Understanding crystal structure

To study crystallographic texture, it is important to understand crystal structure and diffraction from crystals.

**Determination of Miller Indices (denoted by hkl):**

- **Determine the intercepts along the crystallographic axes, in terms of unit cell dimensions**
- **Take the reciprocals**
- **Clear fractions**
- **Reduce to lowest terms**

For example, if the x-, y-, and z-intercepts are 3, 1, and 2, the Miller indices are calculated as:

- Take reciprocals: 1/3, 1/1, 1/2
- Clear fractions (multiply by 6): 3, 6, 2
- Reduce to lowest terms (already there)
Intercepts are: ∞, 1, ∞

Miller indices of the plane are:

$$\left(\frac{1}{\infty} \frac{1}{1} \frac{1}{\infty}\right)$$

Intercepts are: ∞, 1/2, ∞

Miller indices of the plane are:

$$\left(\frac{1}{\infty} \frac{2}{1} \frac{1}{\infty}\right)$$
Representation of crystal planes and the corresponding miller indices
Stereographic projection

- mapping of crystallographic planes and directions in a convenient and straightforward manner.
- two dimension drawing of three dimensional data.
- planes are plotted as great circle lines, and directions are plotted as points.
- Sometimes, planes are also indicated by the normal to them, that is, by a point.

**What do we learn further:**

- geometrical correspondence between crystallographic planes and directions with their stereographic projections.
- important crystallographic directions that lie in a particular plane of a crystal.
What is a pole?

• Let us consider a small unit cell.
• Construct a big sphere, called the Reference Sphere, around the point unit cell taken as the centre.
• Next draw perpendiculars to the six cube faces of the unit cell and extend these till they cut the reference sphere.
• These points of intersection of the plane normals with the reference sphere are known as the poles of the respective cube planes, (100), (1\bar{1}00), (010), (0\bar{1}0), (001) and (00\bar{1}).
• Place a source of light, say at the 001 pole position and then allow the light rays passing through the poles 100, \( \bar{1}00 \), 010 and \( \bar{0}10 \) to fall on a piece of paper put perpendicular to the 001-00\( \bar{1} \) axis.

• The lower half of the reference sphere will be projected as a circle, known as the Basic Circle on the piece of paper which is the projection plane, parallel to the (001) plane of the unit cell.
• The pole 001 will be at the centre of the basic circle, while the poles 100, \( \overline{100}, 010 \) and \( 0\overline{10} \) will appear on the periphery of the basic circle.

• The basic circle, along with the poles of different \{100\} type planes is a stereographic projection of the three dimensional unit cell, placed at the centre of the reference sphere.

• Since the plane of the projection is parallel to the (001) plane, the projection is known as the (001) stereographic projection of the cubic unit cell.
In a similar manner, the poles of the \{100\}, \{110\} and \{111\} planes can also be plotted with, say \{100\} and \{111\}, as the projection planes and the resulting stereographic projections (or stereograms).
Questions

1. Draw the following planes and directions in a BCC unit cell: (001), (113), [110], [201].
2. Indicate the following planes and directions in hexagonal crystal: (1210), (1012), [1120], (1010), (1123)
3. What do you mean by angle true in a stereographic projection?
4. Draw a standard (111) projection of a cubic crystal, showing all the poles of the form {100}, {110}, {111}.
5. What is Inverse pole Fig. (IPF) and how it is different from a pole figure?
6. Show [110] in a (001) pole figure.
7. Why single stereographic triangle is sufficient to represent the orientation in inverse pole figure?