Symmetry and Structure in the Solid State
Prof. T.N. Guru Row
Solid State and Structural Chemistry Unit
Indian Institute of Science, Bangalore

Lecture – 40
Conversion from Direct to reciprocal space, the inverse relations

We will now look into a few more aspects of reciprocal space and reciprocal lattice. So, effectively we look at more on Bragg's law and reciprocal space.

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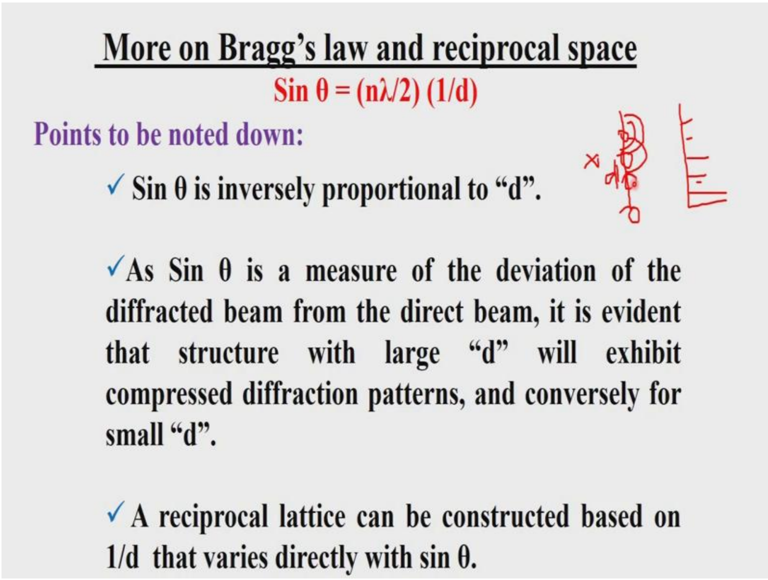

So, we have 2dsin θ = nλ, that can be written in a slightly different way by saying sin θ = (nλ/2)*(1/d). Now why did I write like that, we will know a little while later, because it is essentially to do, deal with how the appearance of the reciprocal lattice is, and how we can get to these various values of sin θ from the d values for a given λ.

So, that what we have done is, we have already discussed the reciprocal lattice. So, some of the points which we should note from the Bragg's law are the following. So, in order to keep this discussion going and also to keep you afresh, as we go further and further, is to remind you of the following points; one is sin θ is inversely proportional to d, so this is seen here. Sin θ is a measure of the deviation of the diffracted beam from the direct beam, it is evident that structure with large d will exhibit compressed diffraction patterns and conversely for small d. Let me take a little time to explain this. Suppose we have a structure with a very large d spacing, this is equivalent of having a multiple slit experiment which we discussed earlier on, we discussed of course, only a two slit experiment, and then we decided to this increase or decrease the distance between these two slits.

We can have any large number of slits, many slits, some 8 or 9 slits. So, I can show you a little diagram of my own which will be very lousy, but I will try to draw it. Suppose you have a source here which is a light source and then we keep a slit in front of it, keep a screen in front of it and then put holes through the screen; 1, 2 and 3 and so on. At equidistance, my diagram does not show equidistance, but you assume that they are all equidistant to each other. Then as we discussed earlier on each one of them now becomes a source, so you will get spherical waves coming out from each one of those like that. And whenever there is an intersection here we will get a bright spot on the screen, which we are going to put here.

So, we will get therefore, the bright and dark images corresponding to this, like that and we know that it is an inverse relationship. So, if the distance is d between these two. If that distance between these two points is d and that is repeated in all in the two dimensional plane, then we will get a large number of indications of bright and spoil dot lines here; that is the interference theory. So, what is said here is an issue where we can have different spacings of these slits or holes. So, each hole is a source, so instead of this we can have a diffraction grating which we have already discussed before, or we can have a crystal which is essentially a three dimensional grating; and therefore, depending upon the type of d spacing we have.

