CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

Prof. Sandeep Sangal
IIT Kanpur

Lecture 09(A): Properties of Planes and Directions in Cubic Unit Cell

In this lecture, I am going to talk about a couple of properties related to planes and directions in a cubic unit cell. One of the first things I want to examine is this: if I have a plane with Miller indices (hkl), and if I consider a vector that is normal to this plane, what would be the Miller indices of that normal vector?

Let's say I have this plane (hkl)**,** and let me also mark the points where this plane meets the **x**, **y**, and **z** axes. Let these intersection points be A, B, and C. Now imagine a vector indexed by [u v w] which is normal (perpendicular) to this plane.

If the vector [u v w] is perpendicular to the plane ABC, that means it must also be perpendicular to any vector lying in the plane (hkl).

So, consider the vectors $\overline{AB}$ and $\overline{BC}$. Let us go back to the previous lecture, where we already found the relationships for the vectors $\overline{AB}$ and $\overline{BC}$. Since those steps are already done, we can skip the derivation and directly write the expressions for $\overline{AB}$ and $\overline{BC}$.

Where the plane (hkl) intersects the **x**, **y**, and **z** axes will obviously be at
$\frac{a}{h}$, $\frac{b}{k}$, and $\frac{c}{l}$.

From the previous lecture, the vector $\overline{AB}$ can be written as:

$$\overline{AB} = -\frac{a}{h}i_1 + \frac{b}{k}i_2$$

Similarly, the vector $\overline{BC}$ can be written as:

$$\overline{BC} = -\frac{b}{k} i_2 + \frac{c}{l} i_3$$

As before, i_1 is the unit vector along the **x** axis, i_2 is the unit vector along the **y** axis, and i_3 is the unit vector along the **z** axis.

Now, we also know that we are dealing with a cubic crystal. Since it is cubic, that means: $a = b = c$. So, we are dealing with a cubic unit cell.

So $a = b = c$, which means I can write the expressions for the vectors $\overline{AB}$ and $\overline{BC}$ replace everything with a.

So, for $\overline{AB}$:

$$\overline{AB} = -\frac{a}{h} i_1 + \frac{a}{k} i_2$$

I can take a common:

$$\overline{AB} = a(\frac{-i_1}{h} + \frac{i_2}{k})$$

Similarly, for $\overline{BC}$:

$$\overline{BC} = -\frac{a}{k} i_2 + \frac{a}{l} i_3$$

$$\overline{BC} = a(\frac{-i_2}{k} + \frac{i_3}{l})$$

(And yes, as you noted, the minus sign in the first term remains intact.)

Now, as stated earlier, if the vector [u v w] is perpendicular to the plane ABC, then this vector n (whose Miller indices are [u v w]) must be perpendicular to both vectors $\overline{AB}$ and $\overline{BC}$.

So, let me write the normal vector n like this:

$$n = a(ui_1 + vi_2 + wi_3)$$

Since the vector n is perpendicular to AB and BC, their dot products must be zero.

Dot Product $n \cdot \overline{AB} = 0$:

Both vectors have a scalar factor a, so together they give a^2.

Inside, we take the dot product:

$$(ui_1 + vi_2 + wi_3) \cdot (\frac{-i_1}{h} + \frac{i_2}{k})$$

Now expand:

- $i_1 \cdot i_1 = 1$
- $i_2 \cdot i_2 = 1$
- $i_1 \cdot i_2 = 0$
- $i_1 \cdot i_3 = 0$
- $i_2 \cdot i_3 = 0$

So only two terms survive:

$$a^2(u(-\frac{1}{h}) + v(\frac{1}{k})) = 0$$

Thus, we get: $\frac{-u}{h} + \frac{v}{k} = 0$

Dot Product $n \cdot \overline{BC} = 0$:

Again, they give a^2.

Inside, we take the dot product:

$$(ui_1 + vi_2 + wi_3) \cdot (\frac{-i_2}{k} + \frac{i_3}{l})$$

Again, only the matching unit vectors survive:

- $i_2 \cdot i_2 = 1$
- $i_3 \cdot i_3 = 1$

So the dot product gives:

$$a^2(v(-\frac{1}{k}) + w(\frac{1}{l})) = 0$$

Thus: $\frac{-v}{k} + \frac{w}{l} = 0$

So, if we take this dot product, then this is what we are going to get. We have two relations now.

Since both quantities have to be 0, this implies, when we club both conditions together:

$$\frac{u}{h} = \frac{v}{k} = \frac{w}{l}$$

So, these ratios all have to be equal.

Let us say that these ratios are equal to a quantity called χ.
Where does this take me? Well, I can write:

$$u = \chi h \qquad v = \chi k \qquad w = \chi l$$

So, I now have the indices u, v, w in terms of h, k, l.
In fact, my direction [u v w] can be written as χ is common…

So, I can just take it out, and I have the direction [h k l]. Since χ is just a scalar quantity (a constant), this clearly implies that the direction [h k l] for a cubic unit cell is perpendicular to the plane (hkl). So, this is the first property that we have looked at.

Therefore, the indices of the direction normal to a plane (hkl) in a cubic system are the same as the Miller indices of that plane.

Now, since this is the case, I can now talk about the angle between two planes in a cubic unit cell as well. So, consider the planes $(h_1 k_1 l_1)$ and $(h_2 k_2 l_2)$. And again, this is for the cubic unit cell.

What will be the angle between these two such planes? The angle would be defined by the angle between their plane normals.

So, just from the previous discussion:

- The normal to the plane $(h_1 k_1 l_1)$ is the direction $[h_1 k_1 l_1]$.
- Similarly, the normal to the plane $(h_2 k_2 l_2)$ is the direction $[h_2 k_2 l_2]$.

And therefore, it is now a simple matter of taking the dot product between the two vectors $h_1 k_1 l_1$ and $h_2 k_2 l_2$ determining the angle between these two planes. So all I need to do is take

$$(h_1 k_1 l_1) \cdot (h_2 k_2 l_2)$$

and this would be equal to the magnitude of $(h_1 k_1 l_1)$ multiplied by the magnitude of $(h_2 k_2 l_2)$ times $cos\,\theta$, where θ is the angle between the two planes.

So, taking the angle between them, I can now write:

$$cos\,\theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\,\sqrt{h_2^2 + k_2^2 + l_2^2}}$$

So now, these two properties that we discussed for a cubic unit cell cannot be directly applied to the other Bravais lattice unit cells.

(Refer Slide Time: 16:16)