Electron Diffraction and Imaging
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Lecture - 11
Tutorial - 02
Interplanar Distances and Angles

Welcome you all to this course an Electron Deflection and Imaging. In today's class we will discuss about how to find out distance between different planes, inter planar spacing, how to determine similarly inter planar angles how to determine we will discuss it. How we can go about is normally what we do is that this can be done in real space as well as in reciprocal lattice space. We have already learned about the relationship between the vectors in real space and the vectors in reciprocal space.

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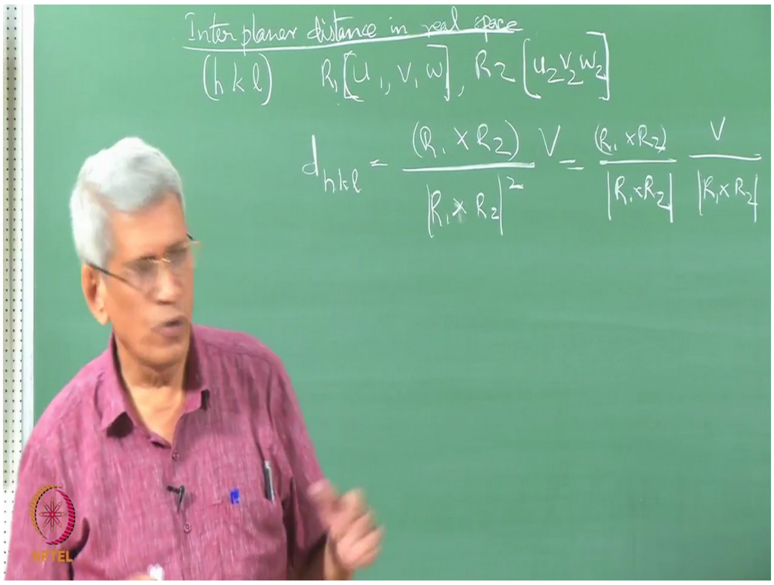

Suppose we wanted to find out angle between a interplanar distance in using the real space concept itself. We do not want to invoke the reciprocal lattice vector At all. Then what we have to do essentially is we should know 2 vectors which are lying in a plane. So, suppose h k l is the indices miller indices of a particular plane; if you know 2 vectors r 1 which is v 1 w 1.

This is how we can represent it, r 2 which is u 2 v 2 w 2, if these 2 vectors are lying in a plane, what we should find out first is essentially the vector which is normal to this plane, these 2 vectors are there we find out the cross product of these 2 vectors. That vector is perpendicular to it find out for that vector what is the unit vector in that direction. Then find out that inter planar distance magnitude then in the vector notation we can represent it. So, that will essentially turn out to be, suppose I wanted to find out d h k l, r 1 cross r 2 divided by r 1 cross r 2 magnitude the whole squared in to v, the volume of the unit cell. Essentially in fact, v is nothing but equal to r 1 cross r 2 by modulus of r 1 cross r 2.

This gives the unit vector in this directions inter planar direction and v is the volume divided by r 1 cross r 2 is that area of the unit cell. So, that will give that distance equivalent because this is essentially a scalar quantity, this is how this expression is being used. So, we have to use this expression, but what is essentially important is that in this case we should know what the volume which is going to be, but generally the lattices could be essentially simple lattices, we know how to find out the volume. If it is a triclinic lattice, there how do we find out the volume? That is the most general case which we can consider it. So, we will come to how to determine this volume. The other way in which these distances could be measured is the using the concept of reciprocal lattice.

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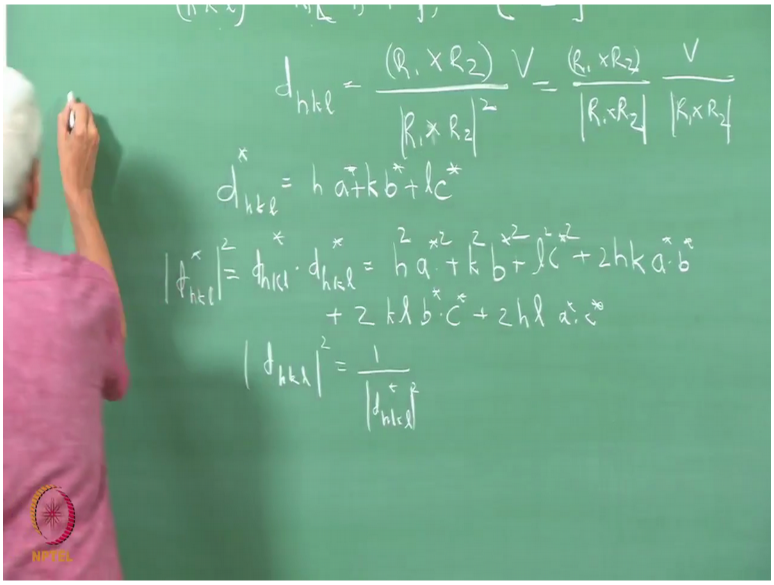

So, the plane h k l is nothing but indices of the vector in the reciprocal space. So, there any vector if I take it, d star h k l this will be equal to h, in to a star plus k in to b star plus l in to c star correct? We can write it this way. And we know d h k l star dot product of this if I take d h k l, this is nothing but equal to d h k l star the mod square it will turn out to be and this will be nothing but h squared.

