CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 07: Miller Indices for Planes in Lattice Space

In this lecture, we are now going to talk about Miller indices of planes. Let us begin with a few examples to understand the concept. I am taking an arbitrary unit cell. Do not assume that it is necessarily cubic. It could be rhombohedral, orthorhombic, triclinic, or any other type. First, let us start with something simple. Sometimes, I can specify my unit cell vectors **a**, **b**, and **c** in this orientation as well.

Now, let us take a plane. I will always take a plane that lies completely inside the unit cell, even though in the infinite lattice the same plane extends to infinity. So, consider a plane drawn by joining three corners of the unit cell. Now, the question is: what do I do next?

So, in order to define a plane, even mathematically, we need to find its intercepts, that is, the points at which it intersects the three axes **a**, **b**, and **c**. In this case, we can clearly see (again using fractional coordinates) that the intercepts with the axes are: along **a**, it intercepts at 1, along **b**, it intercepts at 1, and along **c**, it intercepts at 1. This is the first step we need to take: get the three intercepts for the plane.

The second step is to take the reciprocals of these intercepts. In this case, that gives us $\frac{1}{1}, \frac{1}{1}, \frac{1}{1}$ which again becomes 1, 1, 1.

Therefore, the Miller indices for this plane are (1 1 1). Notice that this time we write these indices in circular brackets, not square brackets. This is important because circular brackets are conventionally used to denote that the indices refer to a *plane*, not a direction.

Let us take another example. This time, we have joined three different corners of the unit cell. Again, we first need to determine the intercepts. Before writing down the intercepts, we should notice that we must shift the origin in this case. By shifting the origin to this new point, we can properly identify the intersections with the axes **a**, **b**, and **c**.

So now, the axes are drawn from here: this is point A, this is point B, and this is point C. If we observe carefully, the plane intersects the **a**-axis at this point; essentially, it intercepts at –1. It intersects the **b**-axis again at –1, and it intersects the **c**-axis at 1.

Next, we take the reciprocals. The reciprocals are simply -1, -1, 1. Therefore, the Miller indices become (since we have negative numbers, we place a bar on top): $(\overline{11}1)$.

Now, let us take a few more examples to understand this. In my first case, let us consider this plane. In fact, let me label it as well: A, B, C, and D. This is basically one of the cube faces. So, what are the intercepts in this case? Again, I have to show my axes: **a**, **b**, and **c**.

It intersects the **a**-axis at 1. Where does it intersect the **b**-axis? Well, it is parallel to the **b**-axis. Whenever two lines or a line and a plane are parallel, we consider their intersection to be at infinity. So, it intersects the **b**-axis at ∞, and it intersects the **c**-axis also at ∞.

Now, we take reciprocals: $\frac{1}{1}\,\frac{1}{\infty}\,\frac{1}{\infty}$. Therefore, the values we obtain are: 1, 0, 0. So, the three numbers become (1 0 0).

Now, you can understand the logic behind why we take reciprocals: we do not want infinity to appear in the Miller indices. Therefore, the Miller indices for that plane simply become (1 0 0).

Similarly, if you look at the other cube faces, the face that intersects the **b**-axis at 1 but the **a** and **c** axes at infinity will have Miller indices (0 1 0). The top face, which intersects only the **c**-axis at 1 and the other two at infinity, will have Miller indices (0 0 1).

Now, consider another example. Let us take a plane that intersects the edges as follows: It intersects edge AD at $\frac{1}{2}$. It intersects the second edge at $\frac{2}{3}$. It intersects the third edge at 1. To find the intercepts with the axes, we again shift the origin accordingly. Along the **a**-axis, the intercept becomes $-\frac{2}{3}$, because this is now the direction of the **a**-axis from the shifted origin. Along the **b**-axis, the intercept becomes $-\frac{1}{2}$. Along the **c**-axis, the intercept is +1.

Just as we did for directions, we want to remove the fractions and convert everything into integers. Before doing that, we must first take reciprocals of the intercepts. So, the reciprocals become: $-\frac{3}{2}\ \ -\frac{2}{1}\ \frac{1}{1}$. The next step is to obtain the Miller indices. Since only the first term contains a fraction, we simply multiply all three numbers by 2 to remove it.