If we have a larger d spacing what does it mean? What does it mean if you have a larger d spacing, suppose 1 0 0 is a very large value then $1/d_{hkl}$ will be a very small value. If the value of a dimension is very large, suppose it is 20 Å then the corresponding 1 0 0 plane will be at 1/20. So, as the unit cell expands, the expansion of the unit cell can go commensurate with the number of atoms which are put inside the unit cell. So, we can put let us say a protein molecule, the cell dimensions could be 100, 200, 300 or whatever. And they also go to their respective crystal systems depending on the symmetry with which they crystallize. On the other hand if you have a just an atom, the unit cell dimensions will be fairly small. So, for a smaller value, the 1/d value will be very very large and for a larger d value the 1/d value will be very very small.

So; that means, for larger unit cells the number of points which you get will be a large number compared to smaller unit cells, you will get a smaller number. So, that is what is meant by this statement. So, the statement looks very profound, but essentially what it means is that, we get a large number of reflections from a larger unit cell, and reasonable number of reflections from a reasonable unit cell and less number of reflections from a smaller unit cell. Obviously, this is not going to hurt our approach, because our approach would be to see as many information, as many scattering directions possible we will identify; that means, as many d values we can accumulate, the better is the result.

So, the idea of looking into reciprocal lattice further now will tell us how we can get this information and how useful that information can be. So, we therefore, talk about the construction of a reciprocal lattice. So, it is based on 1/d. So, we are talking about the d spacing here; that is the spacing on the on the screen here, 1/d is the spacing which corresponds to the reciprocal lattice. So, when we get the reciprocal lattice image, the reciprocal lattice image is we know that it is proportional to 1/d; that is why the equation here is written in terms of 1/d right.

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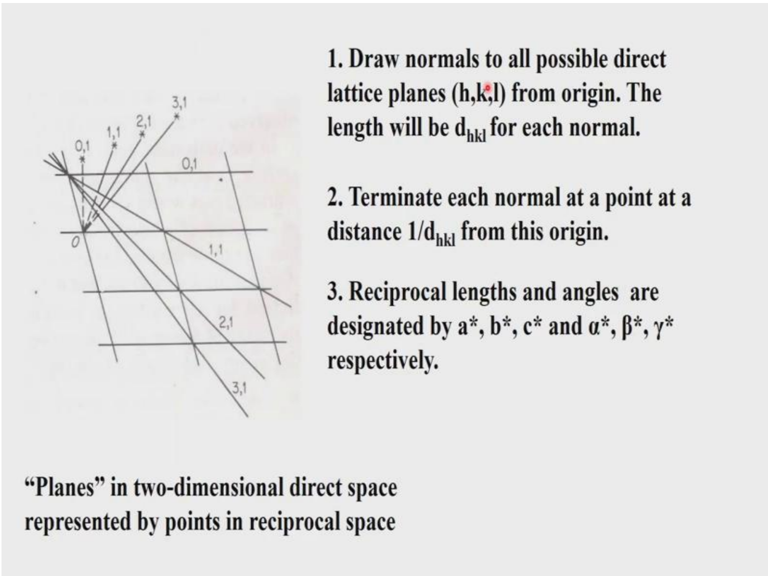

So, let us see a little detail of how these issues come up, let us take a unit cell. So, let us take a unit cell here, this is let us say represents the unit cell, this is the origin of the unit cell. So, from the origin of the unit cell if we now look at the planes which appear; so, suppose you take this as 0. So, 1 unit along this direction you have this plane, and 1 unit.

So, if you consider now the plane which is 1 unit away at 0 then we call this plane as 0 1. We are looking into two dimensions, so this plane will be 0 1, the index of this plane will be 0 1. So, we are looking at the diagram in the with respect to this background.

So, we start from 0, this is the direct space we go up to that point which is 1 unit and then 1 unit along this will represent the 0 1 direction. So, if you now consider 1 unit along this and 1 unit along the second direction then you will get a 1 1 plane, that 1 1 plane is represented in this fashion. So, 1 1 plane is now going through this point. So, the similarly 2 1 plane is now half way along this. Remember the bread analogy, this is half way along this and 1 unit down this, so it will be 2 and 1. So, if you consider this plane this is 3 and 1 ok. So, we now, therefore, have represented 0 1, 1 1, 2 1, 3 1, the 4 planes with respect to the direct lattice.

So, we have a direct lattice with as a have indicated the lattice diagram in the background, we have drawn the lattice net. And using the lattice net we have identified 4 positions 0 1, 1 1, 2 1, 3 1. These are the planes passing through the with respect to the origin of the main cell. Now, the next step that is required, is that. So, what we have done is, next step is to draw normal's to all possible direct planes from the origin.