A star square plus k squared b star square plus l squared c star square plus twice h k l in to a star, b star plus twice k in to l, in to b star dot C star, plus twice h in to l in to a star dot C star. Correct? This is how essentially it will turn out to be. And we know that once we have this magnitude, d h k l the magnitude is essentially is going to turn out to be one by d h k l star correct? Square this will be that whole square. So, using this relationship we can find out.

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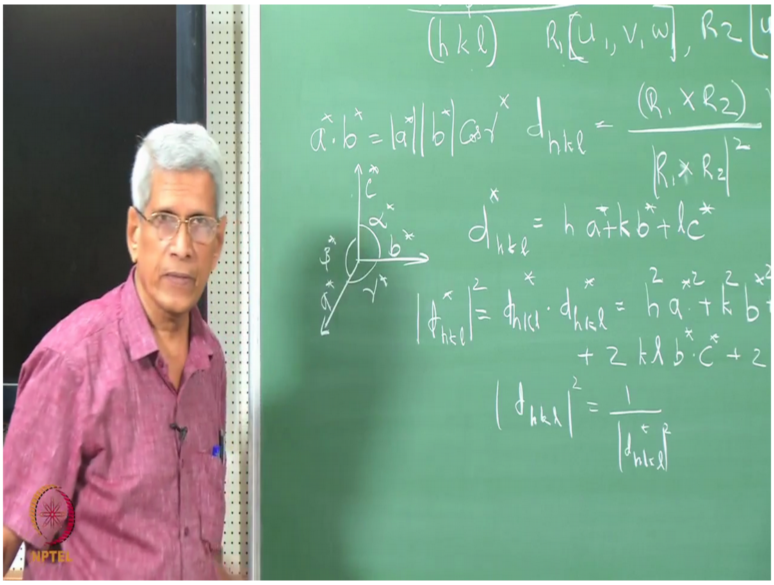

Here again, if you take a star dot B star then it will be equal to for example, equals modulus of A star in to modulus of B star in to this will be cross angle between a and b will turn out to be gamma Correct? So, essentially what we require is this sort of not gamma this is gamma star angle between these 2 vectors. There is essentially if we represent a star b star in terms of a coordinate system, in this direction a star b star and in this direction c star. This is the angle gamma star between them. This will be alpha star angle this will be beta star angle. This way we can utilize it to find out. Now again, that we know the relationship between a star in real space and reciprocal space.

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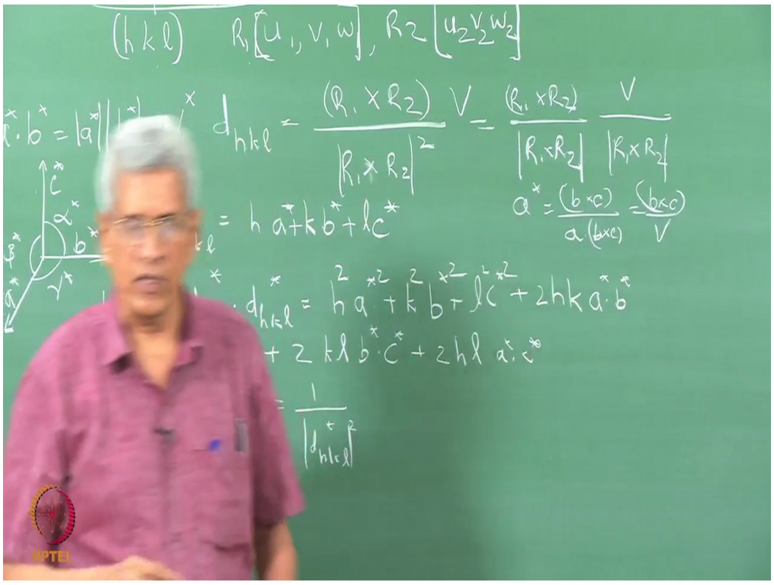

Essentially is a star will be equal to b cross c by A dot B cross c, which we write it as b cross c by v, similarly we can write it for others also this expression can be used to find out cuts essentially, is that what is the relationship between these angles, this is how we have defined it in reciprocal space. Similarly, in real space also we can choose a coordinate system.

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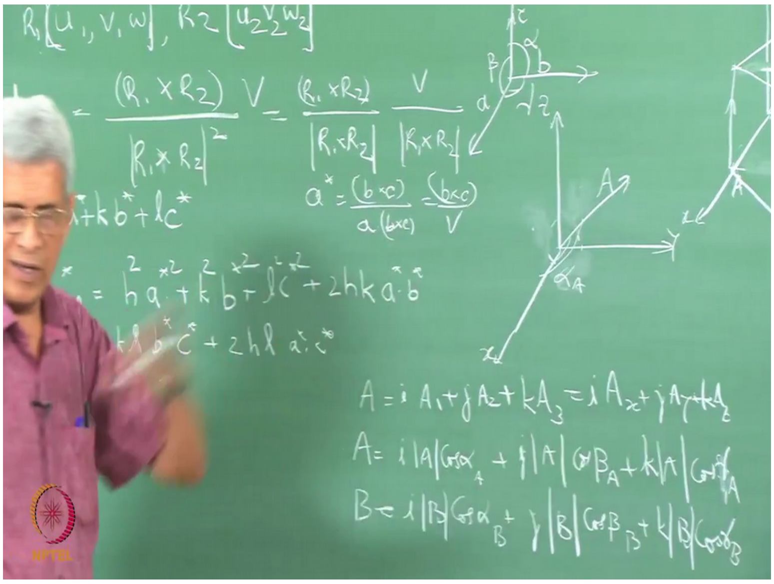

In which we define the unit cell. So, in that if this is a and this b and this direction it turns out to be c, and this angle is gamma, this angle is alpha this angle will be beta.