Multiplying by 2 gives: $-3\ \ -4\ 2$. Therefore, the Miller indices for this plane are $(\overline{3\ 4}\ 2)$. With this, we have covered all the possible situations and should now be able to find the Miller indices for any plane quite easily.

Now, let me revisit the example we discussed earlier. Consider this plane again. The Miller indices we previously obtained were $(\overline{1}\ \overline{1}\ 1)$. If we simply negate all the numbers, the same plane can also be represented as $(1\ 1\ \overline{1})$.

Now, let us see how we can visualize this. To obtain these Miller indices, I had taken this origin. Now I will do a small construction: I draw another unit cell just below it and extend the plane. If I extend the plane and label its intersections, it will be easier to follow. Let us say the original plane passed through points A, B, and C, and by extending it, I reach point D in the cell below. Thus, the same plane continues into the second (bottom) unit cell.

Now, let us concentrate on the plane ABD and try to get the Miller indices for it. The Miller indices for ABD should represent the same plane as those for ABC. For ABD, I must choose the origin appropriately. I will take the origin at the lower corner (the one in the bottom cell). With that origin, the intercepts are: along **a** it is 1, along **b** it is 1, and along **c** it is –1.

Take the reciprocals, and I will get 1, 1, and the same third number. Finally, the Miller indices become $(1\ 1\ \bar{1})$. So we can see that $(1\ 1\ \bar{1})$ and $(\bar{1}\ \bar{1}\ 1)$represent the *same* plane. Therefore, by negating all the indices of a plane, I am still describing the same plane.

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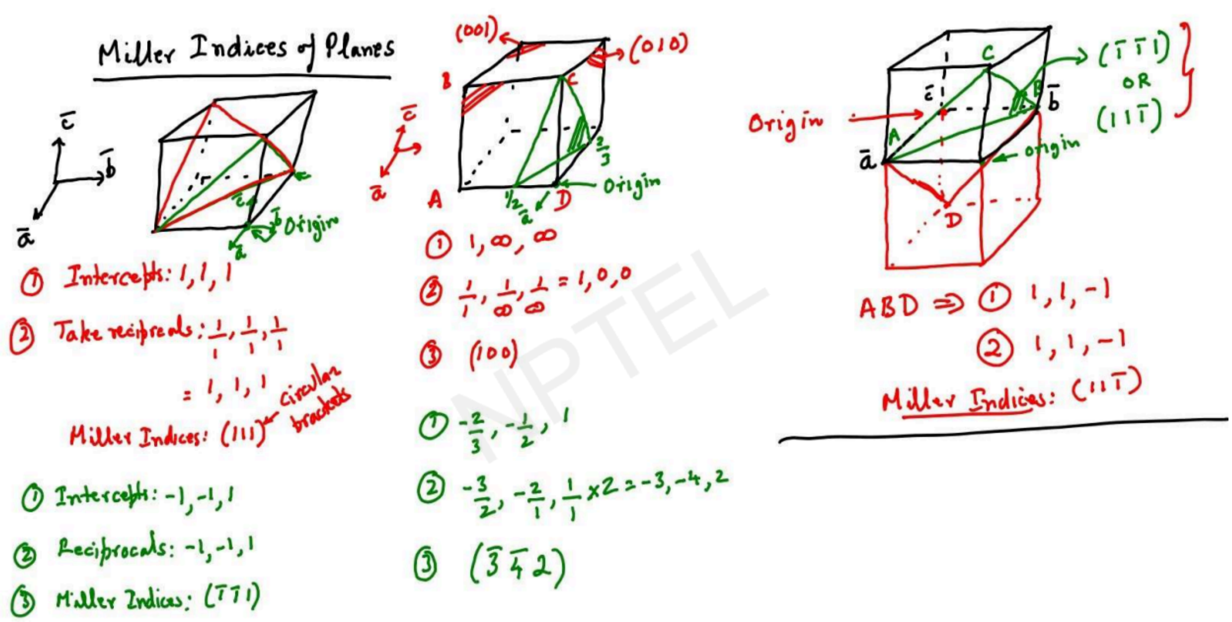

Now, we need to understand one more important point regarding planes. Let us consider an arbitrary plane. Suppose this plane intersects the **a**-axis, **b**-axis, and **c**-axis at certain positions. What will those intersection points be? If the Miller indices of this plane are (h k l), then the intercepts along the axes will be:

- along the **a**-axis: $\frac{a}{h}$
- along the **b**-axis: $\frac{b}{k}$
- along the **c**-axis: $\frac{c}{l}$

Here I am writing the *absolute* intercepts, not the fractional coordinates.

