

Structure of Materials
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Lecture - 13
Miller Indices

Having defined the concept of family of directions, let us go and count the number of the family the important directions.

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Family of directions		
Index	Members in family for cubic lattice	Number
$\langle 100 \rangle$	$\{100\}, \{\bar{1}00\}, \{010\}, \{0\bar{1}0\}, \{001\}, \{00\bar{1}\}$	$3 \times 2 = 6$
$\langle 110 \rangle$	$\{110\}, \{\bar{1}\bar{1}0\}, \{1\bar{1}0\}, \{\bar{1}10\}, \{101\}, \{\bar{1}01\}, \{10\bar{1}\}, \{\bar{1}0\bar{1}\}, \{011\}, \{0\bar{1}1\}, \{01\bar{1}\}, \{0\bar{1}\bar{1}\}$	$6 \times 2 = 12$
$\langle 111 \rangle$	$\{111\}, \{\bar{1}\bar{1}\bar{1}\}, \{1\bar{1}\bar{1}\}, \{\bar{1}1\bar{1}\}, \{\bar{1}\bar{1}1\}, \{1\bar{1}1\}, \{1\bar{1}\bar{1}\}, \{\bar{1}\bar{1}1\}$	$4 \times 2 = 8$

the 'negatives' (opposite direction)

Symbol	Alternate symbol		
$[\]$		\rightarrow	Particular direction
$\langle \rangle$	$\{ \{ \}$	\rightarrow	Family of directions

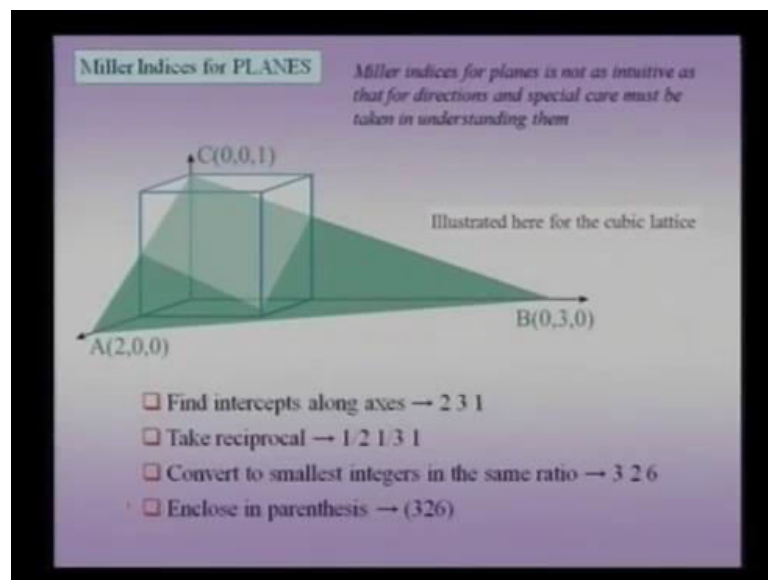
Like the 1 0 0, 1 1 0 and 1 1 1 which are important directions, and we will be dealing with them often when we talk about various properties of crystals, and make a counting of the all the members the family. So, this is for the cubic lattice that we are doing, the simplest of the possibilities, so we have the 1 0 0 family you have the 1, 2, 3, 4, 5, 6 members of the family. Essentially which can be thought of 3 members and their negatives therefore, we have 3 into 2 6 members belonging to this family.

As for as the 1 1 0 goes I can off course write 1 1 0, I can make one of these things negative, I can make the other index negative, and I can permute all the ways. I can put the 0 in the first place and second place the third place and therefore, if I count the positive directions and their opposites, they can have 6 into 2 there are 12 members of the 1 1 0 family. The 1 1 1 family which is also very important family especially with

regard to cubic crystals, and especially face centered cubic crystals, which we call the cubic close pack crystals.

We see that there are 8 members to this family which can be understood as 4 into 2 8, so this numbers are very, very important. And when we talk about especially something known as the multiplicity factors with regard to planes, we need to know the number of such planes and therefore, we need the counting of all the equivalent possibilities. Now, sometimes in literature there are alternates symbols to describe directions for instance the family of directions, and this symbol double square bracket is also used which essentially is similar to the carat brackets we have been using, so far.

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Now, let us go to the concept of miller indices for planes, the concept of miller indices for planes is not straight forward as the concept of miller indices for directions. And we need to play a little care and attention in understand the concept, in other word whenever a miller indices for planes is presented to us we have to understand that is certain procedures have been followed in arriving at those indices, and we have to be careful in understanding them.

So, let us take one arbitrary plane and of course, this is the specific plane, which passes through 3 points A, B and C in for instance cubic system of course, a cubic lattice in this case. Now, the A point is as vertices 2, 0, 0 and B point is 0, 3, 0 and the C has 0, 0, 1 as

it is vertices, I want to find out the miller indices for this planes. So, first thing I write down the intercepts along the axis, which is nothing, but 2, 3 and 1.

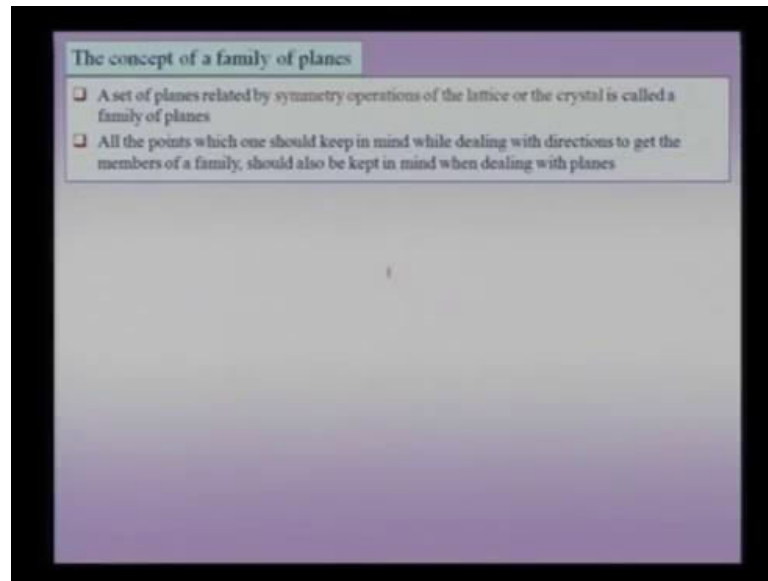
The next thing I take the reciprocal of these numbers, and this is where the fact that miller indices for planes becomes contra intuitive or there not active as see miller indices for directions. And that is why as I mentioned you have to take special care in understanding them, so the reciprocal would be half 1 3rd and 1, I will convert them into smallest integer; that means, I will multiply this entire thing by a factor of 6.

So, this can be this is nothing, but 6 times 3 2 6, so 6 by 2 is 3, and 6 by 3 is 2 and I have got 6. What I will do next is enclose them in the normal brackets and as 3 2 6 I will not use commas in normal cases between these indices, and wherever I may have high order index let us suppose I had 13 to 6 then I would leave a space to make sure that the 13 and the 2 and 6 are distinct. So, let me go through the procedure again I find the intercepts A B and C along the 3 axes I will take reciprocal of these indices, and then I convert them into smallest integers and finally, I will enclose them in brackets.

So, for this plane which is marked in green here the indices would be 3 2 6, and as before when I am writing an index like 3 2 and 6 I mean the complete set of planes, which are equivalent to the plane which are parallel set of planes. So, even though I mention the single plane, except when I want to be explicit about a particular plane I know the indices 3 to 6 refers to the whole set of parallel planes, which have this kind of a property or passing through or this kind of the orientation in space.

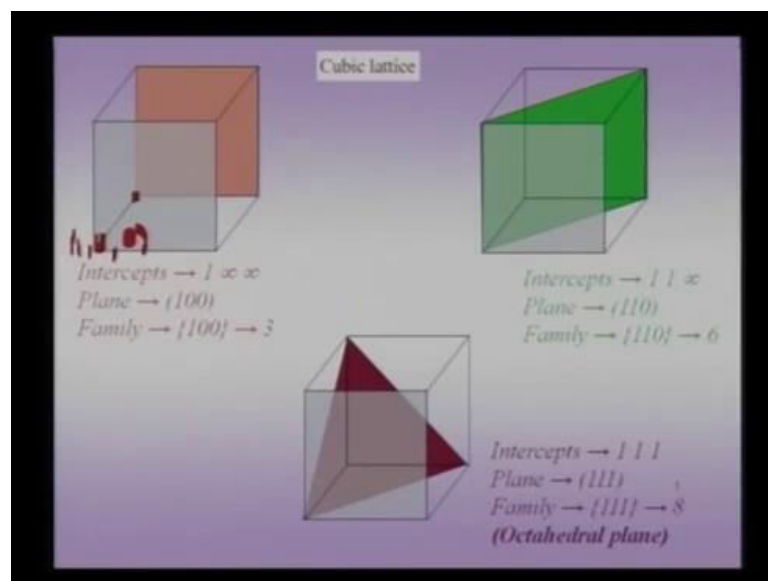
Now, normally when you show a plane you do not show the entire plane, you only show the part of the plane which lies within the units cell, which have been marked in this light shaded green. So, that is the path which is shown in usual diagrams and we have to remember these planes are actually infinite planes and they therefore, pervade entire two dimension space or pass through entire three dimension space.