To use this formula essentially what we should know is, what is the relationship between alpha star beta star gamma star, in terms of alpha Beta gamma that information will be required. Because what we generally have with respect to crystal structure is only in a real space which we have. Similarly what is going to be the general formula for the volume in terms of a b c the coefficients and also in terms of the coefficient in terms of the lattice parameters a b c of the general unit cell which we have considered, and the angle between these various lattice parameters in different directions, translation with it in different directions.

This is the information which is necessary to use this. So, the question essentially is how are we going to determine this. So, we know that any vector now vector Algebra, what we do it is we choose a coordinate system which is essentially the orthogonal system, correct? Where that angle between all these is going to be essentially 90 degree, correct? These are sort of coordinate system which we chose it in this system anyway, since we will be putting other angle say it will just we can consider any vector in this system if we consider this vector which is lying like this. We define this vector as A. How do we find out that magnitude of the vectors essentially suppose this is x y and z? Then what is going to be that is this vector A can be written as I in to A1 plus j in to A2 plus k in to a 3. This way we can write it. This can also be written as instead of A1 A2 A3 essentially represent the component in x y and Az. So, sometimes it is written as I in to a x plus j in to a y plus k in to Az. This is the way also we write this expression correct?

The other way in which we can do it is that what is going to be the projection the angle which it is going to make with respect to this and find out what is going to be the magnitude of A. So, then we can write a can be written as I in to modulus of A in to I will write this angle which it makes as cos alpha A this angle which makes this is alpha with respect to y axis I in to modulus of A in to cos beta A j plus k into modulus of A in to cos beta Cos gamma A. This way also we can represent it there are many ways in which these vectors could be represented. So, in this representation essentially this magnitude is a scalar quantity. And then with respect to the angle which that vector makes respect to various axis this form in which we can write it.

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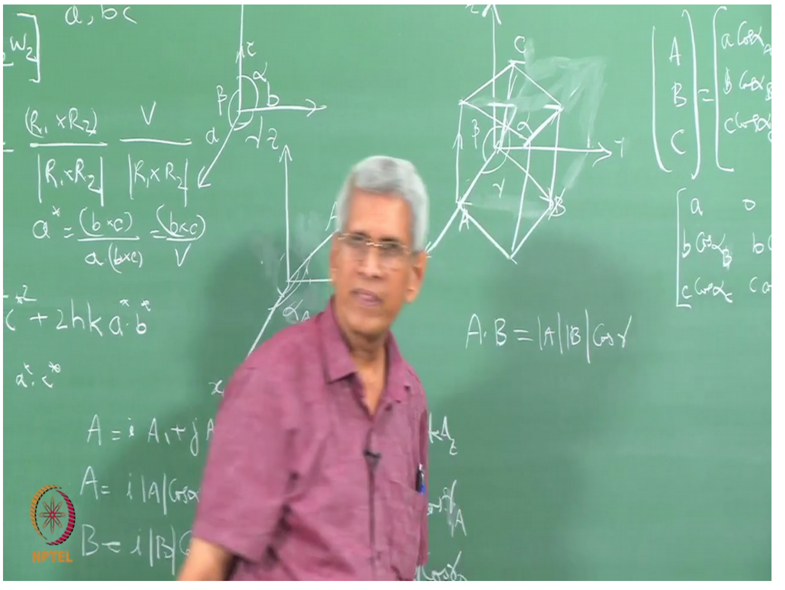

So, now we will come back to the problem of filing of the one thing. Now let us consider x y and the z; suppose I consider a vector A in this direction vector B in this direction. Just I am taking as aspecific case it could be a general one, I am taking it. So, that it becomes a little bit simpler to solve it. And a vector c these are all the translational vector in these directions. If we take this with these vectors we could now construct a unit cell correct? So, what essentially will happen is that, suppose I take this like this. So, this is essentially how the unit cell is no A, what is essentially will happen is, this way it will come like this. From here to here to here and here to here this is how the unit cell will be correct? Now this essentially what it is going to be a b, and this is going to be the c vector this we assume it to be a tricliniclattice.

Now, these vectors a b and c can be in written in terms of each one of them in terms of vector coordinates that is orthonormal system which we have chosen. Then we will be writing an expression like this for A vector. Similarly, we can write an expression like this for B i in to v in to cos alpha B cos beta B plus k in to modulus of B cos gamma B right. This way and this modulus of A B C is essentially the translation vector in this the magnitude which we can assume it to be A B and C.

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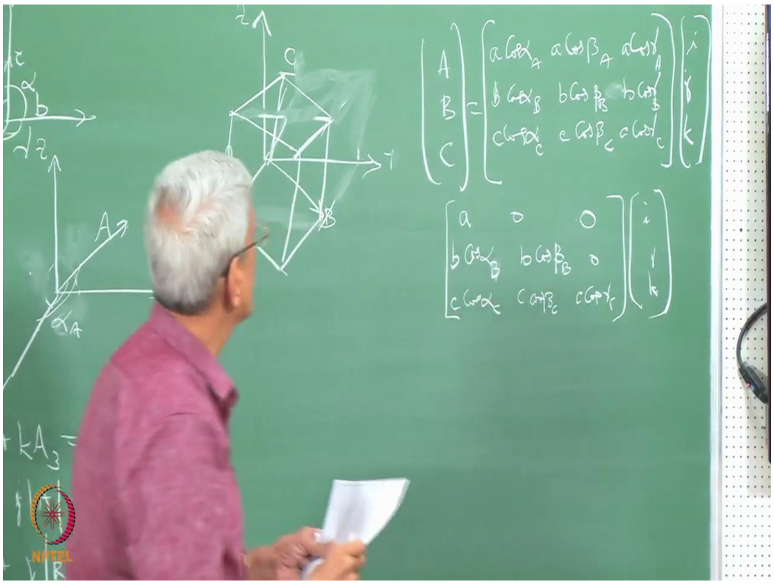

