CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 06: Miller Indices for Directions in Lattice Space

We very often need to define directions and planes in a lattice or a crystal, for which a set of three indices is used, called the Miller indices. So first, let us consider directions and see how we can obtain a set of three indices to represent a direction.

Let us consider an arbitrary unit cell. This is my unit cell, and let us take a specific direction here. Let us take one of the corners of the unit cell, and take the opposite corner of the unit cell, and join them to define a direction. Let me call this vector $\overline{OA}$. So, this is a vector; basically, a direction means we are trying to define a vector.

For a vector, we need three components in three-dimensional space; in two dimensions, we would require only two components. My standard axes are the **a** axis, **b** axis, and **c** axis of the unit cell.

For $\overline{OA}$, the three components would be:

- along **a**, there will be some component,
- along **b**, there will be another component, and
- along **c**, there will be a third component.

Along the **a** axis, you can see that if I look at the absolute magnitude of the component, then along **a** I have a component of magnitude *a*. Along **b**, I will have a component **b**, and along **c** I will have a component **c**, which are nothing but the magnitudes of the edges of the unit cell.

But what we do is make use of fractional coordinates, so that we do not have to specify *a*, *b*, and *c*, because *a*, *b*, and *c* are already specified when you define a crystal. So, we consider *a* to be 1 unit, *b* to be 1 unit, and *c* to be 1 unit, and therefore I can simply write the components of this vector $\overline{OA}$ as (1, 1, 1). Now there are three components, and therefore the Miller indices for this direction would simply be [111], conventionally written inside square brackets. Thus, the direction $\overline{OA}$ has Miller indices [111].

Let us take another example.

Consider the direction $\overline{OB}$. This direction $\overline{OB}$, or this vector $\overline{OB}$, lies in the plane AB itself, and very clearly its three components would be: 1 unit along **a**, 1 unit along **b**, and 0 units along **c**. Therefore, the components are (1, 1, 0). Hence, the Miller indices for this direction become [110].

Let us take yet another example.

Consider the direction $\overline{OC}$, where the vector intersects the edge halfway at the midpoint of the edge (represented by $\frac{1}{2}$). The three components $\overline{OC}$ are: 1 along **a**, $\frac{1}{2}$ along **b**, and 0 along **c**. To remove the fraction, I multiply all components by 2, and the direction becomes (2, 1, 0). Hence, the Miller indices become [210].

Now, let us take one or two more examples. Incidentally, do not assume this is a cubic cell; it can be any unit cell in the Bravais lattice. Consider a vector like this: the vector intersects the top face at its midpoint. How do we define its components? For this, we need to shift the origin. Let me call this vector $\overline{DE}$. So, I shift the origin to point D. Now, what are the three components?

Along **a**, the vector goes halfway in the *negative* direction. So, the component along **a** is $-\frac{1}{2}$. Along **b**, it goes halfway in the *positive* direction, giving a component of $\frac{1}{2}$. Along **c**, it goes one full unit, so the component is 1. To remove the fractions, I multiply all components by 2. This does not change the direction; it only changes the magnitude. Therefore, the indices become: (−1, 1, 2). And conventionally, negative indices are written with a bar on top. So the Miller indices are: $[\bar{1}12]$. This illustrates the simple idea of defining a direction in crystal or lattice space using three indices.

Now, coming to some specific unit cells. Suppose I take a cubic unit cell, and this time I am taking a cubic cell as defined in the Bravais lattice, which is $a = b = c$. Let me first consider a direction like this. Its Miller indices are clear: along **a** it is 1, along **b** it is 0, and along **c** it is 0. Therefore, the Miller indices become [100]. Let me call this the vector $\overline{OA}$.

Now, let me call a second vector $\overline{OB}$. The Miller indices for $\overline{OB}$ would clearly be [010], as it has 0 component along **a**, 1 unit along **b**, and 0 component along **c**.

Similarly, if I define a vector $\overline{OC}$, its Miller indices are going to be [001].

I can also define negative directions. So, instead of $\overline{OA}$, I can say $\overline{AO}$. Then what happens is that I simply negate all the indices to show the opposite direction. $\overline{AO}$ would become $[\bar{1}00]$. Similarly, the opposite of $\overline{OB}$, which is $\overline{BO}$, becomes $[0\bar{1}0]$, and the opposite of $\overline{OC}$, which is $\overline{CO}$, becomes $[00\bar{1}]$.