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So, like before we could have the concept of family of planes, and since we are defining the family meaning that they are the translational in equivalent set. Therefore, I just apply the symmetry operations to a given plane, I get all the symmetry related said therefore, I need to apply all the symmetry operation on this plane, and I would get the symmetrically set of these planes which should be called family of planes. So, this is no difference in that sense from the symmetrically set of directions and, now let me consider important direct planes in a cubic lattices.

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So, there are three important planes, the plane which is shown in orange, the plane which is shown in green and the plane which is shown in brown. Now, as before I take the intercepts of this plane along the three axis, and the intercepts would be 1 infinity infinity and the intercept I do not write it as 0, but I translated by 1 unit. That means, even though the orange plane is actually passing through 0 I do not write it as 0 infinity infinity, I taken transient equivalent set which is this grey plane and write it as 1 infinity infinity.

The reason for doing this transient equivalent set will become obvious, when I do next step which is the reciprocal. So, the reciprocal of this would become 1 0 0 and then I enclose it in brackets and that becomes the miller indices for the plane, and if I want to write the miller indices family I can write it as 1 0 0 within a different kind of brackets, now which is the kind of equal brackets which is meant for planes.

Now, a few important things here number 1 is that if I had started out with 0 infinity infinity, and I have taken the reciprocal then I would again land up with infinity 0 0. So, I do not want to do this, and that is why I do not chooses orange plane, but I chooses grey plane assuming that this is the origin this is now the number here I chosen this point as 1 0 0 as my the passing through the grey plane, and then I find out the miller indices.

Now, also this examples makes this obvious that why do I take reciprocals, the reciprocals is to avoid these infinity, I would not take reciprocals all the infinity in the intercepts vanish and therefore, I get a neat number like 1 0 0. Now, let me do the same process again for the green plane which is shown here, which is another important low index plane which is cubic crystals and cubic lattices. So, the intercepts for this plane would be assuming this is my origin would be 1 1 and infinity in the third direction.

So, it never intercepts the z axis, so my intercepts are 1 1 infinity then I take my reciprocal which will makes 1 1 0, and then enclose it in the bracket for the plane. So, it make it 1 1 0 is my indices for this place which is shown in green, the family of planes I would represent within these kinds of brackets as 1 1 0, and the number of members of the family is 6, while the member 1 0 0 family was 3. Now, I will take another after showing these three examples I have shown the same things actually using a physical models.

So, it becomes very clear where are these planes located, now if I take another kind of plane and try to generate this miller indices. So, this is the plane shown in brown and as usual the my origin n is located here, the intercepts for this plane are 1 0 0 along the x axis, 0 1 0 along the y axis, and 0 0 1 along the z axis. So, my intercepts are 1 1 1, the reciprocal of intercepts will be 1 1 1 and therefore, I will put these kind of brackets to show this is a set of planes, and the miller indices for it.

The family of the plane is showed with these brackets with 1 1 1, and there are 8 members in this family and therefore, I call this the octahedron plane. So, let me go down and pick up the modals to show you these 3 planes, which are important planes in a cubic lattice, and we will often deal with these kind of planes in the cubic lattice.

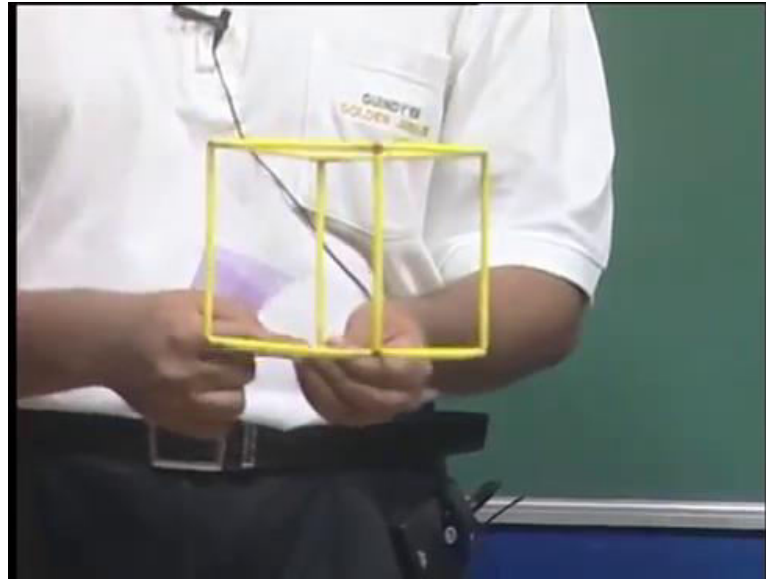
Sowmya ask question.

STUDENT: Sir how will we determine that how many member are there in a family.

Exactly the same way we determine the members the way for family set of for the case of directions, we find the all the symmetrically equivalent set of planes. And therefore, I in other words I take my planes I operate symmetry operations of the crystal or the lattice, and find out all the equivalent set.

Exactly the way you do it for the directions, and for high symmetry ones we saw that we could actually do a very simple, what we mechanical way of doing it. We may put all the negatives, we permute all the indices about because, as in the cubic system therefore, the x axis related to the y axis and related to the z axis in order to the A vector B vector C vector are all related by the 3 fold direction. And therefore, I can just permute them and get all the possibilities, and put negative for all the terms.

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So, let me choose this unit cube to demonstrate for 3 planes we just consider, so my $1\ 0\ 0$ plane is nothing, but any face of the cube. So, this is my face of the cube this is $1\ 0\ 0$ plane, this is another $1\ 0\ 0$ plane which is also to the face of the cube, any one of them is the $1\ 0\ 0$ member. Of course, the exact plane is it the $1\ 0\ 0$ or $1\ \bar{0}\ 0$ or $0\ 1\ 0$ depends on the origin and the orientation of the coordinate axis. But, all belong to the same family, so this three now I am talking about the $1\ 1\ 0$ plane.

That means, that it has intersects suppose this is my origin, this is my x axis, this is my y axis and z axis, it has a intersect 1 along the x axis, 1 along the y axis and infinity along the z axis. So, it will be a plane something like this, so it will interact the z axis, so you can see this, so let me orient this little different let me take this plane, and therefore, you will see that this plane will go to infinity along with z axis.

Now, I have the other modal which actually puts this plane in perspective, so you see here this is the member of the $1\ 1\ 0$ family. So, you can clearly see this is the Perspex box within which I have drawn $1\ 1\ 0$ kind of a plane.

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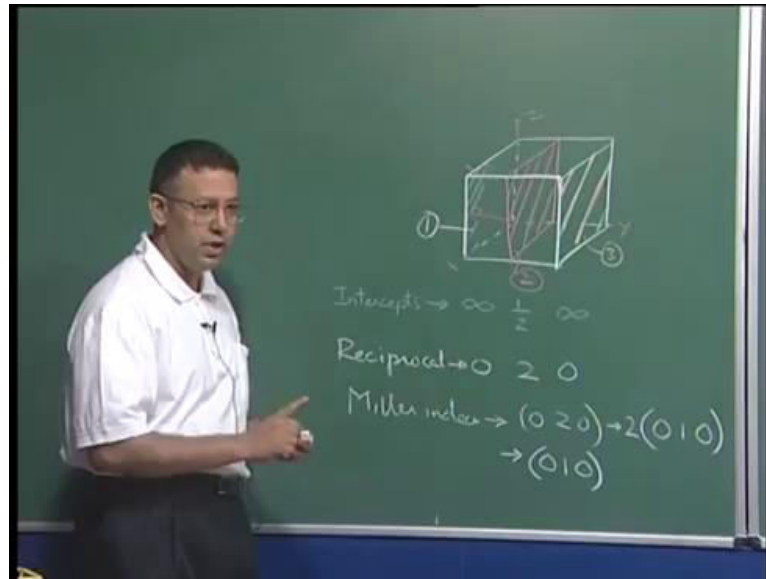


So, you can see this plane, now let me draw the third plane which is the $1\ 1\ 1$ plane, so I have got a triangle, again I have told you that all these planes are infinite planes. But, typically present them by the section of that plane which lies within the units itself and that is why it is looks triangular, otherwise all these planes should be infinite planes. So, this is my original before, so this $1\ 1$ plane intersects the x axis along one point that is $1\ 0\ 0$, $0\ 1\ 0$ and $0\ 0\ 1$ therefore, I can draw my plane which is this plane which is here.

So, this is an inclined plane which has intersects among the 3 axis, so I will just show it to you this in different orientation you can have a look, and as I mentioned before this is a very, very important plane, especially when you are talking about cubic closed pack crystals. So, we will deal with this plane quite a bit when we are talking about the cubic closed pack crystals, and this as you will see it happens to be closed pack plane in the cubic crystal. And in that case these directions will turn out to be the closed pack direction.

Student: Sir, can we find h planes cubic lattice means the lattice which cuts the edge of the indices, means the indices which cut the edges can you find the indices in that edge.