If we take in this form now, what essentially is that this itself can be written as A B C can be written in terms of a cos alpha A cos beta A A cos gamma A B cos alpha B B cos beta B and B cos C cos alpha C C cos beta C C cos gamma C in to i j and k. This type of matrix notation which we can write, correct? The sort of coordinate system which we have chosen a is matching with this. So, what is the angle which it makes it respect to this one it is 0. So, that will cos alpha it will turn out to be 1 correct? Then the other 2 cos beta A and the cos gamma A is going to be 0 get 90 degree angle makes. So, this expression will turn out to be a 0 0 then, similarly here it will be I will just write that expression, but you can work out all this aspect cos alpha beta B cos for B cos beta 0 C in to cos alpha C C cos beta C in to C cos gamma C then in to i j k. So, this is the expression for ABC in terms of the orthonormal system of coordinate system with which we have.

And angle between these will be turn out to be gamma, angle between these 2 axis will be going to be alpha this angle is going to be beta these are all the angles with respect to unit cell which we have, but now we have measured all the angles with respect to the coordinate system with which each of these lattice vector translational vectors of the unit cell is defined, correct?

Now, we know that A dot B will be equal to modulus of A in to modulus of B in to cos gamma, correct?

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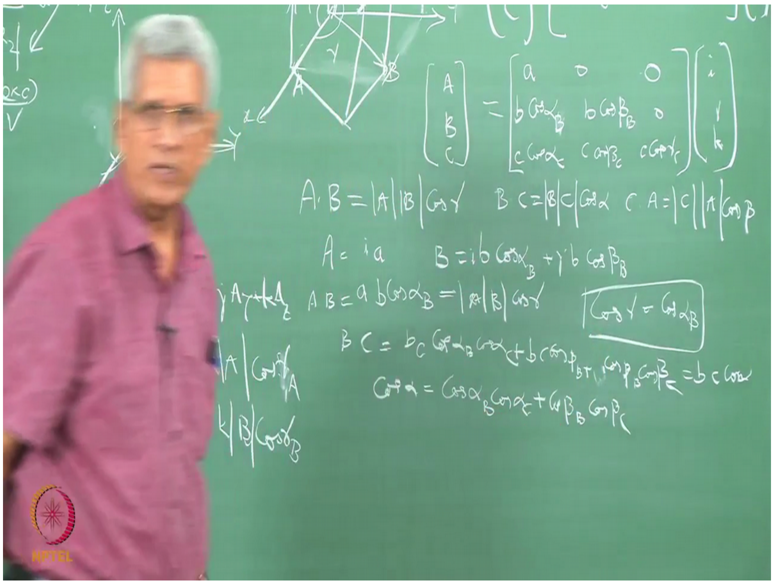

Similarly, B dot C equals modulus of B in to modulus of C in to cos alpha then C dot A modulus of C in to modulus of A in to cos beta. We know this expression. This is one expression which we have. From this equation here it is A B C we can find out the value of A B and C. Then also we can substitute on this side and find out, correct? So, if we try to do that then you know what will happen, A dot B, if you try to do it what is a here is equal to i into a correct? What is b equals i into b in to cos alpha B, plus j in to b in to cos beta B correct? If you take A dot B what is it which is going to turn out to be, this will turn out to be a in to b, A dot B equals to B cos alpha beta Cos alpha B it will turn out to be correct? Because that other ones that j because i dot i only will be equal to I dot j equals 0.

So now, we have this expression this can be equal to modulus of A in to modulus of B, in to cos gamma this modulus is A B. Now we get that expression right cos gamma equals cos alpha B correct? So, now, alpha B we have got it in this matrix in terms of the angle between the 2 vectors to lattice translation with the unit cell we have got that information. Essentially what we have to do it is that information like this for all other angles if you get it now we will have an expression which is connecting A B C in terms of the modulus of A B C and the angle between them that is all this whole game is once that information is available we have again.

Similarly, if you do it I will not go into work out all these details, I will just write that expression which one can work out for oneself. If you take this expression that B dot C this will turn out to be B C cos alpha B cos alpha C plus B C this what it will turn out to be beta B plus cos beta B to cos beta C this equals b C cos alpha from which we will be getting a relation that cos alpha equals cos alpha B cos alpha C plus cos beta B, in to cos beta C. This is the sort of an expression which will be deriving, but if you look here beta B is what it makes with respect to this one correct? This beta B will turn out to be 90 minus gamma, if we use that expression then cos beta B will turn out to be sin gamma we can substitute like this.

Finally, I will just write down the final expression like that it is essentially a working note on algebra, I told what the methodology which has to be good is essentially using this relation, and in which we had already got this is b c in to cos alpha this is C A in to cos gamma and C dot A we have to take the substitute then we will have that relationship finally, what it will turn out to be A B C 0 B cos gamma B sin gamma this is 0.

