CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 08: Interplanar Spacing

In this lecture, we are going to talk about the interplanar spacing between (hkl) planes. This diagram, which you see here, is what I had drawn towards the end of the last lecture. It shows a set of parallel planes that have indices (hkl). As I mentioned in the last class, when I refer to a (hkl) plane in a lattice or a crystal, it actually represents a set of parallel planes that are equally spaced. This diagram illustrates the spacing between those (hkl) planes.

Now, if we look at it, there is a normal vector drawn here, which is perpendicular to all three planes shown. Of course, there is an infinite set of such parallel planes, and they are equally spaced. That spacing is what we call the "*Interplanar spacing*", symbolically represented as d_{hkl}. So, d_{hkl} is the interplanar spacing for a specific set of (hkl) planes.

To understand this concept clearly, let us look at one more diagram by taking a specific set of (hkl) planes.

So, I am just drawing a set of unit cells, and this unit cell can belong to any one of the Bravais lattices. For instance, I have this set of unit cells, and this is my **x**, **y**, and **z** axis. Now, in this set, the **x**, **y**, and **z** directions are indicated, showing which is the **x** direction, which is the **y** direction, and which is the **z** direction.

Let me consider the (0 1 0) planes. So, all of these form the (0 1 0) plane because this is my **a**-axis, this is the direction of the **b**-axis, and this is the **c**-axis.

So, the (0 1 0) planes are all present, and they are all equally spaced. Their spacing, in this specific case, is b. Similarly, I can have a set of (hkl) planes in a more general way, as I have drawn here. This could be any set of (hkl) planes.

Again, you can figure out what the normal would be. The normal, of course, is the **b**-axis in this case for the (0 1 0) planes.

Now I intend to derive a relationship for the interplanar spacing of a (hkl) plane. The simplest case is the cubic system; as we move away from cubic, the relationship becomes progressively more complex, and for the most general case (triclinic,) the spacing is the most complicated and is difficult to derive by simple geometric tools.

First, we will derive the interplanar spacing for lattices whose unit-cell axes are orthogonal (perpendicular) to each other. For clarity: an orthorhombic unit cell has $a \neq b \neq c$ all interaxial angles equal to 90^o (unlike the cubic cell, which has $a = b = c$).

So, let us consider an orthorhombic example. I will draw the (hkl) plane that is closest to the origin. Then I drop a perpendicular from the origin onto that plane. The perpendicular distance from the origin to the (hkl) plane is the interplanar spacing d_{hkl} for that family of planes.

This is some (hkl) plane whose Miller indices are (hkl). This (hkl) plane will intersect the **x**-, **y**-, and **z**-axes at:

- along the **x**-axis: $\frac{a}{h}$,
- along the **y**-axis: $\frac{b}{k}$,
- along the **z**-axis: $\frac{c}{l}$.

Now, drop a perpendicular from the origin. Let the origin be O and let the perpendicular meet the plane at N. Also, label the intercepts on the axes as A, B, and C, respectively. Draw the line AN. Then consider triangle OAN. Because $\overline{ON}$ is perpendicular to the (hkl) plane, any line in the plane is perpendicular to $\overline{ON}$; in particular, line AN lies in the plane and is perpendicular to $\overline{ON}$.

So, $\overline{ON}$ is perpendicular to the (hkl) plane, as drawn, and I need to find the length ON, which gives the interplanar spacing. I can say the vector $\overline{ON}$ is perpendicular to the plane (hkl). The magnitude of this vector, which I will denote by ON, equals the interplanar spacing d_{hkl} for this particular (hkl) plane.

Now, since $\overline{ON}$ is perpendicular to the (hkl) plane, any line lying in the plane is perpendicular to $\overline{ON}$. Thus $\overline{ON}$ is perpendicular to $\overline{AB}$ and also perpendicular to $\overline{BC}$. In fact, $\overline{ON}$ it would be perpendicular to $\overline{AC}$ as well, but it is sufficient to consider just two non-collinear vectors in the plane $\overline{AB}$ and $\overline{BC}$ because two independent vectors completely define the plane.

So, let us now look at a few other vectors. For example, let me consider the vector $\overline{OA}$. The vector $\overline{OA}$ is along the **x**-axis, and let me also define three unit vectors along the **x**, **y,** and **z** axes. These unit vectors are i_1 along **x**, i_2 along **y**, and i_3 along **z**. Normally, the general practice is to use $i,\ j,\ k$, but I am not choosing those symbols because they will get confused with the plane indices (hkl).

