An Introduction to Materials: Nature and Properties (Part 1: Structure of Materials) Prof. Ashish Garg Department of Materials Science and Engineering Indian Institute of Technology, Kanpur

> **Lecture - 11 Miller Indices (contd.)**

Ok; so, we start this lecture 11 today.

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Müller molices (contr)

Which is again on Miller indices; we will continue some part of the previous ones before we move on to the Miller indices for directions.

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Miller Indices
Planes - h k l
Dinections - u v w

So, last lecture we are talking about Miller indices for Miller indices for planes and you also have Miller indices for directions. Now, this is needed to complete the description of the unit cell. So, for plane Miller indices are usually described as h k l and for direction you would describe the Miller indices as u v w.

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▜▗▙▙▓▓▝▓ Plane $\begin{array}{ccccccc}\nh & k & l & \longrightarrow & \text{mtej} & \text{or} & \text{$ Reciprocal of the inter-cepts on respective unit cell lengthes which are convented to smallest set of integers

As we saw that for a plane the procedure is h k l are nothing, but the reciprocal of the intercepts on respective unit cell lengths and which are converted to the smallest set of set of integer.

So, h k l all three are integers they can be positive as well as negative.

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So, I will just go through some more descriptions of h k l in a unit cell ok. Now, let us say you want to draw a plane which is 1, 2, 3 ok. So, what you do for that is you take you go as; so, this is h, this is k, this is l. So, on x axis your intercept is 1 over 1 on y axis your intercept is 1 over 2 on z axis the intercept is 1 over 3.

So, you can see here this is one this is half and this is one third and you can choose this as a origin o because all three are positive. So, if you go in this direction it is plus x when this directions plus y if you go in this direction is plus z. And if you connect all three of them this is your plane 1, 2, 3. Now suppose you wanted to draw a plane which is 1 bar 2 three. So, h h k l could also be negative; so, this bar 2 means it is negative of 2.

So, what this means is that you have interceptor on x axis as 1 along minus y axis you have half and along plus z axis you have.

Student: One third.

One third; So, here there is a problem because you now cannot choose this origin and the and the thing a Miller indices is that that the planes and direction should be represented within one unit cell you should not be needing to go out of the unit cell. So, in this case what you need to do is that you need to shift your origin.

So, if I shift my origin for example, here I go in minus x which is not useful to me; I go in positive y, I go in positive z; if I choose my origin here I can go minus y minus x, but I will not need minus x. So, I choose this as a origin this is o prime let us say. So, if I come in this direction this is plus x if I come in this direction this is plus minus y and if I go in direction one above this is.

Student: Plus z.

Plus z; So, I can now draw the intercept this is along the x intercept, along the a length of the unit cell which is 1. So, it is at a this is at half and this is at one third somewhere here. So, if I now connect these three points; so, this is 1 bar 2 3 plane. Now ah; so, this is how you and you can identify a plane if I told you the as I told you the procedure in the last class.

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That if you have a plane drawn within a unit cell. Now let us say I would want to draw a plane now here, let us say this is the plane or now let me just draw it in green this is the one this is a unit cell whose intercepts. So, if you look at it now what is the origin you are going to choose first of all? You cannot choose this as origin it is very obvious here. So, you need to choose an origin from which you can count the intercepts. So, I choose an intercept which is the origin which is here o prime let us say.

So, I have a intercept which is here which is; so, along x what is the intercept?

Student: 1.

1; along y what is the intercept?

Student: Minus where minus 1.

Minus 1; along z what is the intercept?

Student: (Refer Time: 07:18)

Plus.

Student: Plus half.

Half convert into reciprocal 1 minus 1 and.

Student: 2.

2. So, the plane is.

Student: 1 minus 1.

1 1 bar.

Student: 2.

2 ok; So, this is how you draw and identify a plane. So, now another thing is about the family of planes ok.

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So, if I draw a cube if this is let us say if this unit cell is not a is just a cube ok. So, just a cube would imply; so, this is a cube alright. So, what is this face of the cube this is ?

Student: 0 1.

0 0 1 what is this face of the cube?

Student: 0 1 0.

0 1 0 and what is this face of the cube?

Student: 1 0.

1 0 0 now in a cube all these three are identical. So, in a cube 0 0 1, 0 1 0 and 0 0 1 planes are similar planes because of symmetry. If you turn the x axis by 90 degree then it would look similar to 0 0 1; if we do the rotation of y axis if you do the rotation of z axis by ninety degrees all of them will look same right.

So, I can represent these as 0 1 0 0 planes by these curled brackets ok. So, this would mean family of 1 0 0 type planes, but only valid for a cubic system ok. So, 1 0 0 here would mean it implies 1 0 0, it implies 0 1 0 and it applies 0 0 1 ok. So, you can see that you have; so, likewise you can have. So, you can see that there is a multiplicity right.