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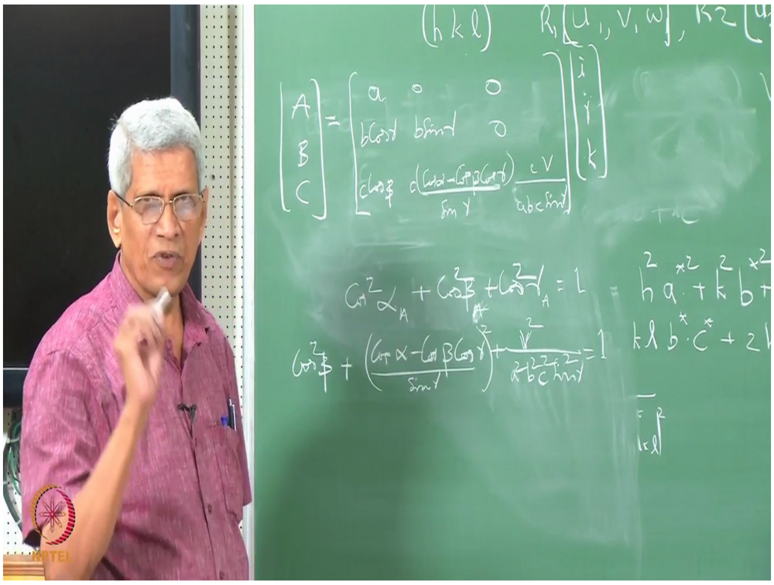

This is C cos beta C cos alpha minus cos beta cos gamma by sin gamma plus no here it will be C V by A B C sin gamma i j k and what is v here this v is nothing but the volume of the unit cell.

And this we know that in the expression which we has written this, cos squared plus cos squared beta A plus cos squared gamma A, this should be equal to 1.

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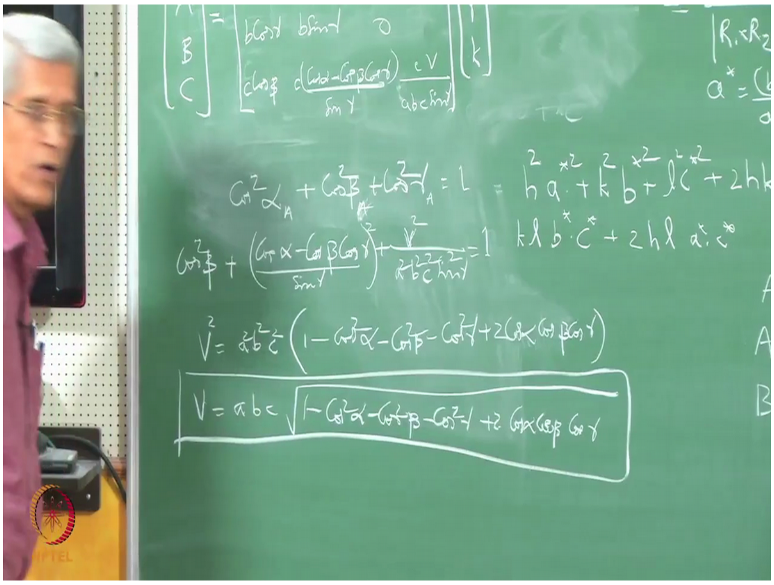

Similar expression holds for all of them. So, then if we write this this term will turn out to be for the last one cos square beta plus cos alpha minus cos beta cos gamma A sin gamma to the whole square plus v squared by a squared b squared c squared sin squared gamma this will turn out to be 1. If we try to solve this equation, what we will get as a final answer is because here v is one term a squared b squared is there then all others are angle between the different translation with different vectors of the unit cell. So, essentially now v squared will turn out to be a squared b squared c squared, in to 1 minus cos squared alpha minus cos squared beta minus cos squared gamma, plus 2 cos alpha cos beta cos gamma.

So, from this we will find that v equals a b c in to root of this temp 1 minus cos squared alpha minus cos square beta. This is essentially is what how the volume of a triclinic structure whether no symmetry is associated with it none of the angles are 90 degree, we can relate them to the angle between that unit cell vectors and the lattice parameters these general formula. So, once we have this formula then it becomes now very easy to find out if we are using a real lattice vectors like the way we have written.

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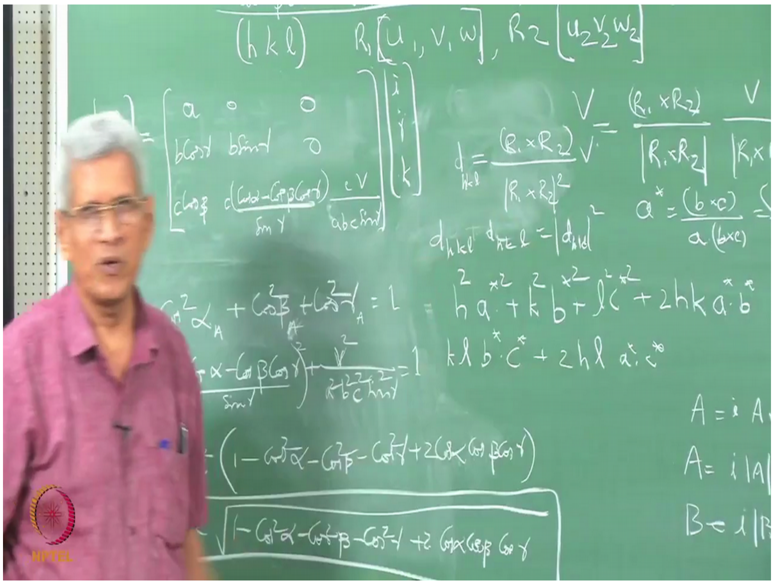

Here it is going to be that d equals that is d h k l will be equal to if 2 vectors, r 1 cos r 2, which are lying in this plane divided by r 1 cross r 2, the whole squared in to v we have. And the r 1 and r 2 are defined in terms of a b c substituting this we can get this expression.