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I try to understand your question and let me draw it on the board and if I am wrong you can correct me, suppose this is my cubic unit cell, and my now I am talking about the cubic lattice, can you come to the board and draw me which I have you are talking about. So, that I will give the different color chock and then you draw the plane, so you are taking about the plane which is cutting the edges right, so you just draw the intersects and I will draw the edge which are the edge.

Student. That means, any edges which cuts the plain.

So, just one edge and where is the other intersects it has to intersect.

Student: That means, any edge we can consider.

So, let me consider the simplest of the lot assuming is the cube now, and now this is an important question. So, because, I have only considered those planes for instance, so far which are at the phases for instance this would be a plane which I considered, now this is an alternate plane which does not pass through any of those and actually cuts the half point very good question. So, let me answer this question let me consider the simplest of the lot it will be consider the translation with the equivalent plane of that, this is my plane now.

And to make sure that this plane actually sits with this system what I will have to do I will have to draw the white line outline. So, in other words if this is my origin this point

inside is my origin, and now my intersects along this is my x axis, and this is my y axis and this my z axis. So, my intersects for this plane along the x axis it would be infinity it will never intersects the x axis, along the y axis, so I will write down the intersects along the y axes is half.

Because, I considered this at the middle of the edge for simplicity, you could of course, also reside anywhere in the edge. So, I will write half for simplicity, and also it does never intersects the z axis, so intersects along the z axis would be infinity, so now I go and find the reciprocal of this. So, the reciprocal of this plane would become 0, so this is my reciprocal becomes $0 \ 2 \ 0$, some miller indices will come $0 \ 2 \ 0$ if I like or if I want to factor I like to common factors, it will become $2 \ 0 \ 1 \ 0$.

And I can of course, write it as $0 \ 1 \ 0$, and important question arises what is the difference between re writing as a $0 \ 2 \ 0$ and the $0 \ 1 \ 0$ they are in other words in some sense equivalent planes. But, there is the certain difference and you will soon come that actually it is the very important questions that's why because, if you talking about any rate of $0 \ 2 \ 0$ planes that would include for instance this planes. So, suppose I got equivalent to this planes.

So, let me now level this planes I call this planes 1, I call this red plane as 2, and just for say of clarity I will able to this plane has 3 I will give them orange color and level this plane as 3. This 3 planes are equivalent if I do not mention anything except this number $0 \ 1 \ 0$, and I could consider any one of them as we already saw, but there is the certain difference between this 3 planes, and what is the difference we will definitely consider after looking the next slide.

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Points about planes and directions

- Unknown direction $\rightarrow [uvw]$
- Unknown plane $\rightarrow (hkl)$
- Double digit indices should be separated by commas $\rightarrow (12,22,3)$
- In cubic lattices/crystals $[hkl] \perp (hkl)$

Interplanar spacing (d_{hkl}) in cubic lattice (& crystals)

$$d_{hkl}^{\text{cubic lattice}} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

So, coming back to the main slides, so let me mention few points about plane and directions you for returning to solving problem. Now, an unknown direction typically is $u v w$, suppose I have I do not have specific planes I have a unknown plane, I have call it $u v w$ sorry an un direction I will call it $u v w$, an unknown as will call $h k l$. And suppose I am talking about high index plane, where have double digit indices I could separate them by compass of course, you could also use the space between the indices, but absolute explicit you can separate them by my commas. A point which will of course the expand point little more in one of the coming slight is that cubic lattices, and crystal $h k l$ plane is perpendicular to the $h k l$ directions, akriti has question has this point.

STUDENT: Sir, $h k l$ plane is perpendicular to $h k l$ directions is the true for on un usual cubic lattice or other...

Very good question, so we will return to this questions becomes we have complete slide on this very aspect alone. So, we will return to this and the process we will consider another issue of what is known as the wave zone law, when we have a set of planes I would also like to include what is the known as the inter planer spacing, which is written as the subscript $h k l$ and I do not usually put the brackets on the $h k l$ the usual brackets. But, I have to understand that I still mean the miller and I am referring to the plane $h k l$ within brackets.

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In other words when I am writing d_{hkl} what I mean is $d_{(hkl)}$, so that this actually implicitly means that I am actually contributing the Miller indices. So, what is the formula for d_{hkl} for the cubic lattice.

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Points about planes and directions

- Unknown direction $\rightarrow [uvw]$
- Unknown plane $\rightarrow (hkl)$
- Double digit indices should be separated by commas $\rightarrow (12,22,3)$
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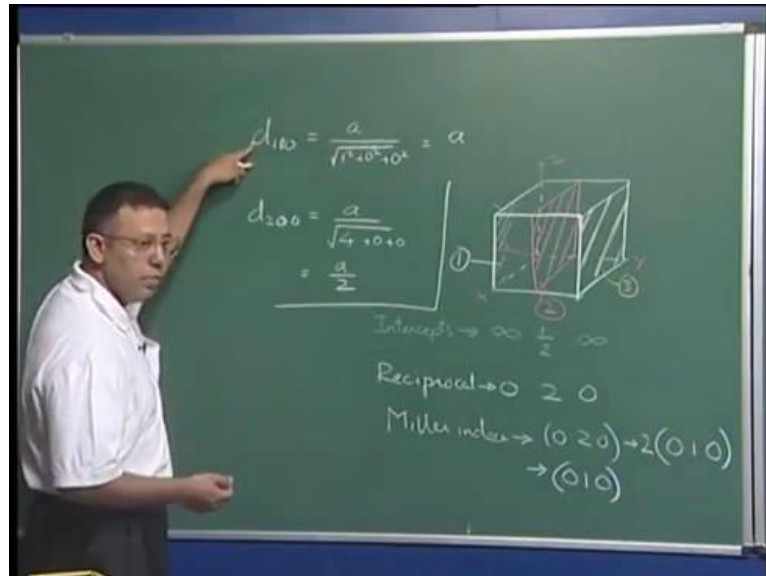
Interplanar spacing (d_{hkl}) in cubic lattice (& crystals)

$$d_{hkl}^{\text{cubic lattice}} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

And as you can see have explicitly mention it is the cubic lattice, and the formula is a is the lattice parameter the cube, and the formula for the inter plane spacing is a divided by root of $h^2 + k^2 + l^2$. Now, let me written to the problem is in

hand and try to calculate inter plane spacing, for the two kinds of planes we have just now seen.

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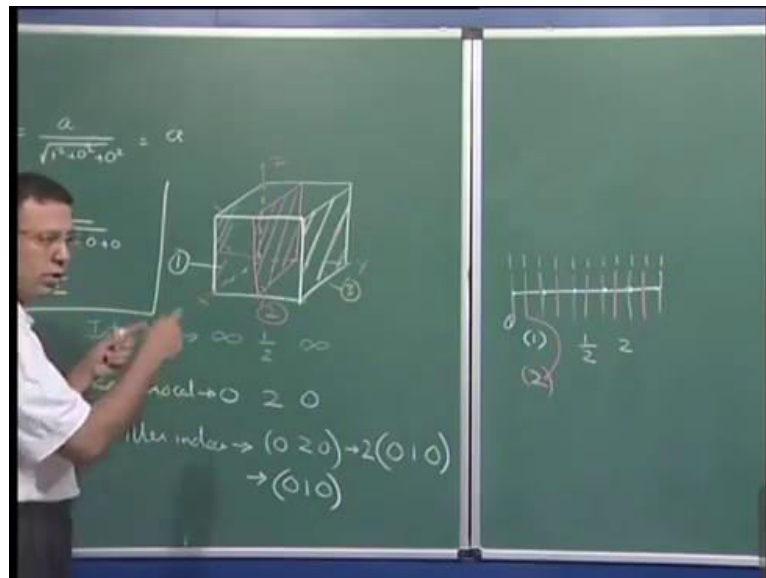
So, we have 2 planes here the d_{100} , and the other plane we have in consideration which is nothing, but either this 1 plane or the 3 plane and I also have this red plane which is the as I calculate the indices is d_{200} through $0\ 2\ 0\ 0$ sorry the plane has d_{100} on the other plane is d_{200} . So, given by formula the this is a by square root of 1 square plus square plus 0 square that is equal to a.

In the inter plane of spacing is a if I write it as $1\ 0\ 0$, we can clearly see as for as the orientation goes the red plane is no different from the white plane 1 or the 3 plane. So, d_{200} by the formula will be a by square root of 4 plus 0 plus 0 therefore, it is a by 2 in other words the inter plane spacing out the $2\ 0\ 0$ plane is half that of the $1\ 0\ 0$ planes. Now, what does it means, it means that the $1\ 0\ 0$ plane is a sub set of the $2\ 0\ 0$ planes, if I consider single plane just as single how 1 plane.

Of course, I can position that plane here or here or here, and I would use an indices like $1\ 0\ 0$ for that pane I could you place it some anywhere between. But, when I am talking about real crystals I would not arbitrary spaces plane I would place is at unit cell in a very specific way. And the specific way could be somewhere between the 2 that is half along the y direction or it could 3/4'th along y directions etcetera therefore, I am considering the specific plane I need to worry about what is this explicit.