So, in case of cube 1 0 0 implies; you also have bar 1 0 0, 0 1 1, 0 0 and 0 0 bar 1. So, you have depending on how you look at it there are three different types of which are identical three different plane; I mean it is sort of oxymoron in some sense I can just say three planes which are identical.

Similarly, if you look at 1 1 0, 1 1 0 would imply ? 1 0 1 1 1 0 0 1 1.

Student: (Refer Time: 11:13)

It would also imply 1 0 bar 1.

Student: 1 0.

1 bar 1 0.

Student: 0.1

0 1 bar 1 and you can make some more combinations out of it. So, I will just leave them to you. So, these are called as family of planes and this is. So, if you look at the number of planes here this is called as multiplicity of the planes. So, in a in a in a cubic system your if you look at just 1 0 0 type at 6 planes, but crystallographically speaking it is six planes if you include the negatives into account [FL].

Similarly, if you look at if you look at hh 0 you have hh 0 will have you have 12 of them. So, you can have 1 0 1, 1 1 0 and so, on and so, forth you can have bar 1 0 1, you can have bar 1 1 0 and 0 bar 1 1 and you can have bar 1 0 bar 1, bar 1 bar 1 0 and 0. So, there are 12 of these ok.

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Similarly, if you go to h h h which is nothing but let us say.

Student: 0.

1 1 1 kind of plane. So, 1 1 1 would mean? 1 bar 1 1, 1 1 bar 1, bar 1 1 1 and you will have other options as well 1 bar 1 bar 1 bar 1 1 bar 1 and bar 1 bar 1 1 and so, you have in total of 8. So, you have 8 multiplicity.

So, similarly for a cube if you if you took if you like take h k l; h k l kind of planes will be 48; if you look at h h l it will be 24 if you look at h k 0; it will be 24 and so on and so, forth ok. So, this is for cube if I do the same exercise now in a tetragon; let us say I take it tetragon ok. So, this is the tetragon; so, here a is equal to a is not equal to c ok. So, a is equal to b is not equal to c. So, you have two lattice parameters a and a and c.

So, here now which one is ah; so, this face is this is 0.

Student: 1 0.

1 0 this is.

1 0 0; now what is this? 0 0 1.

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 712.999879 ■ 图 Tetragmel $A - B + C$ $a \neq c$ (100) 2 (010) are equivalent (000) hoo, oho, hoo, oho 100 4 $h00$ 2012001 \rightarrow 2 $00l$ d_{100} hkl ohk $h\nmid D \rightarrow \# h \circ k$

Now, this plane of course, because of tetragonal symmetry is different as compared to the other two planes; this has a fourfold these two have a twofold and in terms of atomic density in terms of spacing, it is different. So, in case of tetragonal system; so, this is tetragonal. So, in case of tetragonal 1 0 0 and 0 1 0 are?

Student: Same.

Equivalent, but 0 0 1 is not. So, in case of tetragonal you draw h 0 0 multiplicity will be 4; this will imply h 0 0, 0 h 0 and then you will have 0 0 l; this will have a multiplicity of 2. So, 0 0 l and bar l similarly there are other planes as well. So, when you have h k l or h k 0.

So, h k 0 will not be equivalent to h 0 k or 0 h k because of tetragonal symmetry because the third indices is along the c axis which is c c lattice parameter which has different length has compared to a and b and things become. So, you can see the multiplicity will go down in tetragonal system and you will also see that d 1 0 0 and d 0 1 0 are same ok, but d 0 0 1 is not same as d 1 0 0 and d 0 1 0.

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So, the formula that we saw d is equal to a divided by square root of h square plus k square plus 1 square this is valid only for.

Student: (Refer Time: 17:27).

For tetragonal; So, this is d h k l for tetragonal system this d h k l would be 1 over square root of h square plus divided by a square k square divided by a square plus 1 square divided by c square. So, this is for tetragonal if you look at orthorhombic it will be.

Student: (Refer Time: 18:14).

So, now formula looks very similar for these three are orthogonal systems orthogonal systems. For non orthogonal systems these are different d h k l are different and I I will refer you to principles of X-ray diffraction by B P Cullity. So, at the back there is appendix on these planers inter planar spacing's as well as inter planar angles.

So, if you look at inter planar angles they will also be different, they will not be the same ok. So, similarly you can you can also look for inter planar angles also have different?

Student: Relations.

Relations; so, this again you can find in cullity now. So, this is about the tetragonal system now if I go to now directions; so, here we have finished the plane part ok. So, what we have learned is how to draw a plane, how to determine a plane, how to basically

the mirror indices of a plane which is drawn, how to find the inter planar spacing and how to find the inter planar angles.