Then once we here have we have that that is d h k l dot d h k l will be equal to modulus of d h k l the whole square and from which we have been able to find out. And general expression that is what it can be done or as I mentioned the reciprocal lattice vector also that concept if we use it.

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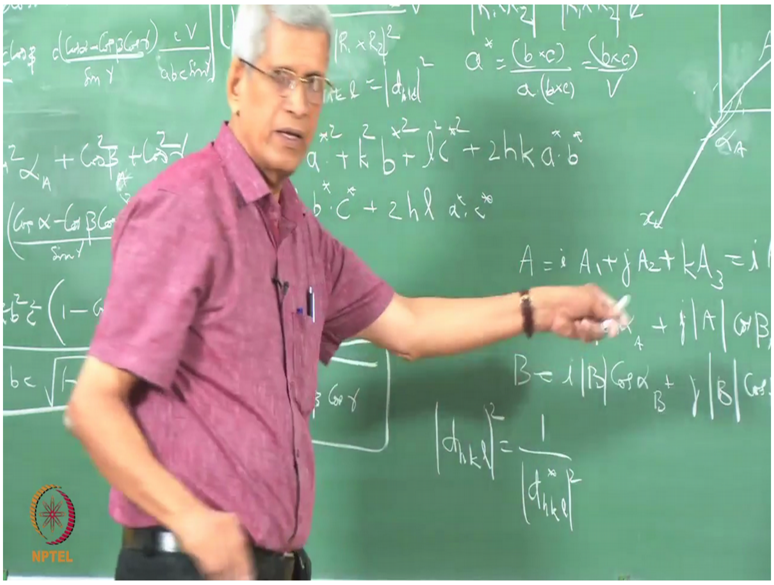

Then d h k l the whole squared equals one by d h k l star, the whole squared, this expression also we have written it in this expression what we know that a star b star and c star we know the relationship.

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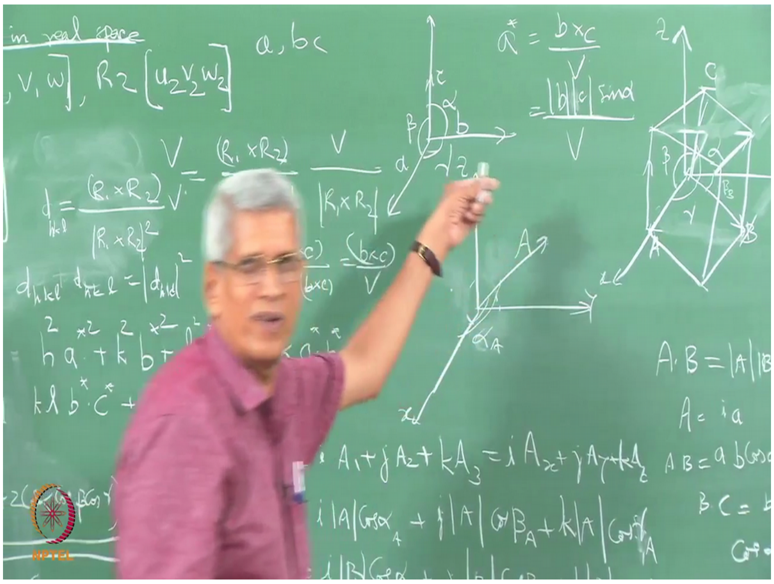

In that relationship essentially what we require is that a star will be equal to b cross c by v, that we have this expression which is there. This will generally turn out to be what is b cross c b cross c will be modulus of B in to modulus of C in to sin alpha divided by v.

So, now, this b c sin alpha divided by volume we know. So, now, we get all the information a star. So, we can use this and then an algebra which we have to work out.

That way we can get information about the inter planar spacing, we can get a general expression which one can derive, but if we use the reciprocal lattice vectors, we have to get another relationship and that relationship is nothing but what is the relation between the angle alpha star beta star and gamma star.

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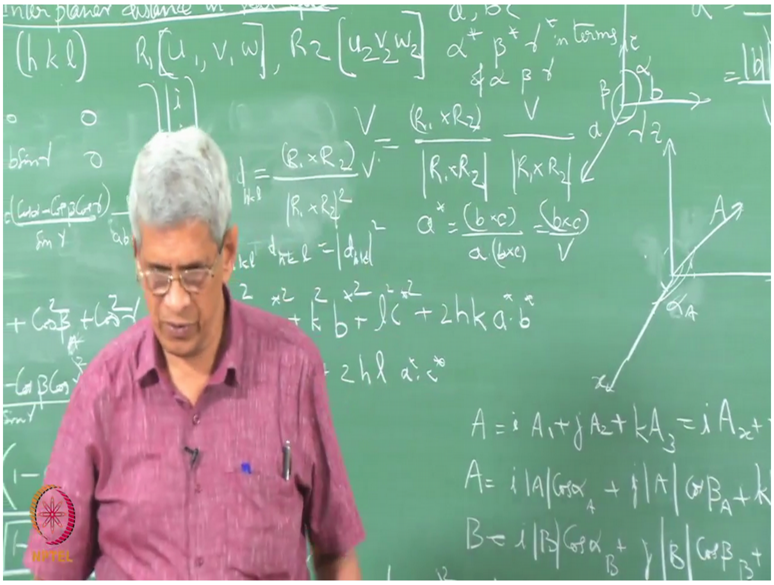

In terms of alpha beta and gamma we have to get that relationship correct? That is a must without which we cannot do that. That relationship also I will just write it down, but as an exercise one can work out that relationship essentially is cos gamma minus cos alpha.