And the reason is that there could be attendance which could be explication on this planes, which could actually began some detraction of some other effect. Therefore, I need to worry about, now what I mean that the inter plane spacing of the 2 0 0 plane is half the other 1 0 0 plane, and what I do mean also that h this is 1 0 0 is a sub set of the 2 0 0 I will explain here.

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And let me do it in one dimensions first implicitly, so this are my lattice points approximately equal. So, now, what will be the for instance suppose this has just one dimension therefore, I cannot have planes here, but let me just consider that this is plane that I am considering, they have only one index to describe that pane. So, this set of plane should be the y planes, and I call the one set, and index for this would be simply one right.

Now, the other set of planes which is here let me draw the other set on super post on this top here. So, the other set of plane means which is now actually includes not only the plane which have between, but also the plane which are related let me draw them, now let plane are 2 and close it with in brackets. So, miller indices of this planes would be 2, as you can clearly see that my red planes are located 0 half 1 1 and half 2 and 2 and half etcetera.

But, my white planes are located only at $1\ 2\ 3\ 4$ etcetera; that means, that the red planes are super set of the white planes. That means, if I just delete half the red planes I can get the white planes.

Student: Sir, near there are lot of planes, so every each planes are the sub set of every one.

I am not very sure what you are asking, but let me explain the concept go over concept again the subset and superset and this spacing, I have clearly seen that $d\ 2\ 0\ 0$ has half the spacing or $d\ 1\ 0\ 0$. Now, question is what is $d\ 2\ 0\ 0$ plane, it is not just this one red plane, but it is series of red plane because, this understood, now the when I am talking about $d\ h\ k\ l$ I am talking about the inter plane or spacing. That means, it is a spacing between all those set of planes.

And, now I am asking a questions let I am only considering this planes which are located in the front and in the back, which are like the $1\ 0\ 0$ planes or I am also talking again into account planes which per weight at the middle. So, now, talking about the $2\ 0\ 0$ planes I am talking about planes in the middle, but also a plane in the corner, it is not that I would explicit this planes, this are now my $2\ 0\ 0$ planes this, this, this right.

And what is the inter plane spacing half right, half that if my planes are located in this ends and this ends right. So, this is my $1\ 0\ 0$ set as you can see, my $2\ 0\ 0$ set as plane of middle also right therefore, it has got half the inter plane this spacing, now since this is the $2\ 0\ 0$ set is not just this plane, it is this plane, this plane, this plane all of them belongs $2\ 0\ 0$ cell and that is inter plane now spacing is now this distance.

Now, therefore, by $1\ 0\ 0$ set you only includes the y in the z , so let me write planes belongs to the $1\ 0\ 0$ set, it is 1 plane in the diagram the $2\ 3$ plane etcetera $2\ 0\ 0$ set actually includes the 1 the 2 and also the 3 right. Therefore, it is a set which is half the spacing and therefore, with density of number of planes right therefore, when I like in the case of vectors in directions that set if I am just to worried about just expression, then I can factor out all the component in factors for the directions.

But, if I worried about the length and this directions then I cannot co factor of the common factors. Similarly, for planes if I no worried about what is the interplant of spacing or where plane I just worried about the orientation then I can fact of all common

factors. But, also additionally worried about the interplant spacing and there exact positions the unit cell, then I need to consider I can factor out the 2 I have to keep the two within the numbers. So, the this is the important point note and this becomes a absolutely clear when specially when we do, the equations to understand diffraction.

Student: Sir, as they are all 2 planes 1 0 0 in 2 0 0 then how we will conform at the time of the plane this is the super set and this is the sub set.

See, 2 0 0 is the plane, this plane, this plane all of them are 2 0 0 plane, the 1 0 0 is the center, so 1 0 0 containing with the 2 0 0. Because, now if I have my 2 0 0 set I just drop this I get the 1 0 0, so this is the superset; obviously, the this has more number of entities twice number of entities compare to the this.

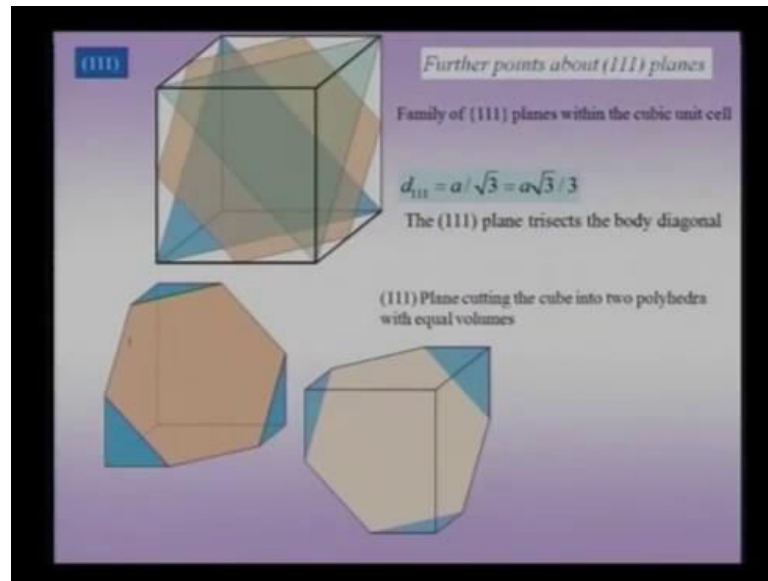
Student: Sir, this is the things are there is a lot of place are there, so if we taken one hits why do so this why do sets are the super sets of there one.

Initial we of course, there present this planes only within the unity cell, but we have to always remember they are pervading entire space, they are translations equivalent set or set of planes which this for status this also bring us to an another point perhaps not often discuss is that, that I have 3 indices in 3 directions. As you know from the cosine law that actually there is the question connecting the three indices.

That means, the two independent data that what is suffixed in three dimensions; that means, that when you use 3 indices rotation as you are doing miller indices. There is some extra information that this third index is giving us, what is the extra information, this is the extra information that actually embedded within my h k l plane is also the inter planes spacing.

And that is why even I would supply varityping the in two index notation in three dimensions because, now I am equations connecting the 3 which means I have a production of number parameter, which should be 2 sufficient. But, I still in insist of using 3 index notation v can three dimensions because, of the fact that I can actually calculate d h k l, which is embedded within the information on the planes.

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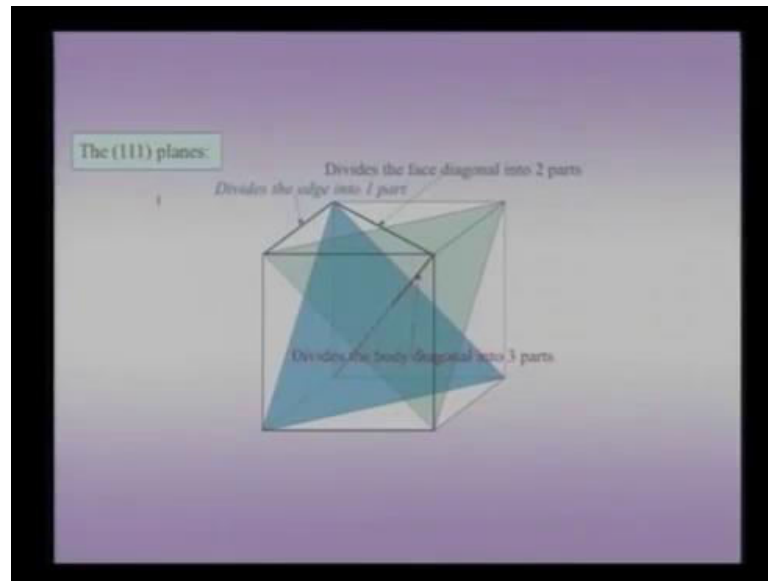


So, let us now consider as I told you the 1 1 1 plane and try to illustrate some more problems properties of this 1 1 1 plane in cubic crystal. Now, when I talk about the 1 1 1 plane for instance in some sense I say pointed out the blue plane, the orange pane and the green plane are all one, one planes. But, I have to take little care specially suppose I am calculating the atomic density on this plane, I have to take certain care in choosing the appropriate plane otherwise I make a wrong atomic density.

Suppose, I was talking about FCC crystal Cubic Close pack crystal, and atoms were actually present on the this planes. Then and of course, cubic crystal you know there will be FCC plane there will be atom here, and atom here, and atom here atom here on this blue plane and, so for. Because, now atom the face center of part from the vortices, this and carefully choosing plane for making the calculations, in some sense all the this 3 I have the same orientation this 3 planes.