So, we have drawn now 4 direct planes 0 1, 1 1, 2 1 and 3 1, and we are now going to draw the all possible normal's to these draw normal's. What do we mean by normal, it should come at 90^{o} to the diagram which we have drawn. So, you get a 0 1* a 1 1* a 2 1* and a 3 1*, so these are now perpendicular. So, you draw the perpendicular to 0 1, perpendicular to 1 1, perpendicular to 2 1, and perpendicular 3 1.

So, these are now the star the stars are now the points which are normal, which are drawn with respect to the various d_{hkl}. Now where do we stop it? We have to have a stopping point and the stopping point will be $1/d_{hkl}$. So, the length of each of these now we stopped at $1/d_{hkl}$. So, we know the value of the d_{hkl} now. And so at $1/d_{hkl}$ from this origin this is now the origin of the reciprocal lattice. So, the origin of the reciprocal lattice is here, so we now draw these lines. Normal to the various planes which we have shown intersecting at that point; so, this therefore, will give us the collection of all the reciprocal lattice points which are indicated by star mark.

So, reciprocal lengths and angles are designated by a^* b^* c^* α^* β^* γ^* respectively, similar to the star marks on these values, so these are the $1/d_{hkl}$ values. So, what we have to see also here is that whenever we consider planes in the two dimensional direct space, the plane 0 1, the plane 1 1, the plane 2 1 and is a two dimensional case. The normal's now are ending up with a point and therefore, they are represented by points in the reciprocal space.

So, when you get a diffraction pattern, we have already discussed that in the previous our that way with a diagram. Here again this diagram is making it more clear that from a diffraction from a plane, is essentially like reflection, and so when X rays fall on a plane, any point on that plane on which it falls will scatter at the same phase and as a result the scattering direction is determined and that scattering direction now is fixed at $1/d_{h\ k\ l}$ which now forms a point and that is the reciprocal lattice point.

So, if you take therefore, a collection of all these reciprocal lattice point. In principle it also represents a three dimensional lattice and therefore, we call it as, not just the points in the reciprocal space, we call it as a reciprocal lattice. So, given the direct lattice and the planes associated with the lattice, since the planes are associated with the direct space lattice. The points which are now normal's to those planes which are now the collection and the representation of the reciprocal space, in reciprocal space, they define the reciprocal lattice.

So, therefore, the reciprocal lattice, reciprocal points also form a three dimensional lattice. So, this is very important, they do not form a two dimensional lattice, they form a three dimensional lattice, because this direct space, these normal's now are with respect to the planes. So, the planes are all in various orientations with respect to a b c. And therefore, we have the reciprocal lattice characterized by a^* b^* c^* and α^* β^* γ^* or the interaxial angles.

So, how does that develop? In what context we can see they are developing into these three dimensional lattices in various crystal systems. So, we will examine that a little carefully and closely, because that is something which will clearly tell us how this concept of reciprocal lattice has developed. It is not just that you know if you have a = 100 Å, $1/a$ how is it getting represented, will it become 0.01 something. In fact, this question has been asked when we have taught several times by students. So, we thought we will make it clear in the context of how this is really coming up, and these two pictures will tell you clearly how these develops.

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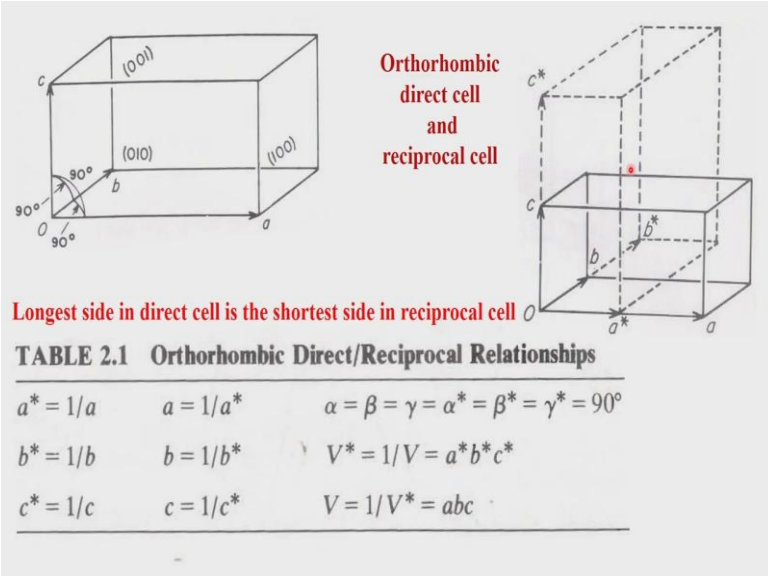

