Crystals, Symmetry and Tensors
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Lecture 6c
Transformation of direction and planes

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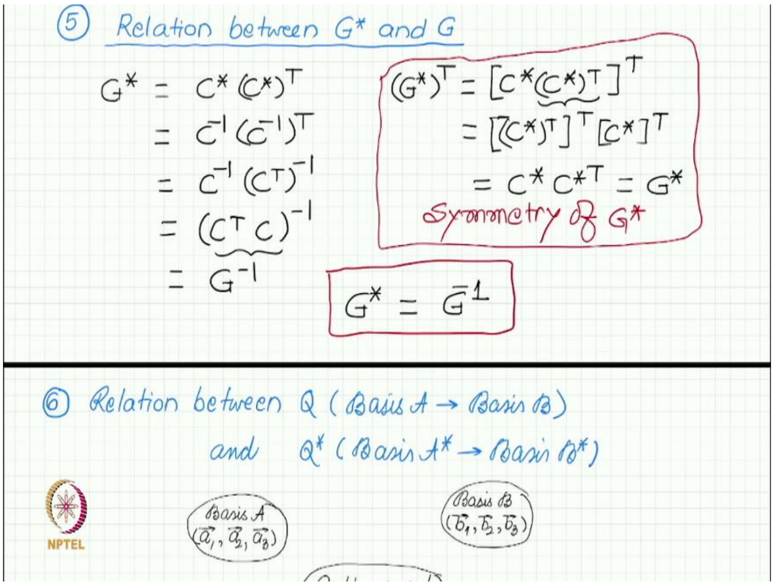

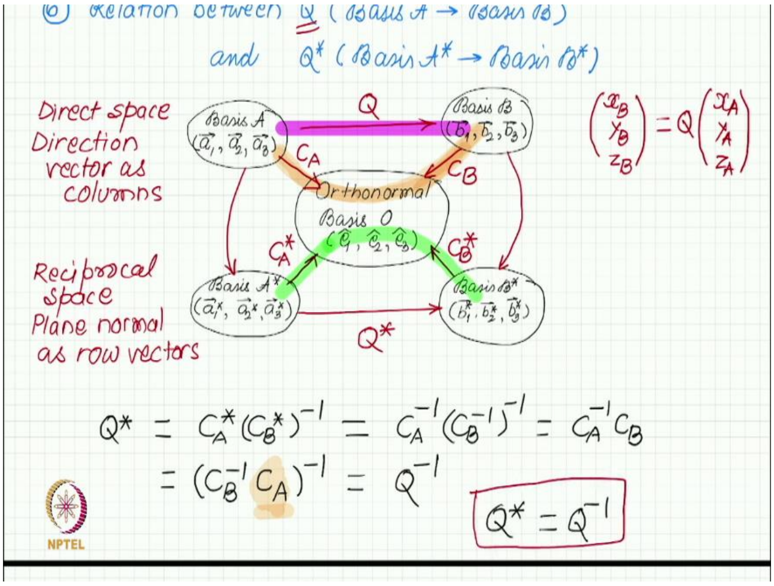

Now, we do little bit more juggling with this coordinate transformation, so let us do this, let us now introduce 2 bases, when we said Q Matrix, transformation from 1 basis to another basis. So, we have 2 basis, basis a, defined by a1 a2 a3 and basis b defined by b1 b2 b3, and we defined a q Matrix, coordinate transformation matrix which will transform any vector in the a basis to its component, it will transform its component in the a basis to its component in the b basis, that is what Q does.

And we have decided to write use these bases as the direct space where we are writing vectors as columns, so these may be a direction vector as columns. So, the job of Q is to give you xB, yB, zB, from xA, yA, zA, where xA, yA, zA, and xB, yB, Zb are components of the same vector, but refer to different coordinate system different bases A and B, and Q is my transformation matrix which does this matrix.

Now, for every basis A, I can calculate its corresponding or determine its corresponding reciprocal basis. So, this is the reciprocal space, so we are using it for example for plane normal, here the vectors, the common vector which we will be using is plain normal and we will be writing them as row vectors, similarly, for B there is a B star.

Now, A can be related to the orthonormal basis, so we have already 4, 2 direct basis A and B, which are talking through each other through Q. We have 2 reciprocal basic, corresponding reciprocal bases who we want to know that in what language they are talking, so their communication language will be some other Matrix Q star, and we want to find out what is that Q star.