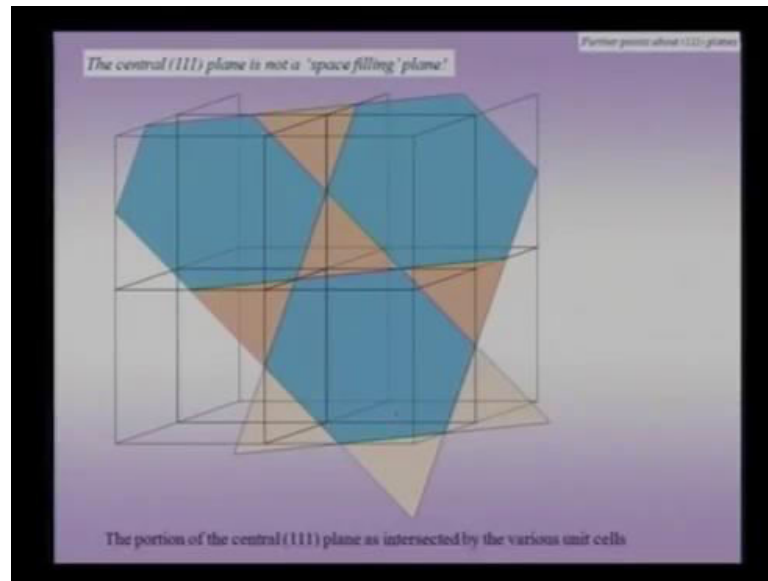
But, I have to little careful, so let me calculate the d 1 1 1 plane, so these are all 1 1 1 planes, the 1 1 is a by square t root of 1 square plus 1 square plus 1 square, which is d a by root 3, I can write this also as a root 3 by 3. Now, what is a root 3 a root 3 or a root a is the body diagonal of the cube, now what is a root by 3 is 1 3rd of the body diagonal the cube, in other words by 1 1 1 planes will trisect the body diagonal, so that mean with that one of the slide coming up, let me see.

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Here, so if have the body diagonal of the cube $1\ 1\ 1$ plane actually divides the d body diagonal into 3 parts, and this is important because, now that $1\ 1\ 1$ plane which will actually trisect the body diagonal will be the blue plane, and the green plane. So, that means, the orange plane truly not speaking belonging to the same set, it has got the same orientations, but I will not consider the rate when I am actually considering $1\ 1\ 1$ planes, it because, if I am talking atoms line on $1\ 1\ 1$ plane, I only consider upon the blue plane and the green planes to be equivalent and not the orange planes. And I have seen that the blue plane and green plane together will trisect the body diagonal as given by the $d\ 1\ 1\ 1$ information. Now, however, I may want to c consider the orange plane, because this actually speaking the middle plane of this cube.

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Along the 1 1 1 directions this mid plane as the cube actually breaks this poly, this cube into two half of the poly heats which are this plodder shape here and therefore, I can get two half and if I want to do that operation, then I will have to consider the orange plane. Now, talking about the atomic density, you want to make a calculation atomic density, have to be clear the kind of plane I have to choose has to be a space feeling planes. In other words, those planes themselves should assonate space, in other words contain of the units cells should if extended all the directions, should form the complete plane.

Suppose, I chose the central plane can clearly see central one plane was form of an hexagon, so I have choose different color, but do not get confuse this blue color was the original orange color in this plane. So, this is shape on hexagonal, but you can see that you can extended the cross units cells, the hexagon then cells do not feel the entire two dimensional plane 1 1 1 kind of a plane. That means, I have to add additional triangle to make the complete base fields, therefore I make atomic density calculation or a those calculations based on this kinds of blue 1 1 1 which is shown as hexagonal here, I will get my number wrong.

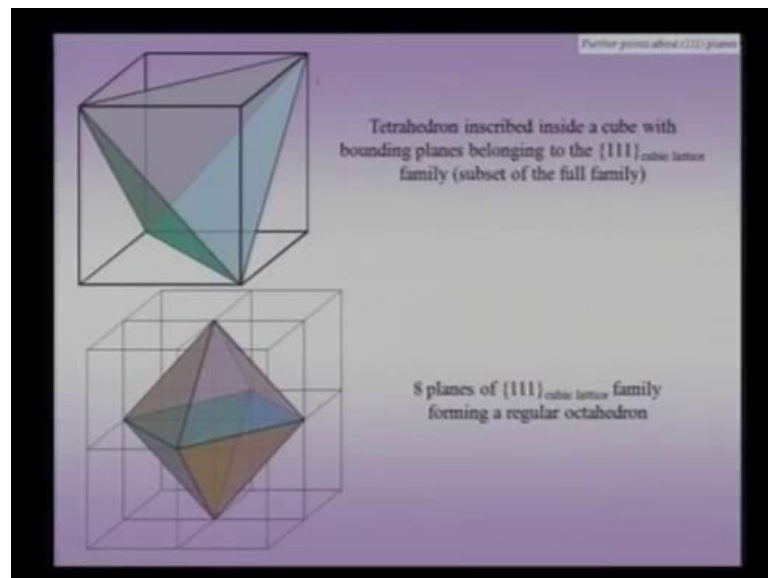
So, this point has to be kept in mind, that I have to also additional worry which plane unit cell have to choose, and clearly the correct choice for this cubic crystal system would be the blue plane or the green plane. And suppose, I am talking about addition of the poly hydra, then in to a mid plane, then this all orange pane is the mid plane which

actually by shapes my body types. I was mentioning about family of directions and I was also trying to related to a concept of origin like the $1\ 1\ 1$ planes in the octahedral planes, the $1\ 1\ 1$ planes is the octahedral planes for the cubic lattice; and as I mentioned it has got the highest symmetry and therefore, there are 8 members.

Now, therefore, I can think of these $1\ 1\ 1$ planes all the equivalent set of $1\ 1\ 1$ planes which will include planes like $1\ 1\ 1$, $1\ \bar{1}\ \bar{1}$, $1\ \bar{1}\ 1$, $1\ 1\ \bar{1}$, and so forth there are 8 members in the family. And those are the 8 members, which are shown in the diagram, in other words it is in the shape of the octahedron, so I can actually understand it by taking a cube and trying to put the octahedral planes. So, this octahedron should reside within the cube, so let me break the cube little bit to get the octahedron inside.

So, I will see that this plane, if exactly this octahedron at fitted within the cube then these will be octahedral planes. So, you can clearly see this so these are the $1\ 1\ 1$ planes, in this case of course I am just considering the orientation, I am not considering the exact position of the $1\ 1\ 1$ planes. But, I have to remember the whole family of these $1\ 1\ 1$ planes form an octahedral like this, and all these are triangular phases and therefore, they are octahedral planes.

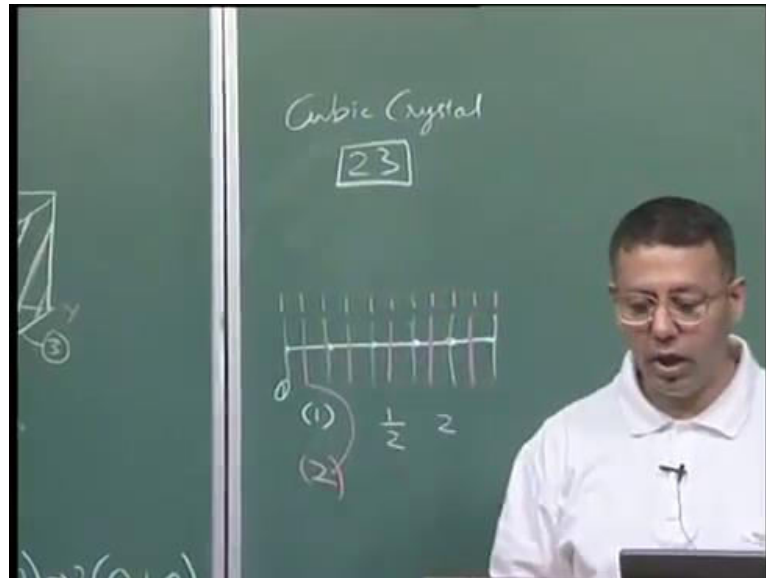
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If I have to truly represent this octahedral planes I will have to go outside the unit cells, and look at the way I have done it in this diagram, where in the 8 unit cells, each one of them having one of the members in the family is shown therefore, form a octahedral

plane. Now, as I mentioned the family of planes is symmetrically related set, it could happen the cubic crystal I am talking about actually has only 2 3 symmetry.

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That now suppose I am talking about the cubic crystals that is with 2 3 point group symmetry; that means, it is a lower symmetry than the and this is nothing, but the tetrahedral symmetry. Then in such a crystal there will be the 4 members in the family which will form a tetrahedron, and you can see the 4 members in that family inscribed within the tetrahedron. So, you can see here there are 4 members in this 1 1 1 family which go inside the cube, and they form a tetrahedron.

So, let me show this tetrahedron which is inscribed and of course, here it I am not inscribed it, but will show you the relative orientation in the cube. The way to construct the tetrahedron within the cube is to consider, one phase diagonal which is on the one direction, the other phase diagonal which is perpendicular to it. So, I can inscribe a tetrahedron within the cube of course, in this case I am not inscribing it I am just nearly positioning it. So, you can see that by doing that I can actually see where is the orientation of the planes with respect to the cube.

So, this is my tetrahedron and now clearly this crystal since as only tetrahedral symmetry it has got only 2 3 fold axis this 1 3 4 and this 2 3 fold second 3 fold and 3 fold and such a crystal clearly does not have any 4 fold axis. Therefore, it is important to understand that this 1 1 1 plane has very important roles in many kinds of crystals, even of lower

symmetry. And typically if you are talking about FCC crystals are body simple BCC crystals this will be 1 1 1 plane will be an octahedral plane we are having 8 members.