The first picture tells us that we have a unit cell and this particular unit cell is described with respect to the origin here. This is an orthorhombic direct space lattice. So, we have therefore, Oa is the distance along the *x* direction, Ob is along the *y* direction and Oc is along the *z* direction. So, by definition the plane up here is 1 0 0. So; obviously, by the plane if you consider a planar half point, it will be half that is 0.5 0 0 the position and this plane will be identified as 2 0 0; that is the Miller index revision.

So, we can therefore, have this as the unit cell. So, this represents now $a\ b\ c\ \alpha\ \beta\ \gamma$. $\alpha\ \beta\ \gamma$ in this example is 90 90 90. So, how does the reciprocal cell come up? Reciprocals cell in this particular case comes up by this definition. The table d below shows, the relationship between the direct space in the reciprocal space associated with a orthorhombic unit cell.

So, the unit cell dimensions are $a\ b$ *and* c, the corresponding dimensions will be $a^*\ b^*$ *and* c^*. So, the point to note here is that the longest side in the direct cell; that is a here in this example, will be the shortest in the reciprocal lattice. So, we take the same origin, the origin is the same for the direct space lattice as well as the reciprocal lattice, and we now show the picture of the reciprocal lattice; that is we have already discussed and found out it is also a three dimensional lattice. And so if there is a behaviour of atoms and molecules in such a way, that they are restricted to the orthorhombic symmetry. The symmetry that is reflected in the direct space must also be reflected in the reciprocal space.

So, we therefore, indicate this unit cell if this is a^*, the short one becomes longer it is b^* and this third one is c^*. So, this will be now the unit cell of our reciprocal lattice. The fact that α β γ are 90^o, will ensure that these values are equal to 90^o. What is also important to note is that they are interconvertible; that means, if you have a^* b^* c^* as $1/a$ $1/b$ $1/c$, the corresponding a b c will be $1/a^*$ $1/b^*$ *and* $1/c^*$. So, what happens to the volume of the unit cell. The volume of the unit cell is a . (b * c), and therefore, we can now calculate the volume of the reciprocal lattice which is 1/V and that is a^* b^* c^*.

So, the volume also is invertly inversely related to each other and that is how this relationship develops; a very straightforward case in case of the orthorhombic symmetry. Any symmetry higher than orthorhombic symmetry, particularly if it is cubic can also have this kind of a situation or tetragonal will be a similar situation, because the angles α β γ are 90^o with respect to each other. So, crystals belonging to orthorhombic tetragonal and cubic will have this feature; a^* is equal to $1/a$, b^* equals $1/b$, c^* equals $1/c$ and so on.

Remember in the case of tetragonal and cubic in particularly in case of tetragonal $a = b$. So, your a^* and b^* will be 1 and the same from the distance point of view, but they are oriented at 90^o with respect to each other. Same thing they extended to cubic system $a = b = c$ and therefore, you will have $1/a$ $1/a$ $1/a$ as the reciprocal lattice values for the reciprocal lattice in the cubic cell.

So, otherwise these crystal systems will have this kind of a behaviour. So, this is the direct space lattice and that is the reciprocal space lattice and the relationship between them is shown here.