So here is the important point I want to highlight: a plane with Miller indices *(h k l)* does not represent just one plane. Because the lattice extends infinitely, these indices actually represent a set of parallel planes.

Now, where will the *next* parallel plane appear? If I move another distance $\frac{a}{h}$ along the **a**-axis, the new intercept becomes $\frac{2a}{h}$. Similarly, along the **b**-axis it becomes $\frac{2b}{k}$, and along the **c**-axis it becomes $\frac{2c}{l}$.

If I draw a plane through these new intercepts, I get a second plane that is: Parallel to the first plane, and has the same Miller indices. Let us check this. The intercepts of the second plane are: $\frac{2a}{h}$ along **a,** $\frac{2b}{k}$ along **b**, $\frac{2c}{l}$ and along **c**. If I now take the reciprocals of these intercepts (and ignore the absolute lengths *a, b, c*), I get: $\frac{h}{2}, \frac{k}{2}, \frac{l}{2}$. To remove the fractions, I simply multiply all of them by 2, returning me to: $h,\ k,\ l$.

So indeed, the second plane has exactly the same Miller indices as the first. This shows why a single set of Miller indices corresponds to an infinite family of equally spaced parallel planes.

These planes repeat periodically. We can move in the positive direction to get the next plane, and we can also move in the negative direction. This means there is also a plane that passes through the origin, and then many more planes continue beyond it in the negative direction as well.

Now suppose I drop a perpendicular from the origin onto the set of planes. This perpendicular will meet the first plane at one point, the second plane at another point, and so on. You can imagine that it will continue intersecting the third, fourth, and further planes.

From the way these planes are drawn, you will see that they are equidistant from each other. So, if this point is O, the next intersection is A, and the next is B, then the distances $OA = AB$, and similarly for the next pairs.

This perpendicular distance between successive parallel planes is called the interplanar spacing, denoted by d_{hkl}. It represents the spacing between the set of planes with Miller indices $(h\, k\, l)$.

In a later lecture, we will see how to calculate this interplanar spacing. The formula for d_{hkl} depends on the type of unit cell, and the relationships will be different for different Bravais lattices.

One final comment on the planes is that, just as we had symmetry-equivalent directions, we also have "*symmetry-equivalent planes*". To understand this, let us consider the cubic system.

Consider the plane whose Miller indices are (1 0 0), the second plane whose Miller indices are (0 1 0), and the top plane whose Miller indices are (0 0 1). Of course, once you consider this front plane, the plane at the back, which is a parallel plane, would also be part of the same set of parallel planes.

Now, these three planes, because of the symmetry of the cubic lattice, are equivalent. Suppose there are only lattice points at the corners; or even if you take the face-centered cubic structure, you will see that all these planes have the same set of lattice points at the corners. And if it is a primitive cell or a face-centered cubic cell, then one will see lattice points at the corners and at the centers of the faces for each of these planes.

So, all of these planes can be grouped together into a "*family of planes*". In the case of directions, we use angular brackets. In the case of planes, we are going to use curly brackets, and we will write it as {1 0 0}, representing all the planes of that family. We can write specific planes in circular brackets. A lot of times you will also see that the negative indices are written, but essentially there are only three sets of planes.

If I had, let us say, instead of this plane, talked about this particular plane, then we know that the Miller indices for that plane are (1 1 1). The family of planes will be written in curly brackets as {1 1 1}. What are the planes in this family? I can write (1 1 1), I can write $(\bar{1}\ 1\ 1)$, I can write $(1\ \bar{1}\ 1)$, and $(1\ 1\ \bar{1})$. I can also add, if I want, the corresponding negative indices. But they all represent the same set of symmetry-equivalent planes.

So, with this discussion, the method of assigning indices for directions and planes is now covered in this lecture and in the previous lecture.

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