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Members of a family of planes in cubic crystal lattice

Index	Number of members in a cubic lattice	d_{hkl}	
{100}	6	$d_{100} = a$	
{110}	12	$d_{110} = a/\sqrt{2} = a\sqrt{2}/2$	The {110} plane bisects the face diagonal
{111}	8	$d_{111} = a/\sqrt{3} = a\sqrt{3}/3$	The {111} plane trisects the body diagonal
{210}	24		
{211}	24		
{221}	24		
{310}	24		
{311}	24		
{320}	24		
{321}	48		

So, let me write down list of various indices of the cubic lattice or a crystals for instance, and write down the number of members in the family. The 1 0 0 has 6 members which nothing but, forms a phase of the cube so simplest, the 1 1 0 has 12 members and we can see that the 1 1 0 plane actually bisects the phase diagonal. The 1 1 1 member has 8 members and the 1 1 1 planes actually trisects the body diagonals, you go to higher index plane like 2 1 0, 2 1 1, 3 1 1 or 3 2 1 you will see that the number of such members actually increases from 12 to 24, you can go 48 members this plane.

This has so many members, because now so 3 2 1 planes has 48 members in the family and that is the maximum any member in the cubic lattice can have. Because, now all 3 indices are different, you can permute all the 3 indices and that will lead to 3 factorial ways, you can make them negatives and therefore, you will end up with 48 distinct members in this family, the largest family. Sometimes, if you are looking at certain older texts or certain journal papers, you might have can come across some alternate notations for a of family of planes or directions. So, this is just a summary of them, but more often them all we will stick to the kind of notation, we are being using.

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Summary of notations

	Symbol		Alternate symbols		
Direction	[]	[uvw]		→	Particular direction
	< >	<uvw>	[]	→	Family of directions
Plane	()	(hkl)		→	Particular plane
	{ }	{hkl}	{ () }	→	Family of planes
Point	· ·	·xyz·	[]	→	Particular point
	::	::xyz::		→	Family of point

A family is also referred to as a symmetrical set

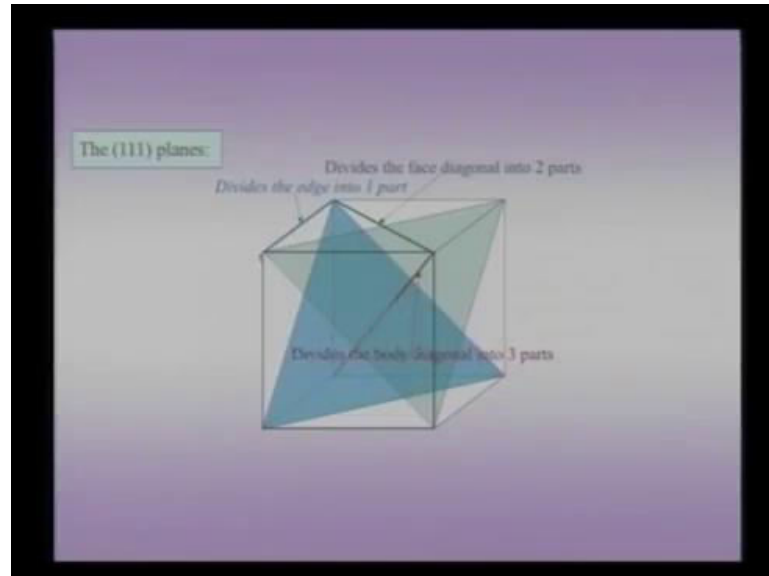
So, far direction this is single member, this is family, sometimes an alternative symbol for family, like this is also used; single member for a plane is like this and for a family is below that. Sometimes a double bracket is also used for a family of planes, additionally they may also use a concept for a point and for a family of points, like you could have point for x, y, z which is put within dots, and family of those points. Now, which will be a symmetry little set of points as between a symbol, which looks like a colon, so certain order these symbols may be useful in a specially reading journal papers.

Briefly we will go over this topic of a certain points about h k l planes, and this may not be at this point of time very interesting, but it is worth were to note this points. If you have a translational is a equivalent set of lattice plane, that will divide for distance the cell edge, the a edge due, it will along the 1 0 0 directions, we have h k l planes will divide it into h parts. Along the 0 1 0 directions which is the b direction, the h k l plane is divided into k parts, along the c plane it is divided into l parts.

Now, this is the cell edge divisions, suppose if you are talking about how the diagonal how the face diagonal which is divided along the h k l planes for instance, we will divide the 0 1 1 direction into k plus l parts, the l 1 1 0 into l plus h parts and 0 0 1 planes into h plus k parts. The body diagonal is divided into h plus k plus l parts, in other words for the 1 1 1 planes, suppose the body diagonal will divided into three parts, 1 plus 1 plus 1 3. So, let me take an example to show you what happens, suppose I am taking about the 1 1

1 plane, then my face diagonal is divided into 1 plus 1 2 parts; if I am talking about edge it is just divided into one part, so this whole thing remains one part.

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So, then the body diagonal is divided into h plus k plus l parts, so therefore, we can get some more useful information, in terms of the divisions of the edge the face diagonal and also the body diagonal from the $h k l$ index.

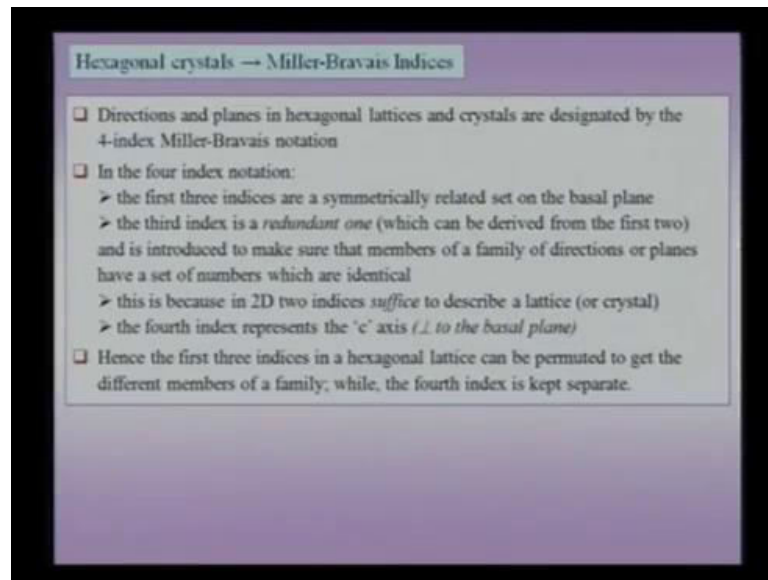
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Condition	(hkl) will pass through
h even	midpoint of a
$(k + l)$ even	face centre (001) midpoint of face diagonal (001)
$(h + k + l)$ even	body centre midpoint of body diagonal

Additionally will notice is that h is even, then their will it will pass through the midpoint of a , and if it is k plus l is even it will pass through, the h plus k will pass through the

face centre $0\ 0\ 1$. And $h + k + l$ is even it will pass through the body centre or the midpoint of the body diagonal. So, we have to note, there are additional information we can obtain from understanding these miller indices, though at this point of time I am briefly mentioning it, I am not going into the details of this analyses.

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Instead I will take up the next important topic, which is the concept of Miller-Bravais indices, which is especially used for hexagonal lattices, and hexagonal crystals. Now, the Miller-Bravais indices is on the same kind of the footing as the miller indices, but has an additional index which has been put in to describe these hexagonal lattice and crystals. So, it is four index notation, the important point to note in this four index notations is that, the first three indices are symmetric related set of all the basal plane.

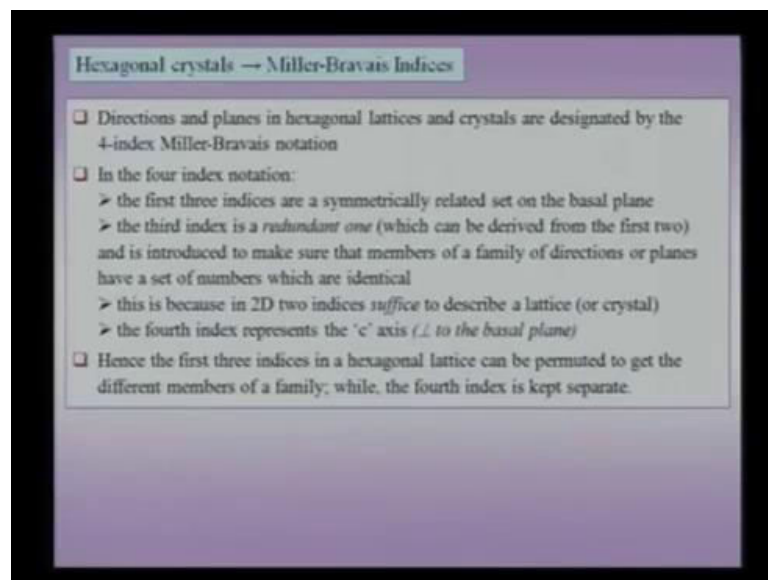
So, we will see what is the basal plane and we will see that the first three indices which are related to a 1, a 2 and a 3 direction all lie on this basal plane. And they are symmetric related by the 120 degree rotation, which is symmetry operation for all hexagonal lattices, the third index is the redundant role. And why is that redundant because, we know that in two dimensions which is now the plane I am talking about, the basal plane of the hexagonal lattice for instance, so let us pick up the hexagonal lattice.