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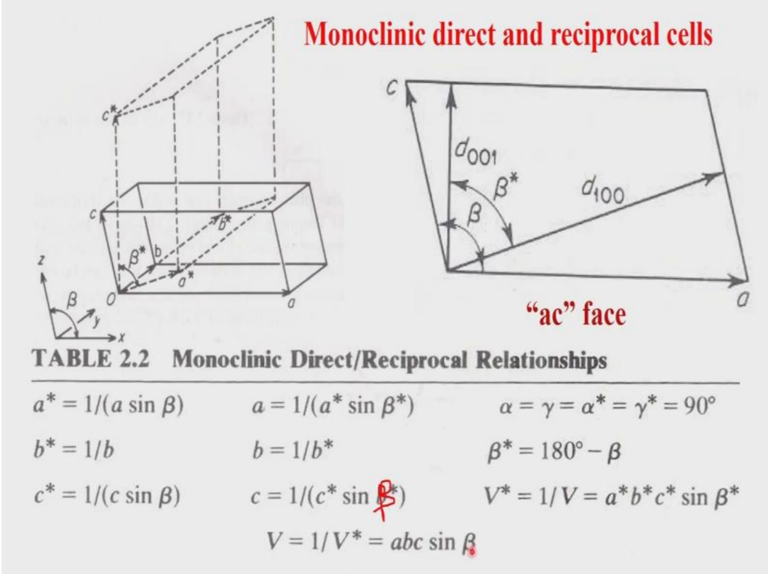

Now, we go to the discussion on the next crystal system which is a monoclinic system. So, in the monoclinic system we have a little bit of a deviation, the deviation comes because of the fact that $\beta \neq 90^\circ$, considering *b* axis as the unique axis. So, when once we consider *b* axis of the unique axis, the angle between *a* and *c* will be β. So, β is the angle between *a* and *c* which is indicated in this diagram. So, we have the *x*, *y*, *z* directions indicated here, the *x* direction is taken up by *a*, the *y* direction is taken up by *b* and the *z* direction is taken up by *c*.

So, this volume of the unit cell will therefore, be ***a* . (*b* * *c*)**, there is no change in that. Remember I am using the vector notation, so when I say volume of the unit cell is ***a* . (*b* * *c*)**, you should remember that there is a certain relationship between the involvement of β as well in this calculation. So, let us look at what happens to the reciprocal lattice in this situation. The reciprocal lattice will be now differently oriented than the case of an orthorhombic system, it is not going to be coincidental with the directions of *a b* and *c*, because now what happens is, a^* now will become the reciprocal lattice will now be *1/a* sin β; that is because we have to now consider the normal to the plane. You remember the previous picture where you saw four normal's being drawn to four different planes.

So, we have to consider the normal to the plane and therefore, if we consider the normal to the plane, this is the plane which is now represented, this is *ac* projection and therefore, if you consider this is the plane, this will be now the plane corresponding to, the plane corresponding to the *c* axis. And therefore, if we now consider the d value associated with it, the $d_{0 0 1}$ is perpendicular to this direction. So, therefore, this angle is β and we get the $d_{0 0 1}$ which is the normal to the plane, not associated with the *c* axis.

The normal to the plane is 90° with respect to the plane, and therefore, we come get this issue that we have now 0 0 1 in this direction, 1 0 0 is in this direction, because this is the 1 0 0 plane. If you consider here this is the 1 0 0 plane. So, what you have done is you have taken the origin and drawn a line like that and that is1 0 0. And similarly along the *b* axis you have taken and drawn a line like that; that is $d_{0 0 1}$.

So, these two now well be making an angle and because of the fact that we have a β angle between *a* and *c*, the angle between $d_{1 0 0}$ and $d_{0 0 1}$will also follow β, but now that will be β*; that is because it is going to be 180° - β. The reason is obvious, the reason, it would have been ideally β equals β if it were 90°. Since we now deviate from 90° this diagram is showing an obtuse angle greater than 90°, the β* will now be an acute angle.

So, that is because it is greater than 90°, 180 - 90 greater than 90° will be shorter than 90°. So, we therefore, get the β*. So, the conversion from *a** to *a* to *a** will be *a** equals 1/*a.* Now since this is involving β we bring in the issue of sin β. How does that come about? this is drawn at 90°, so this angle will come into picture, the β angle and you see that these two are at 90° and these two are at angle β, and therefore, you get *a* * sin β, because the 90° angle is here and this is the value which we have to calculate, this is the angle β.

And therefore, we get 1/(*a* sin β), *b** will be remaining the same, because this is the direction of the twofold axis; that means, that both α and γ are 90° with respect to each other. So, it will remain as such like in the case of an orthorhombic system. So, *b* does not change *b** will be 1/*b.* Whereas, *c** will follow the same diagram as we have here. So, we get *c** is equal to 1/(*c* sin β). So, this now is the representation of the reciprocal lattice associated with monoclinic systems. So, if this is the case then what happens to the relationship between these two. The reciprocal relationship will still remain and in fact, this should be β* is little error here, maybe I will correct it right away.