In between there is an orthonormal basis which is a sort of communication hub, which communicates through different matrices as you know so that we are calling them C, so C A takes basis a to orthonormal basis, C B takes basis B to orthonormal basis, similarly C A star will take A star to orthonormal basis, and C B Star, B Star to orthonormal basis, so Q C A C B C A star C B star and Q star, we have six matrices connecting these five different bases, and we want to find, the goal is to find Q star in terms of Q.

If we know the Matrix which transforms direct space A to direct space B, what is the corresponding Matrix Q star which connects reciprocal space A star to reciprocal space B star?

So, let us do this exercise. So, let us write this Q star, so Q star will help us to go from A star to B Star. Now, suppose there is an obstacle there is a landslide on that path, so we will like to take a diversion, we first go to the orthonormal basis, and then come back to B Star, so the net result of these 2 transformations should be same as the Q star transformation.

But what is going from A star to orthonormal doing? It is multiplying by C A star and what will take us from orthonormal to B Star? Yeah, C B Star inverse, I am happy all of you are with me, will be C A star inverse. So, these two, the product of these two matrices should be same as Q A star, because the end results are the same.

Now, I can write C A star as, I know C A Star is C A inverse, and C B star is C B inverse, so inverse of inverse is C B, so we have C A inverse C B, we can write this as, again using the Matrix inverse properties, C B times C A whole inverse.

Now, let us see what C B times C A will do for us? C A takes us to orthonormal basis and C B inverse, so from A, I come to orthonormal basis using C A and then C B inverse takes me to basis B from the orthonormal basis, so this is this path which is equivalent to the net result is this path. So, I can write this simply as Q, CB inverse C A is Q, to Q inverse. Yet another verification of the reciprocal space name is fully justified.

So, for any transformation, so what we had initially seen that transformation to orthonormal to a transformation to given orthonormal basis C A star was inverse of C A, for a given pair A and A star. Now, we are finding that even a was being taken to B to some other basis through Q, then a star will be taken to B Star, again by its inverse.

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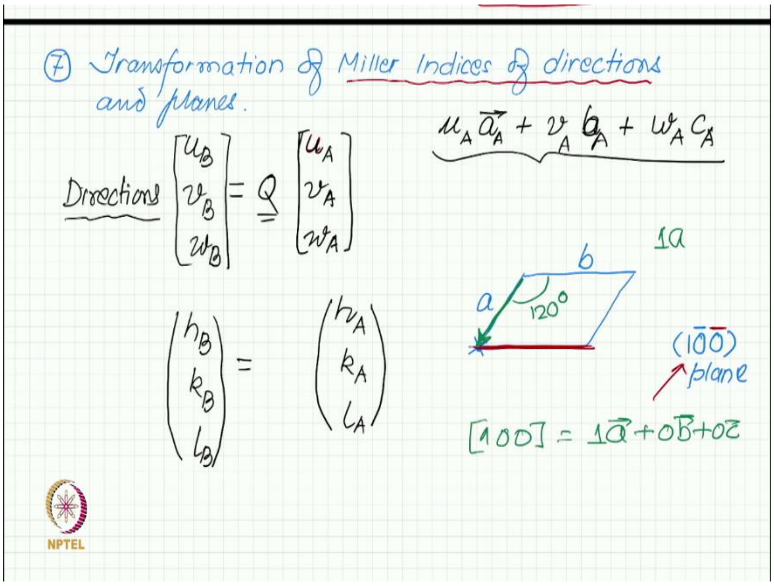

Now, just a comment, not a new result, you have already derived that how will you transform, in fact I can take a quiz now, that given Miller indices of a direction, how will you transform 1 Miller index with respect Miller indices with respect to one coordinate system to indices of the same direction with respect to another coordinate system. If I have UA, UA VA WA has the Miller indices of 1 direction, then I just multiply it by that coordinate trans, because it is a vector.

Miller indices are nothing but what was UA VA WA representing? It was representing a direction UA times A Plus VB times BA, sorry VA times BA plus WA times CA, so it is a vector, and it is a vector in real space, and for real space is what we have set up Q for, so we will get UB VB WB. And how will you transform the Miller indices, so this is for Direction? how will you now transform a Miller indices of a plane? So, suppose I give you the Miller indices of a plane h k l, I give you hA kA La, how will you get hB kB Lb.