Now, all of this, since this is a cubic cell, implies that all of these directions. If you notice, suppose it is drawn in a lattice with lattice points only at the corners (that is, a primitive cubic lattice). Then, along the direction $\overline{OA}$, the lattice points are going to be spaced with a distance of a, equally spaced by a. Along $\overline{OB}$, since it is a cubic cell again, the spacing

would be a. Similarly, along $\overline{OC}$, the spacing of lattice points along that direction would be the same as for $\overline{OA}$ as well as $\overline{OB}$.

Therefore, we can put all of these six directions that we have here into a form that we call "*Symmetry-equivalent directions"*. They can be represented by three indices placed inside what are called angular brackets or triangular brackets, indicating that we are not referring to just one particular direction, but all the symmetry-equivalent directions. So, all six directions are defined by these three indices written within triangular brackets.

So, these brackets are very important when we talk about Miller indices for directions as well as for planes. We have to use specific brackets so that we are clear whether we are talking about a specific direction or about symmetry-equivalent directions, which are also known as a "*Family of directions"*.

Let us take another example. Let us say this is $\overline{OD}$. Now, for $\overline{OD}$, we have already seen that its Miller indices are going to be [110]. Now, I can define many other directions that are symmetry-equivalent to this in a cubic cell. Let us consider this one.

If I look at the Miller indices for this, I need to take the origin at point A. Then, there will be −1 component along **a**, +1 component along **b**, and 0 component along **c**. Therefore, the Miller indices for this direction would become $[\bar{1}10]$.

Take a third example. If I take this as the direction $\overline{AC}$, its Miller indices would now be: −1 along **a**, 0 along **b**, and +1 along **c**, and therefore the indices become $[\bar{1}01]$.

You can clearly see that I can define similar directions on the third plane as well, the third cube face plane, like that. If I want to indicate the symmetry-equivalent directions, they

will be represented by the three indices <110> enclosed in triangular brackets. So, what are the various directions?

I can simply permute the indices and write all the symmetry-equivalent directions. So, from <110> I can write [101], [011], and one can write the negative directions as well. Then there are other directions like $[\bar{1}10]$, $[\bar{1}01]$, $[0\bar{1}1]$, and one can write all the negative directions for these as well: $[1\bar{1}0]$, $[10\bar{1}]$, $[01\bar{1}]$, and so on. So, I have written all the possible symmetry-equivalent directions along the face diagonals.

Now, sometimes we may want to specify an absolute magnitude for a particular direction. Usually, for direction indices, we are not concerned about the magnitude of the vector, only the direction. But if I want to give a specific magnitude, I must mention which vector of the unit cell I am referring to: vector **a**, vector **b**, or vector **c**.

If I don't specify that, the directions become meaningless because there is no reference. So, let's take a specific direction, like $\overline{OA}$. Here, A is the midpoint of the face. So, if I want to write the Miller indices for this direction, I can say it has a $\frac{1}{2}$ component along **a**, $\frac{1}{2}$ a component along **b**, and 0 component along **c**. If I simply multiply these by 2 to remove the fractions, I get the direction [110].

But now, if I want to write the specific magnitude, we already know what the magnitude of this direction is because this is a cubic unit cell, where $a = b = c$. So, for this direction, the magnitude is half the length of the face diagonal. And the full face diagonal is $a\sqrt{2}$, so half of that is $a\sqrt{2} \times 0.5 = \frac{a}{\sqrt{2}}$.

Therefore, to write the specific vector with its actual magnitude for $\overline{OA}$, I can express it as: $\frac{a}{2}[110]$. Here, the Miller indices are [110], and the factor $\frac{a}{2}$ adjusts the vector to the

correct physical magnitude. If I want to calculate the magnitude explicitly, I can write OA (without the bar) as:

$$OA = \frac{a}{2}\sqrt{1^2 + 1^2 + 0} = \frac{a}{2}\sqrt{2} = \frac{a}{\sqrt{2}}$$

So, this method allows me to represent the direction with its absolute magnitude as well.

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