So, this will be β*, same as this. So, a is equal to now 1/(*a** sin β*), 1/*b** and 1/(*c** *sin* β*). So, you see that the volume of the reciprocal lattice is now somewhat shrunk with respect to the volume of the unit cell, because unit cell volume is *abc* sin β. it is it depends upon therefore, this diagram. In this diagram you will see that the volume of the monoclinic cell with a β value greater than 90^{o} will have a certain volume, and that volume will be different from the volume of the reciprocal lattice. I just want you to think about it and tell me which of these two volumes are bigger in terms of the value values you have, because V* will be $a^* b^* c^* \sin \beta^*$.

Maybe you can take it as a numerical example, let us say $a = 10$, b is equal to maybe $b = 5$ and $c = 12$. So, take a unit cell $a = 5$, $b =10$ or $a = 10$, $b = 5$ and $c = 12$, and the β angle you take it as 95^{o} or 98^{o}. So, let me give you the values $a = 10$, the unit cell dimension a is 10, unit cell dimension b is 5 and unit cell dimension c is 12 ok. And β angle you take it as 98^{o} calculate the volume. Now I want you to check whether the reciprocal lattice volume is smaller or larger ok.

So, you calculate for calculate the a^* value b^* value c^* value and find out what is the value of V* and see whether you can get to the value of V*. So, what is important is to remember that β^* is of course, 180 - β, so that will help you in this calculation. The reason why I want you to do it yourself at home is just to get an hang of how these relationships come up between the direct space and the reciprocal space. And how the unit cells now changeover in case when we have the angles other than 90^{o}; I am not going to discuss the next crystal system in full detail, because; obviously, you see with one angle being away from 90^{o} it gets a little complicated, the case of triclinic is extremely complicated.

So, I will show you the diagrams which luckily for me is taken from the book of Stout and Jensen which is a nice picture. In fact, all these pictures are from that book, but the $a^* b^* c^*$ values and $\alpha^* \beta^* \gamma^*$ values associated with the triclinic system, we will just take it for granted and that is in the next slide.

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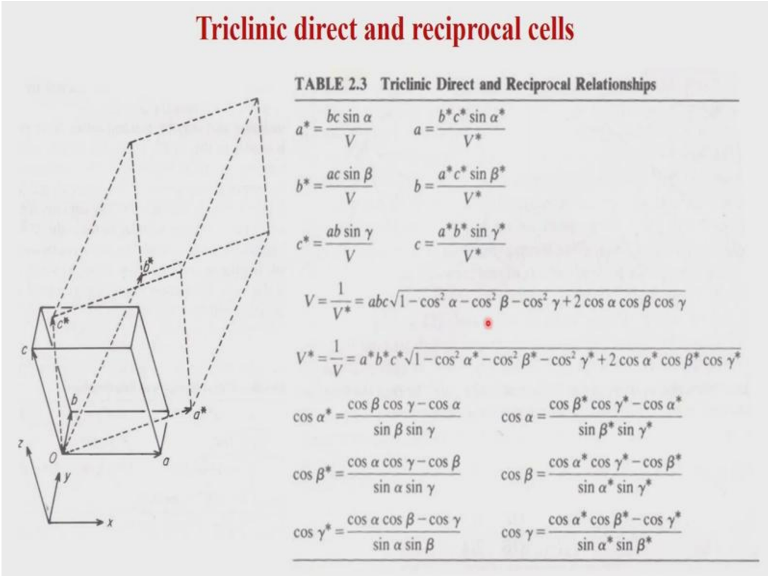

The next slide therefore, shows you the triclinic direct and reciprocal cells, you see the complications. I did not want to show you and then say it is complicated, you already anticipated the complication. So, we therefore, have in this case *a* b* c** values getting values of this kind, where you see that the volume of the unit cell still controls it. I think this diagram is already sort of giving way to what problem I gave you by just looking at it, but I want you to work it out.