Suppose we have a unit cell like this a b and c perpendicular to the plane of the paper, then let us say 100 plane, 1 on the x axis, so it will cut the x axis here at a, 0 means infinite on the b axis, so it is parallel to the b axis, the plane should do something like this and parallel to the c axis, so it is perpendicular to the plane of the paper. So, it is a plane like a prism face it is standing on the plane of the paper perpendicular and is cutting the a axis at 1, this is what is 100 plane, but the 100 direction, here is a direction which is 1a, 100 direction 1a plus 0b plus 0c, so it is this direction.

And you can clearly see that unless and until this angle I have did not say anything about this angle, let us make it a hexagonal unit cell so this angle is 120 degree. So, if this angle is so in hexagonal Crystal 100 direction is no more parallel to or, sorry, no more perpendicular to 100 plane.

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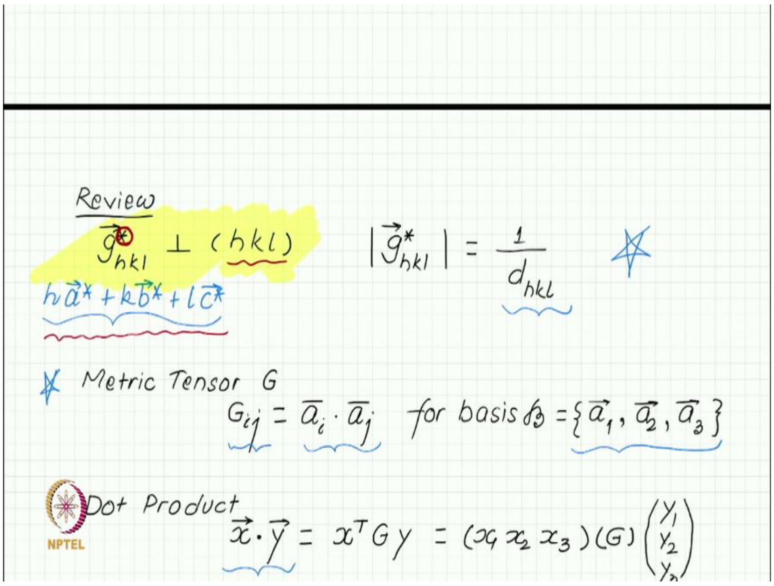

So, if you want that perpendicularity, that was, let us go back to our review that is why that result is so important do not take it lightly, so this result needs to be now, needs to be painted all red, but I do not have a red painting option, so let me paint it all yellow, so it is the g star, this star is very, very critical not any arbitrary vector, but if you want in general for the hkl direction to be perpendicular to the hkl plane, the direction has to be in the reciprocal space that is h k l have to be referred to a star, b star and c star.

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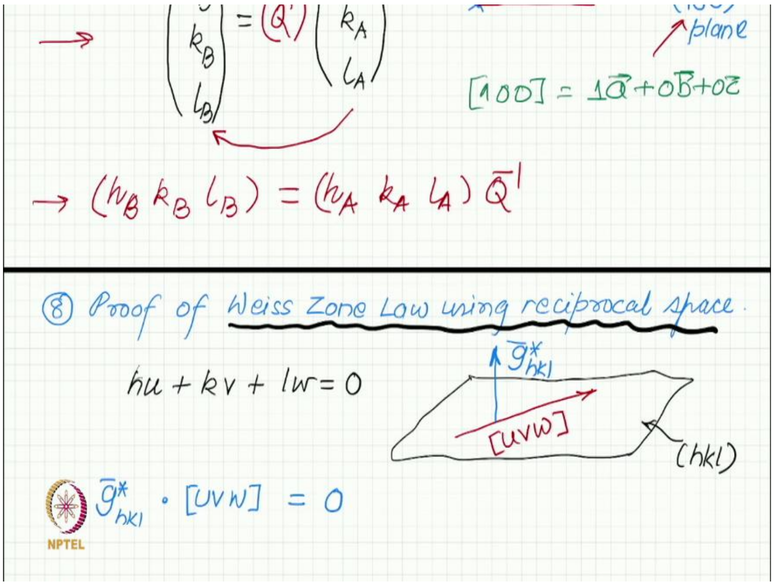

Now, we come back again to this exercise, so now, so we can consider them as plane normal, but we are in we should remember that we are in reciprocal space, so that means we are transforming now not direct space vector but reciprocal space vector, and we have established that relation that how do we transform the reciprocal space vector by Q star or Q inverse only keeping in mind that we should write them as row vector.