So, my hexagonal lattice is blue color here, so I am talking about this plane which I call the basal plane, additionally later on we will see that will also define other kind of planes. So, this is my basal plane either the top plane or the bottom plane, I call them the

basal plane, I will call them these planes as prism planes and planes which are inclined are pyramidal planes, the planes which are inclined like this, they are called pyramidal planes. Now, even I am talking about the basal planes I am going to define three vectors, so these three vectors 1, 2, 3 vectors all lying on this plane.

And what I am trying to tell here is that, one of these indices is transient, because we know in two dimensions we need just two indices to describe lattice or a crystal, and the third index obviously, has to be redundant. What is the reason that we include such a redundant index, it this is introduced to make sure that the members of the families of the directions of planes have a set of numbers which are identical.

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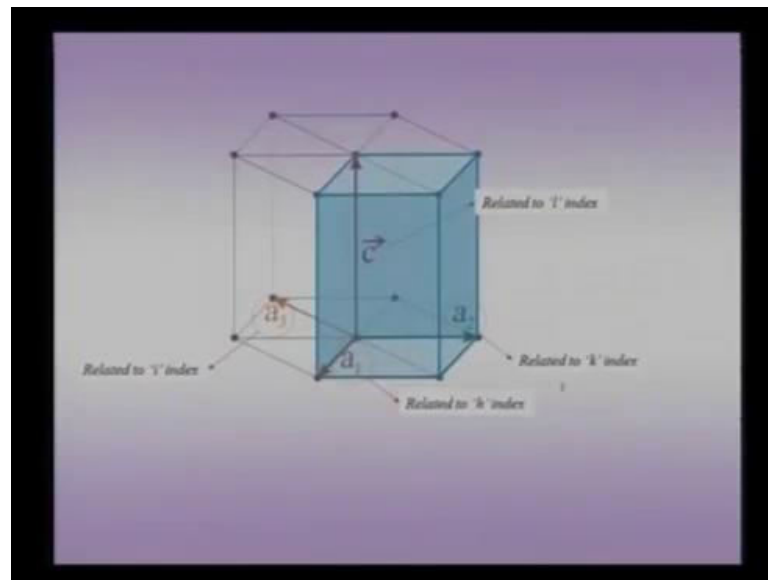


I will explain this concept by taking examples, but what I am trying to say here, in other words I should be able to permute the three indices, and get all the symmetrically related set of directions or planes. Like we did for the cubic lattice for instance, if I have for instance 1 1 0 planes, then I can actually, because these now for a cubic lattice the first index, second index and third index are all in equivalent, I can actually permute them.

So, as I get by merely looking at 1 1 0 plane and I have 1 0 1 plane, I know they are identical kinds of planes as far the lattice course. I should be able to do a similar kind of thing and I can only do that, if I have this redundant index. The fourth index is along the c axis, suppose this is my hexagonal, fourth index is the c index is alone, so this is that direction which is vertical in this. So, whenever I am dealing with hexagonal lattices or

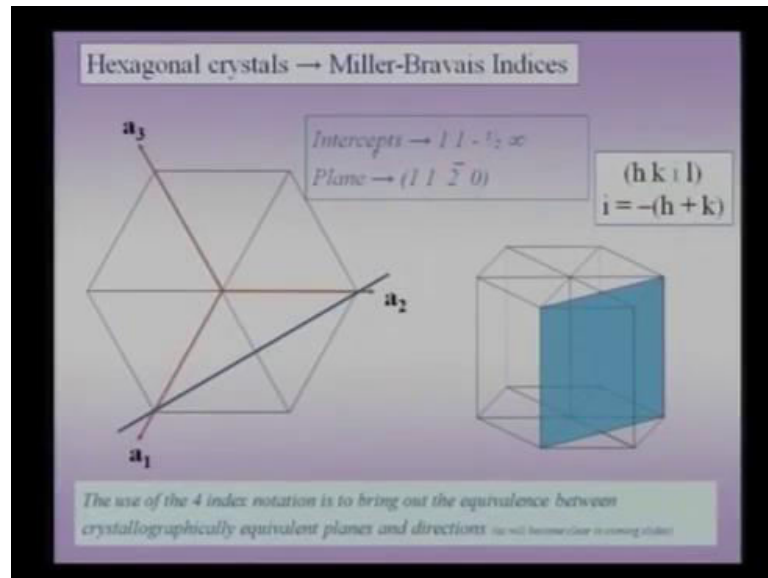
crystals, I can permute the first three indices to get the distinct members of the family; and the fourth index is kept separate, ((Refer Time: 43:25)) fourth index is separate crystallographically as compared to the first three indices, in the Miller-Braveries notation.

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So, I have the a one direction, the two direction, and the three direction all lying on within the basal plane, they are related by the 120 degree rotation, the 6-fold rotation which hexagonal lattice have. And therefore, they can be permuted this, so the h index is relate to the a 1 direction, the k index related to the a 2 direction and the l index related to the a 3 direction, and the a 1 index which is the separate one index is related to the c direction, which is perpendicular to the basal plane.

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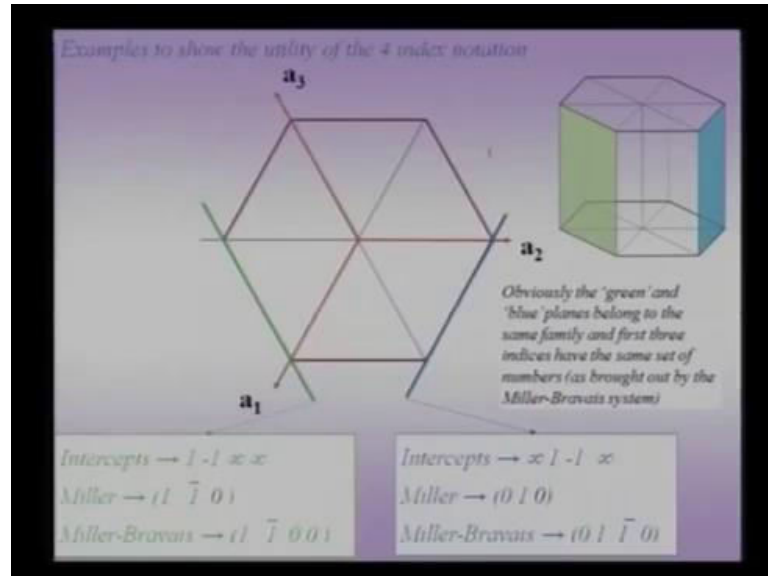
So, let us now try to generate some planes and try to derive their some Miller-Bravais indices, and this examples will also make it absolutely clear, that why we need a four index notation, and what is the concept of redundancy. So, for instance, this is my plane in projection the blue plane and in proper orientation, you can see this blue kind of plane, so let me show this in figure also. So, this is my hexagonal kind of unit cell, so I am considering a plane which is now passing through this orientation to make it clear, this is my plane.

So, it is actually is like the diagonal of the basal unit cell, the present rhombus unit cell which is of course extended upward, now I will try to derive the miller indices, so I start miller bravais indices, so I start with intercepts. So, intercepts along the a 1 direction is 1, intercepts along the a 2 direction is 1, now I have an additional redundant index a 3 and my intercept along the a 3 direction. So, the a 3 direction is in this direction, so it is along minus a 3, so it is half the distance at this point is minus half.

So, it is 1 1 minus half and along the c direction it is infinity never intercepts the c direction, as before to get my Miller-Bravais indices, I will take reciprocals of these ((Refer Time: 45:42)). And these are now 1 1 2 bar 0 and first of course, I will write it as 1 1 minus 2 0 then, as we know in miller indices and Miller-Bravais indices as in this case, I would not leave the negative outside, but I have to put it as the bar. So, the indices

for this plane would be $1\ 1\ \bar{2}\ 0$, now I will take one more example, before we understand the concept of this fourth index.

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Now, suppose I have two planes, the blue plane and the green plane as shown in this cube, it is absolutely clear as far as the hexagonal lattice course, they are equivalent planes, they are related by the symmetry operations of the hexagonal lattice. Therefore, if I look at the indices of these planes, they should look identical to me, so that I am not confused that I am not talking about different kinds of planes. So, now, what are the indices of this blue plane, and what are the indices of this green plane, let me start up with green plane intercept along the a_1 direction is 1, the a_2 direction is minus 1.

Because, a_2 direction is in this direction it is minus 1, the intersects along the a_3 direction is infinity, it never intersects this green plane never intersects as it is infinity. Obviously, the intercepts along the c direction is as you can look on the screen plane, along the c direction also it never intercepts the c direction, therefore it is infinity, to make the Miller-Bravais indices I make the reciprocal. So, I will write it as $1\ 1\ \bar{2}\ 0$ both the infinity it becomes 0 and therefore, they are as before I could have put this out screen plane passing through the origin, that means I could have drawn the green plane like this plane here.