So, what is the vector $\overline{OA}$ now in terms of the (hkl) indices?

Very clearly, it should be $\frac{a}{h}$ (its magnitude) multiplied by the unit vector i_1. Similarly, $\overline{OB}$ is $\frac{b}{k}i_2$ and the vector $\overline{OC}$ is $\frac{c}{l}i_3$.

Now, what are the vectors $\overline{AB}$ and $\overline{BC}$?

So, let us first consider the vector $\overline{AB}$. If I look at it, to go from point A to point B, I can go along the vector $\overline{AO}$ and then along the vector $\overline{OB}$, which means I can write:

$$\overline{AB} = \overline{AO} + \overline{OB}$$

Now, I know what the magnitude of $\overline{OA}$ is, which is $\frac{a}{h}i_1$. So, what will be the magnitude of $\overline{AO}$? It will just be $-\ \overline{OA}$.

So this becomes $-\ \overline{OA} + \overline{OB}$, which gives me the vector $\overline{AB}$ as:

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

Similarly, if I take the vector $\overline{BC}$, it is the sum of the vectors $\overline{BO}$+ $\overline{OC}$, which take me from point B to point C.

So this would be, as before:

$$\overline{BC} =- \overline{OB} + \overline{OC}$$

So this becomes:

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

Now, let us look at the vector $\overline{ON}$ itself.

The direction of a vector $\overline{ON}$ can be defined by three angles, which are called the *Direction cosines.*

- The angle α that the vector $\overline{ON}$ makes with the **x**-axis.
- The angle β that $\overline{ON}$ makes with the **y**-axis.
- The angle γ that $\overline{ON}$ makes with the **z**-axis.

So, basically, *cos α, cos β,* and *cos γ* become the direction cosines.

Let us now try to write an expression for cos α.

Remember that in the right-angled triangle, cos α is nothing but ON / OA.

Here, $\overline{OA}$ is the hypotenuse, and the 90-degree angle is at N, so:

$$cos\ \alpha\ = \frac{ON}{OA}$$

But we know that ON = d_{hkl}, and OA = $\frac{a}{h}$.

Hence:

$$cos\ \alpha\ = \frac{d_{hkl}}{\frac{a}{h}} = \frac{hd_{hkl}}{a}$$

Similarly, for *cos β*, I draw a line from B to N to form another right-angled triangle.

Then:

$$cos\ \beta\ = \frac{ON}{OB} = \frac{d_{hkl}}{\frac{b}{k}} = \frac{kd_{hkl}}{b}$$

Analogously, for *cos γ*:

$$cos\ \gamma\ = \frac{ld_{hkl}}{c}$$

Now I use one of the properties of the direction cosines:

$$cos^2\alpha\ +\ cos^2\beta\ +\ cos^2\gamma\ =\ 1$$

I substitute the expressions for *cos α, cos β,* and *cos γ* into the relation

This gives:

$$\left(\frac{hd_{hkl}}{a}\right)^2 + \left(\frac{kd_{hkl}}{b}\right)^2 + \left(\frac{ld_{hkl}}{c}\right)^2 = 1$$

Rearranging the terms (and noting that d_{hkl} will also be squared), I obtain:

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

This is the expression for the interplanar spacing for an orthorhombic unit cell. Now, it is easy to see the corresponding expressions for other systems:

- Tetragonal system (where $a = b \neq c$):

$$\frac{1}{d_{hkl}^2} = \frac{h^2+k^2}{a^2} + \frac{l^2}{c^2}$$

- Cubic system (where $a = b = c$):

$$\frac{1}{d_{hkl}^2} = \frac{h^2+k^2+l^2}{a^2}$$

For other systems like rhombohedral, hexagonal, or structures such as triclinic and monoclinic, where the angles are not orthogonal, the expressions for interplanar spacing will also contain the terms involving α, β, and γ. In fact, in the case of a triclinic system, all six lattice parameters appear in the expression for the interplanar spacing, making it difficult to derive using the method applied for the orthogonal systems.

For these non-orthogonal systems, the expression for interplanar spacing is usually obtained using the result from the reciprocal lattice concept.

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