So, I should not write, I will deliberately writing it as column vector to challenge you, I should write it as row vector, and then I can happily transform them by Q inverse, if you insist that my vectors are column vector, then you could have used Q inverse transpose, so if you say Q inverse transpose here, then you are fine. So, either will give you the same numerical result it is only algebraically writing a style is different.

Now, this fact, we have established this fact, that highlighted fact, yeah, so this equation or this relation we have worked very hard to prove it, so we can now much more easily prove that same relationship, so let us try to do that. I am talking of proof of Weiss Zone Law, Weiss Zone Law if you remember Weiss Zone Law was hu plus kv plus lw is equal to 0 as a condition that you have a plane hkl, you have a plane hkl and you have a direction u v w, and we wanted to prove this.

So, for this proof also, means I got little diverted there it is not regarding that perpendicular property, there also we used something like that, but for proving the Weiss Zone Law also we used something similar that we constructed two vectors in the plane and then we showed that UV W is a combination of those two vectors, the u v w vector is a combination of those two vectors. But now, using our reciprocal Magic 1, we can do much better, so what is the vector normal to this plane? Yeah, vector normal to this plane, g star hkl and if g star hkl is normal, what will be its relation to u v w? So, g star hkl dot uvw is 0.

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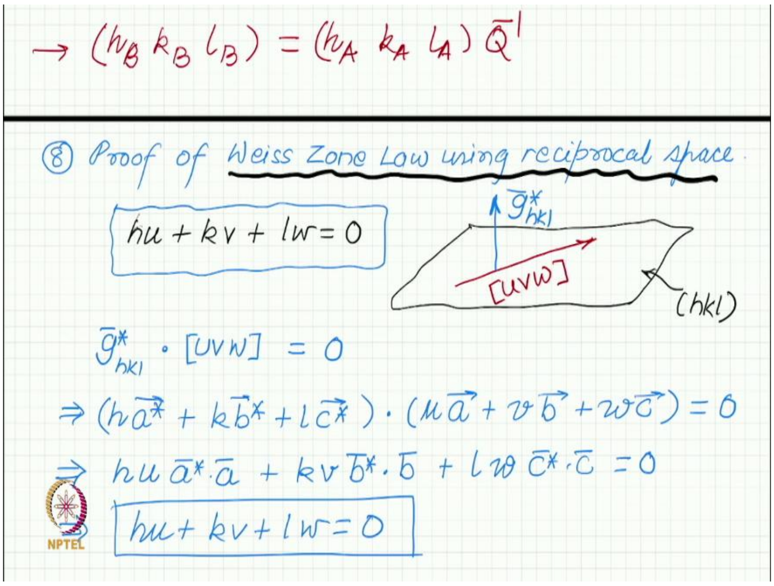

But g star hkl is just a short form, we have just said it is short form of ha star plus kb star plus lc star and uvw inside bracket is just a short form of ua plus vb plus wc and this is 0. Now, this appears to be giving nine terms, but you know the nice property of a reciprocal space, that a star, only a star dot a will survive as 1, a star dot b is 0, a star dot c is 0.

Similarly, b star dot a is 0, b star dot c is 0, c star dot a is 0, c star dot b is 0, that is the definition of the reciprocal lattice. So, this gives you then only hu a star dot a star, kv, sorry, thank you, thank you Ayan, kv b star dot b plus lw c star dot c, other terms are 0 and these terms also are just 1, so hu plus kv plus lw is 0, one line proof for Weiss Zone Law.

You can compare this proof with the previous proof which we gave living totally in real space, somebody was asking that day, why bother about reciprocal space in the first place? why cannot we do everything in real space? In fact, you can do everything in real space because real space is real, there is a reciprocal space is in sort of imaginary construct, but the imaginary construct is to assist you in computation and assist you in many such simplifications, so this is one example.

You can prove Weiss Zone Law, everything is in the quantities themselves are in real space, there is no need of reciprocal space here, hkl is a plane in real space, uvw is a direction in real space, so the relationship is existing in real space, but a proof can be constructed, a simple proof can be constructed by lifting yourself up in the reciprocal space and then coming back again to real space.