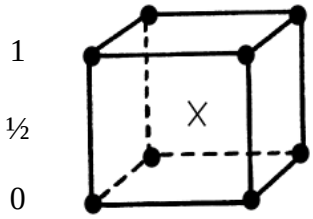
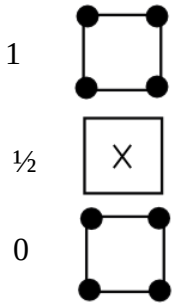
Topic 2-2: Slices

Summary: We now need to be able to visualize 3D crystal structures without the use of technology. In order to do this we introduce slices. Examples of slices of cesium chloride, perovskite and wurtzite are shown.

- The way we visualize crystal structure, without software, is by slicing the crystal into layers
- We can use slices to visualize any crystal with one axis *perpendicular* to the other two
- This technique isn't very useful for Bravais lattices where this doesn't hold true (eg triclinic crystals) because then the slices would be off set. Luckily, these crystals are the exception.
- There are three basic steps to this technique
    - Identify the perpendicular axis
    - Identify the height of each atom
    - Construct 2D cross sections
- A good beginning example is cesium chloride as seen below, where the x is the chlorine atom and the dots are the cesium atoms

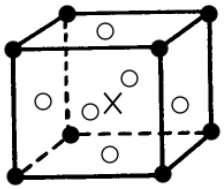


- We see there are atoms as $\vec{a}_3$= 0, ½, 1 so the slices look as follows

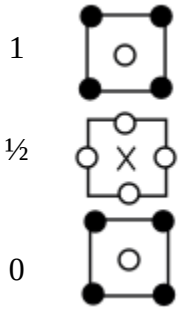


- We can see from this stack that the chlorine atom (X) has a coordination number of 8

- A more complicated structure to study is the perovskite structure (ABO_3) structure, as shown below where the dots are A atoms, the X is the B atom and the Os are the oxygen atoms



- We see that just like cesium chloride there are slices at $\vec{a}_3$= 0, ½, 1 as seen below



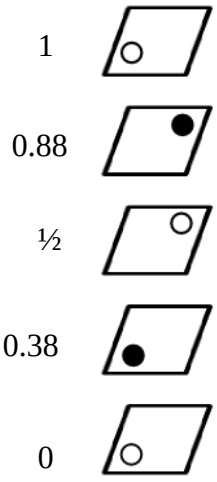
- There are six atoms within equal distance of the B atom (x) which, when put together as seen below, creates an octahedra

- Properties of crystals are rationalized qualitatively from bond type and coordination number
- An example of this is that an ion conductor may exhibit channels or layers for ions to move in
- We use the coordination number as a qualitative description to relate bonding to properties
- A non-cubic example is the wurtzite structure which is hexagonal

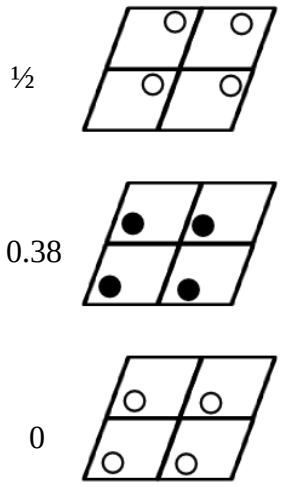
- This structure consists of zinc and oxygen atoms at the $\vec{a}_3$ heights in the table below

Zn (denoted by dots)	Oxygen (denoted by Os)
1/3, 1/3, 0.38	1/3, 1/3, 0
2/3, 2/3, 0.88	2/3, 2/3, 0.5

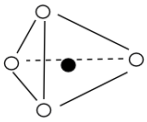
- We first create the usual slices with $\vec{a}_3$ heights 1, 0.88, 0.5, 0.38 and 0 from top to bottom



- We can then tile our slices in 2 by 2 squares to better see the coordination of our atoms



- We can then see that the zinc atoms (black dots) sit in the center of a tetrahedral, as so



and visa versa.

Questions to Ponder

1. Going back to perovskites, some are tetragonal instead of cubic, with a long $\vec{a}_3$ axis and exhibit piezoelectricity. When piezoelectric the A and B atoms are displaced along the $\vec{a}_3$ axis by delta and delta prime. Draw this in slices and rationalize why the macroscopic crystal is a piezoelectric material.

2. What happens if we put a voltage along $\vec{a}_1$ of the perovskite structure?