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 $d_{100} = d_{010} + d_{001} - 04$
 $d_{100} + d_{010} + d_{001}$ A_{100} 7 = 10
 L_{100} 7 = $\frac{h_1 h_1 r_1 h_2 h_1 r_2 f_1 h_2 r_1}{\sqrt{h_1^2 + h_2^2 + h_1^2 + h_2^2 + h_1^2}}$

So, inter planar spacing; so, d 1 0 0, d 0 1 0, d 0 0 1 are all same for cubic; in case of tetragonal d 1 0 0 is same as d 0 1 0 but it is not same as d 0 0 1 for tetragonal. In case of orthorhombic and things are even different for other planes other systems. So, this is just for orthogonal systems.

Similarly, angles in case of tetragonal system in case of cubic system we saw the angle was cos theta 1 1 over.

Student: (Refer Time: 21:09) h.

h 1 h 2.

Student: Plus k 1 k 2.

Plus k 1 k 2 plus.

Student: (Refer Time: 21:16).

2 divided square root of?

Student: h 1 square.

h 1 square plus k 1 square plus?

Student: (Refer Time: 21:22).

Into square root of plus k 2 square plus l two square; this is again only for cubic system, it will be different for tetragonal orthorhombic system. Now, let us go to what we call as directions ok.

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Now, directions are nothing, but vectors alright and they are denoted as I said earlier denoted as u v w.

So, basically we call as lot of people also call them as crystallographic directions; crystallographic directions. So, basically; so, it is nothing at a vector. So, you resolve the components.

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Student: (Refer Time: 22:31).
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So, resolve the vector components and then along the crystallographic axis and then reduce them to smallest set of integers let us see how we work along this.

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So, you have a; I will again draw a unit cell one thing that I forgot to mention is that that representation h k l is independent of the crystal system. The multiplicity may change, but how you determine a plane, how you draw a plane that is independent of the crystal system ok. So, that is applied to all the crystal systems as long as you have a unit cell, 3D unit cell you draw a plane identically in identical fashion irrespective of type of the crystal system.

Student: (Refer Time: 23:42).

So, if I draw a crystal direction a is unit cell ok. So, let us say I want to draw; so, if I take u v w as 1, 2, 3 ok; then what basically it means is that you have one interceptor on x. So, this is one translation, one lattice translation along x 2 lattice translation; now as opposed to plane it is not half, it is 2 of lattice translation along. So, basically what this means is that and this 3 of along z.

So, basically it is 1 of x plus 2 of y plus 3 of z that is how you will represent a vector right if it was a vector R that is how you will represent a vector right 1 of x plus 2 of y plus 3 of z; the problem is if you want to draw in this fashion, you will have to go once. So, this is origin let us say O you will have one here then you will have to go two steps in sorry this was y this was z then you will have to go two steps here and then you will have to go three steps 1, 2, 3.

So, you will go out of the unit cell; that is not desirable what we want to do instead is I can what I can do is that I can convert these back to. So, if I have 1, 2, 3 I divided by the largest integer which is 1 by 3.

Student: 2 by 3.

2 by 3 and.

Student: 1.

1. So, what I now do is that. So, if I now do 1 by third in x direction.

Student: 2 by third.

2 by 3 in.

Student: y.

Let us say y direction and somewhere along here y 2 and on here somewhere here. So, this will be coinciding with this point somewhere here ok. So, this is one third two third and 1 and here now you connect the end point. So, this is a this is the direction OA; so, OA is nothing, but 1, 2, 3.

Student: Direction.

Direction alright; so, this is the direction. So, direction a single direction is determined by these square brackets that family of direction is given as 1 u v w. So, this is single direction. this is family of directions now let me tell now take a few more examples. So, basically if you just look at it objectively this O is the origin which has a 0.000 this is a point which is u v w direction is nothing, but u minus.

Student: Origin.

Origin u v w minus origin basically ok; so, if it was x 1, x 2, x 3 if this was y 1, y 2, y 3 and all you need to do is that you need to find out y 1 minus x 1, y 2 minus x 2, y 3 minus x 3 and then convert them back to integers alright. So, that will be the direction because it is a vector right. So, vector that is this is how you draw a vector as you have studied in your in the school ok.

So, basically now we will finish this lecture here and in the next lecture we look at some more examples of how do we draw the directions. And we will also look at a little different system which is hexagonal system. In hexagonal system the directions are and planes are can be drawn in a different manner because depiction of them can be done in 4 digits rather than 3 digits.

Because as we will see hexagonal system can also be characterized by 4; 4 axis which is which can be reduced to 3 axis, but fourth axis is drawn just for the sake of convenience which is nothing, but related to 2 axis. So, there is a third axis in the basal plane of hexagonal system. So, we will discuss that in next lecture.

Thank you.