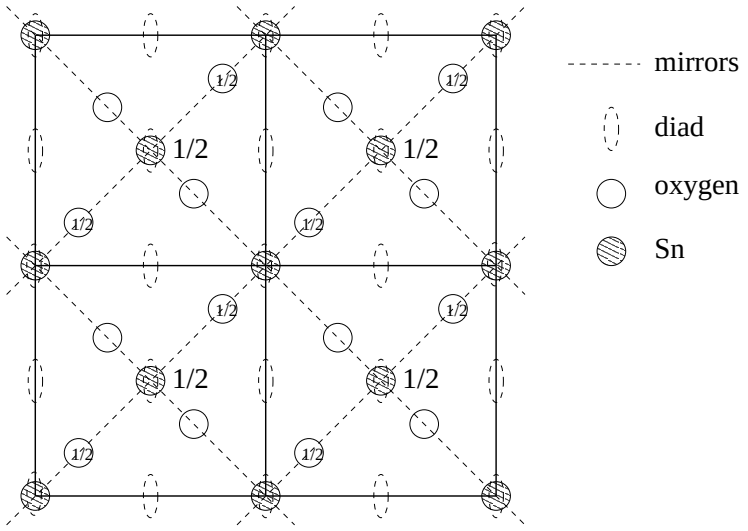
Question A2

Lattice: a 3D array of points, each has exactly the same environment. Each point is related to another by certain translational symmetry.

Motif: atom or group of atom that is associated with each lattice point; represented by fractional coordinates.

Crystal structure: description of the arrangement of atoms in a crystal. It is a superposition of motif over each lattice point.

$$\text{structure} = \text{lattice} \otimes \text{motif}$$



There are **2 unit formula** per unit cell (SnO_2, 4 oxygen in one unit cell).

Oxygen atoms form a **slightly distorted octahedron** around Sn atoms (see central Sn: two oxygens at $\pm[u, u, 0]$, 4 at $\pm[1/2 - u, 1/2 - u, 1/2]$)

To get the **distances** we just need to calculate the amplitudes of the two vectors above:

$$\sqrt{(ua)^2 + (ua)^2 + 0} = 2.077\mathring{A}$$

and

$$\sqrt{(0.19a)^2 + (0.19a)^2 + (0.5c)^2} = 2.038\mathring{A}$$

The angle between [110] and $[0\bar{1}2]$ is given by:

$$\cos\theta = \frac{-a^2}{\sqrt{2a^2}\sqrt{a^2 + 4c^2}} = 115^o$$

Finally, using Weiss equation for a vector [UVW] contained in a plane (hkl0:

$$h + k = 0$$
$$-k + 2l = 0$$

gives $(hkl) = (\bar{2}21)$.