So, it has a fair bit of plane passing through the origin, and I do not do that for the same reason as I mentioned for the normal miller indices, that I will end up with infinities with

reciprocals. So, I will always translate it, so that it is one unit away from the origin, so I have $1\ 1\ \bar{0}\ 0$. Suppose, I were not using four index notation, I were using just three index notation that means, I do not have this third index, which is the redundant, I do not have this third index then, I will write it as $1\ 1\ \bar{0}$.

Now, let me look at the blue plane and try to derive its miller bravais indices, it intersects along a 1 direction is infinity, it never intersects a 1 direction, it is parallel to the a one direction. It intersects a 2 direction at a distance $1/2$, it intersects the a 3 direction at a distance $1/3$, so this is a 3 is positive a 3, this is negative a 3 at $1/3$ intersects, so this is my point along intersection along the a 3. So, I have infinity $1/2$ minus $1/3$ infinity, as usual at c direction, it never intersects.

My miller indices or the miller Bravais indices would be $0\ 1\ \bar{1}\ 0$, I take my reciprocals at this becomes $0\ 1\ \bar{1}\ 0$, this becomes $1\ 1\ \bar{1}\ 0$, which I write as $1\ \bar{1}\ 0\ 0$ and this is $0\ 1\ \bar{1}\ 0$. So, my miller indices is $0\ 1\ \bar{1}\ 0$, but suppose I were using just three index notation the miller indices that means, I do not have my third index here, this would be $0\ 1\ 0$. Clearly the green plane and the blue plane, as far as the lattice goes are identical, in other words, I can use the six fold rotations, which will take me blue plane to this plane, which I have not shaded here and then, I will take it to this green plane.

So, let me show these planes in a model, so one of my plane was this plane, the other plane was the plane like this. So, this was my green plane, this was my blue plane, so this plane is rotated by the six fold to this plane, which is rotated by six fold to this plane. So, all these planes are identical as far as the lattice goes now and therefore, my miller indices should reflect that symmetry. But, looking at the miller indices in three index notation, the first plane would be called $1\ 1\ \bar{0}$, second the blue plane would be $0\ 1\ 0$.

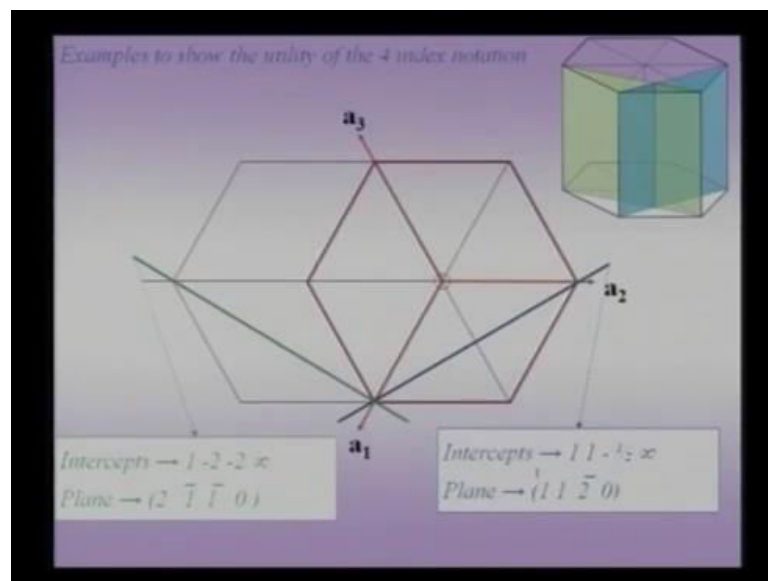
Clearly, even though they are equivalent, the miller indices seen non equivalent, to avoid these kind of ambiguity and therefore, now my question is that, how do I generate my family, given the high symmetry for the hexagonal lattice which is... Therefore, to avoid that ambiguity, I will write a four index notations and in the four index notation, it is $1\ 1\ \bar{1}\ 0$ and this is $2\ 1\ \bar{1}\ 0$. Keeping the l index separate, I can clearly see, there is $1\ 2$ there is 1 and $1\ \bar{1}$ and the 0 and there is a 1 and a $1\ \bar{1}$ and a 0 in both indices.

So, using a four index miller Bravais notation, where in the first three indices are referring to the basal plane, which is the plane shown here. I will actually see that, I will

bring out equivalents between equivalent planes, so this is why the additional index is there. And now, then I can go ahead and permute and generate all the equivalent set of planes. For instance, now I want to generate the equivalent set, ((Refer Time: 50:35)) this plane or this plane or one of these planes, for instance there will be $1\ 0\ 1\ \bar{0}$ or $0\ 1\ \bar{1}\ 0$.

So there all, by just permuting the first three indices, I can get all the equivalent planes, that is why we have the utility of the miller Bravais indices, where in we include the i th index. Now, we said that, the i th index is related to the remaining two index, that is why it is redundant. I can derive my i th index as minus h plus k , so in this case for instance, it is minus 1 plus 1, which is 2 bar. In this case, my i th index, third index is minus of 1 plus minus 1, which is 0, therefore this is 0.

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Therefore, I derive the third index from the first two indices.

Student: ((Refer Time: 51:31))

Which one?

Student: ((Refer Time: 51:35))

Which one, which plane?

Student: ((Refer Time: 51:46))

This one?

Student: Here, you taken zero one 1 bar zero and just before it, you ignored 1 bar and you taken 0 1.

So, this is the three index notation, which is called miller indices notation, wherein I do not have my a 3. So, I only talk about a 1 and a 2, which should have been sufficient, because in the miller indices, we have only three indices notations and for three dimensions, three index notation is more than sufficient. We just introduce an additional redundant index to make things very clear, so it is always, even if you write it here, the third index always exist, which is nothing but, minus of 0 plus 1, which is to 1 bar, which I write as 1 bar.

So, to make it absolutely clear, I index additional index I, which is the redundant index, good question, but this is why the whole purpose of introducing a redundant index. Now, let me consider one more plane and you can see that, again we are considering green plane and the blue plane, which are identical to illustrate the concept of miller Bravais indices for the green plane. So, the intercepts are 1, in this direction a 2 direction is minus 2 and in the a 3 direction, again it is I am not showing the intercept, it will go and intersect at minus 2.

The intercepts are 1 minus 2 minus 2 infinity, at the c direction it will never intersects, the intercepts for the blue plane are one along the a 1 direction, one along the a 2 direction and minus half as before along the a 3 direction at infinity. So, I can derive the miller indices from the intercepts as reciprocals 2 1 bar 1, so actually it will become 1 half bar half bar 0 and I will multiply throughout by 2 and I will take the half factor outside, it will become 2 1 bar 1 bar 0.

For this plane, the reciprocal of this will become 1 1 2 bar 0 and that is what it is 1 1 2 bar 0. And since these are equivalent planes, as obvious from the figure on the right hand corner, you can see the equivalents straight away by looking at the miller Bravais indices. So, this is got 1 1 2 and 2 1 in first three indices and the 0 of course for the last and here it is got again 1 2 bar and 1 1. As far as the negative goes, in other words suppose, I want actually see the equivalents, I may have to multiply this by minus 1.

And that can be done, because now we are not distinguishing planes on other side of the origin. Suppose, a plane had $h k l$, in other words I would looking at the specific plane $h k l$ and now I am not worrying about the whole set of those planes $h k l$, the $h k l$ sides will lie on the positive side of the origin, while the $\bar{h} \bar{k} \bar{l}$ plane would lie on the other side of the origin. But, if I am talking about the set then, I did not distinguish these two planes.

So, let me also consider some examples of pyramidal planes, for instance this pyramidal planes, in other words wherein the c index is, what you might call finite and the c intercepts is not infinity. So, let me take this blue example, so the intercepts of this plane along the a_1 direction is 1, along the a_2 direction is 1 along the c direction, this is again one actually, a a_3 direction is the one direction, which I am talking about the third direction is minus half.

In other words, this is my intercepts here, it is the direction is minus half and along the c direction it is 1, so let me switch to my highlighter now, so my intercepts are 1 1 along a_1 and a_2 , one along the c direction. And the redundant index intercepts is here, which is minus half, so I can write down the miller indices of this plane as $1\ 1\ 2\ \bar{1}$. So, let me consider this plane which is shown here, and so in the right hand diagram and the left hand diagram it is exactly the same plane.

Only thing I have done the different is that, I have only marked the part of the plane, which is the slice in the units cell and here, I have marked the part of the unit, which lies between the complete hexagonal representation, which we normally choose to reflect the hexagonal symmetry. So, the intercepts for this planes are along a_1 direction 1, along the a_2 direction it never intersects that means, it is infinity, along the a_3 direction is minus 1 which is along this direction and finally, along the c direction it is 1.

So, I take my reciprocal and put brackets to the miller bravais indices, which becomes $1\ 0\ 1\ \bar{1}$, so this is my miller bravais indices for the plane. And therefore, I can clearly see that I can use the four index notation in the case of hexagonal crystals, and hexagonal lattices to direct the Miller-Bravais indices.