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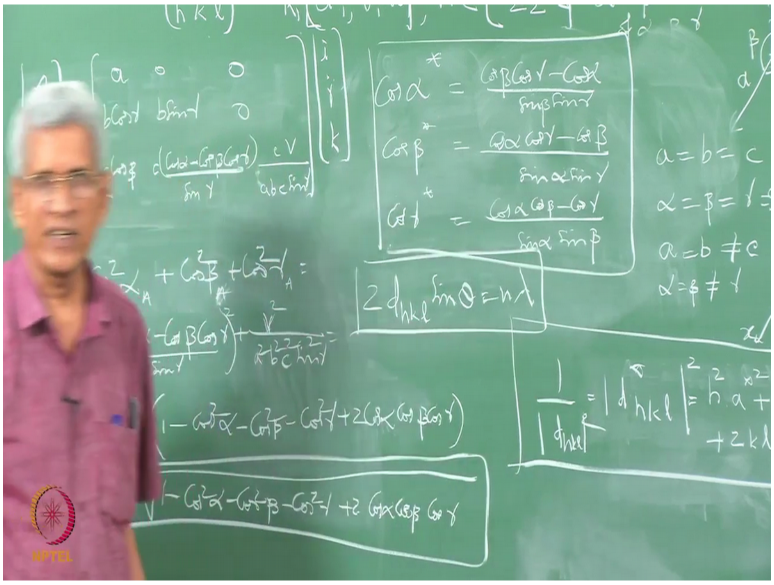

Sin beta sin gamma, similarly cos star equals cos alpha Cos gamma, minus cos beta then sin alpha sin gamma cos gamma star equals cos alpha cos beta minus cos gamma divided by sin alpha sin beta. So, this gives the relationship of alpha star beta star gamma star in terms of alpha and beta in real space unit cell. Similarly, this expression gives a star b star and c star in terms of a b c and the angles alpha beta and gamma in real space system. And now the expression which we have written for this star h k l, I will write down that expression again.

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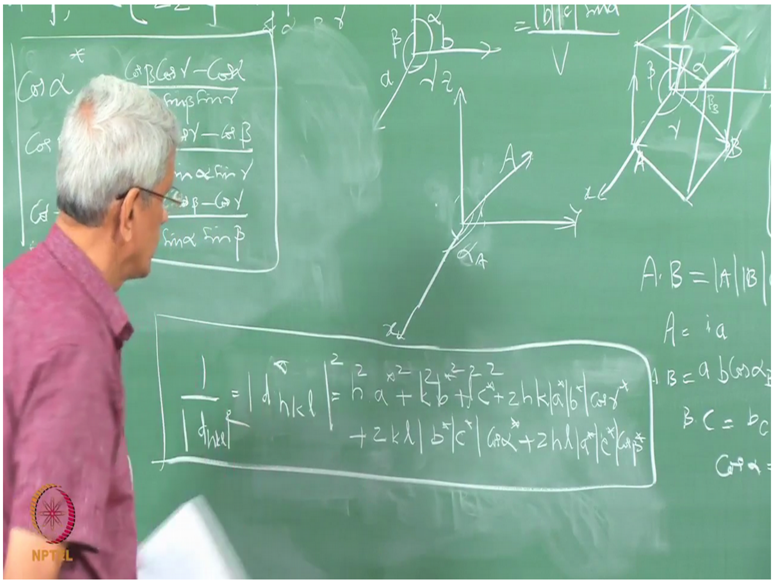

Whole squared equals h squared a s r square plus l, squared c star square, plus 2 h k in to a star mod in to b star, cos gamma star, plus 2 k in to l in to b star, c star alpha star, plus 2 h in to l, in to a star in to c star, cos beta star. This is equals 1 by mod d h k l the whole square correct? So, in this expression now we know a star b star and c star in terms of and we have angle between alpha beta and gamma star in terms of alpha beta and gamma we have.

So, using this expression now one can this is the most general expression to find out inter planar spacing for any crystal structure where there is no symmetry is involve. And using that symmetry how the angles alpha beta and gamma we know how it is being defined like.