So, take the case of a triclinic cell which is, this is *a* this is *b* that is *c*, *α β γ* are all different from 90°. And you see now again what we have to do is to draw normals to planes. So, when we draw normals to planes these planes are not associated with any 90° angle and therefore, they are acute or obtuse depending on *α β γ* being acute or obtuse, you will have the reciprocal lattice appearing with something like this.

So, it is not that when you say reciprocal lattice. The idea is to, you know this nicely done by is the book Stout and Jensen. So, nicely done in the book Stout and Jensen and so because, the idea is to give you that there is a dimension for the reciprocal lattice. You may think if there is *a* = 100 Å , *b* = 200 Å, then the reciprocal lattice volume will be very very small, because its *1/a* 1/a* and *1/b*; that is the logic. The logic is shown here the volume of the unit cell will be very different the of the reciprocal lattice cell. And you can calculate the values of *a b c a* b* c** by using these expressions.

And these involves so much of trigonometry associated with it, the orientation angles come in and those go as products of cos α, cos β, cos γ and therefore, you will get these expressions. You will see the volume now which is simply again written as **a . (b * c)** in vector notation, will be equal to $a\ b\ c$ and square root of this quantity which involves the cosine square functions and also the cosine functions associated with $\alpha\ \beta\ \gamma$. So, basically the take home lesson here in the last few minutes which we have our discussions are, is that there we have different. So, I want you to also work out the case of hexagonal and hexagonal system ok, hexagonal and trigonal (Refer Time: 27:44), in both cases we have an angle 120^{o}.

So, it is effectively like monoclinic, so that is why I have not shown you, it is almost effectively like a monoclinic system, except that there are more conditions than in a monoclinic system. So, the angle being now $\gamma = 120^{o}$ are not β, the unique axis is along the c axis. So, the diagrams and the way in which you work out the direct space and the reciprocal space vectors and their corresponding volumes will be like very similar alike to (Refer Time: 28:16) what we do with a monoclinic system.

So, let me recapitulate what we have done today in this case. We started with the use of the Bragg's law and the reciprocal definition. We indicated that as we increase the distance between in the between the planes, we find that the distances between the reciprocal lattice points shrink and vice versa. And we also said that the one once we have the $1/d_{hkl}$ values we can directly generate the reciprocal lattice, and we showed with examples the generation of the reciprocal lattices with respective various planes, and then we said that in case of the orthorhombic system, the monoclinic system we calculated the direct space and the reciprocal space relationships, and also assumed the values associated with the triclinic system.

This is like the, all of it has been taken from the book of Stout and Jensen in this discussion and I am very grateful to the that book, because drawing these diagrams will be a very difficult task for me. The way I draw things you have already seen, it becomes a very difficult task for me. So, what do we do next?

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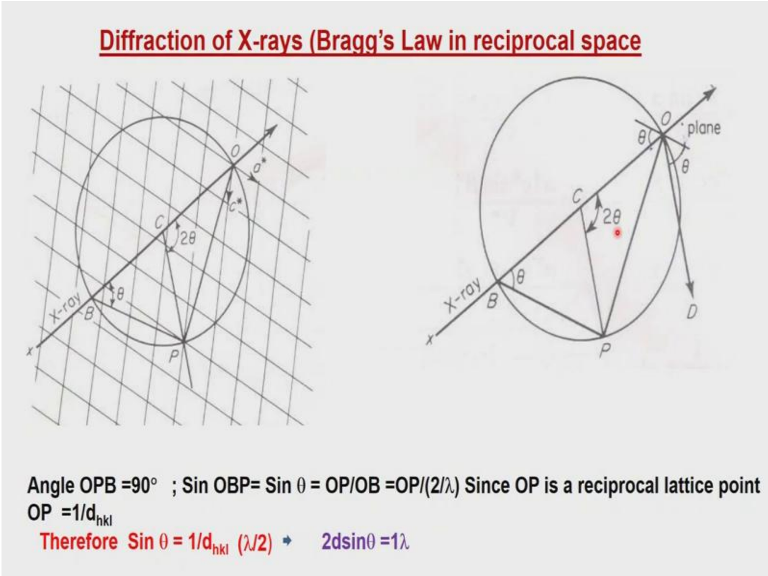

Next we will see what happens to Bragg's law in reciprocal space. This is something which we will take up in the next round.