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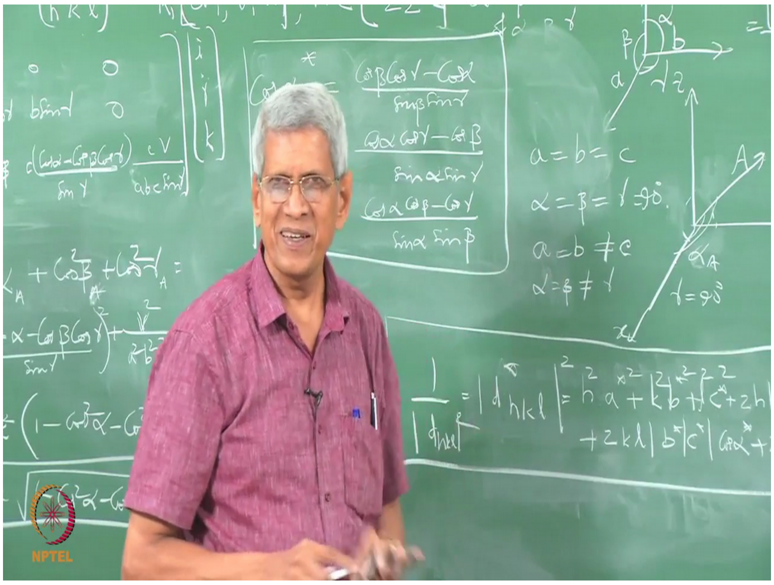

For example, if it is a cubic system we know a equals b equals c. And alpha equals beta equals gamma equals 90 degree. Using these expressions substituting in it we can get that value and find out an expression. Similarly, if it is a monoclinic structure then we know a equals b not equal to c. Alpha equals beta not equal to gamma, and gamma equals 90 degree correct? So, now, we know how these expressions using this we can derive from these expressions for the d spacing, formula for d spacing for various crystal structures. This I am not going to do that yes I had already given a very general formula which has to be used and how to derive that, and using this formula one can find out expressions for the inter planar distance for various crystal structures.

Why we require this formula is that quite often when we wanted to find out or when we wanted to index the fraction patterns, we should be able to find out what the inter planer spacing is because we use the brat condition which is nothing but 2 d 2 d h k l sin theta equals n lambda, to define the diffraction condition diffraction pics, correct? So, from this that information which we can get, the information which we get it is for a particular value of lambda which we use what is the value of theta which we get it from each the information experimentally what we get it is only the d h k l information.

So, these formulas will be the 1 by d h k l information what we get it under reciprocal space from which we can get this information. This way one can derive formula for various structures. Similarly inter planar angles also when we have to find out how do you how can we go about.

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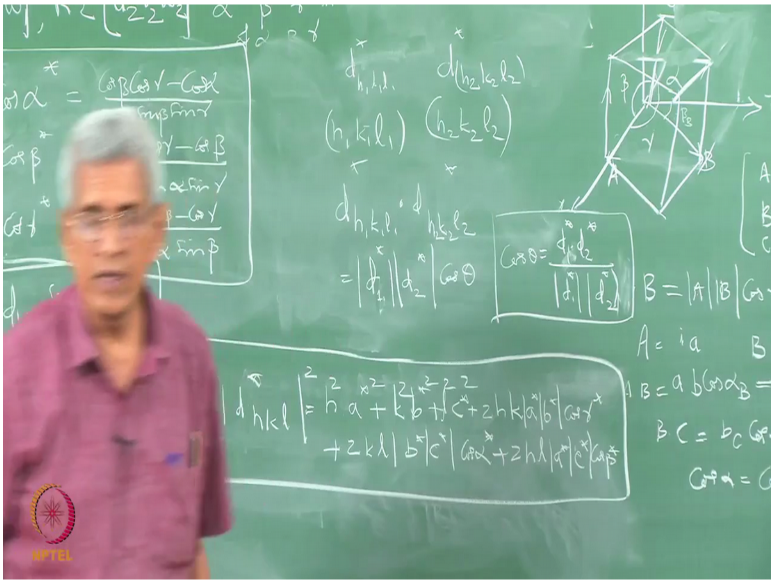

That is if we know, cos theta is that angle that is essentially what we do is if 2 vectors which we define, d star h 1 k 1 l 1 another vector is d star, h 2 k delta r we can define 2 reciprocal lattice planes. So, let us consider the case 2 reciprocal lattice 2 planes, one with miller indices h 1 k 1 l 1 another with miller indices h 2 k 2 l 2. If you wanted to mathematically derive an expression for the angle between these planes. So, what we normally do it is find out what is the plane normal corresponding to this for which you should know 2 vectors in that plane find out once we know, these 2 vectors, you know it and then find out the plane normal for each of this plane. The angle between the plane normal is what it is going to be defined correct?

For a cubic system plane normal it is easier to do it, but not for other systems. Other way we can consider it is that, if you take a reciprocal lattice vector reciprocal lattice vector is in the same direction as the inter planar vector plane normal plane only difference between plane normal is in real space, and reciprocal lattice vector is in reciprocal space, but each of these vectors are parallel to each other, only difference is that the coefficients when we consider it is inverse of the other that is the only difference. So, since the directions are the same the same direction they are angle between 2 reciprocal lattice vectors if we take it, that also we can find out how do we find out the angle between 2 reciprocal lattice vectors suppose if one reciprocal lattice vector is there d star h 1 k 1 l 1, another the dot product if we take it d 2 k 2 l 2, this dot product will be nothing but equal to modulus of, I will just for a simplicity take I will write d 1 star in to this is d 2 star angle between them we write it to be cos theta this we know.

So, how we can find out this values cos theta cos theta is nothing but d 1 star dot d 2 star divided by modulus of d 1 correct? In to modulus of d 2 correct? Using this expression we can derive the angle between the different ways. Now we know d 1 star d 2 star already how to get that information, we have worked out for a general case then one can derive a formula for angle between planes for 2 vectors in reciprocal space. That can be used to get information about them this; what I will do is I can give you some exercise which one can work it out.

So, that is the best way in which because once you people derive it, this will be permanently etched in your memory and you will not the forget it. So, only a general formalism which has to be followed with whatever is a necessary algebra, that is what I have discussed in this class I will stop here now.