

**PROFESSOR:** OK, ready for more? I defined a problem for you. Now let's address it. Said that if we have one coordinate system, and if we have some vector,  $q$ , that's defined as a second-rank tensor,  $a_{ij}$  times some other vector  $p_j$  and let me digress in passing. I am very careful to say "a second-rank tensor" and not a "second-order tensor," because higher-order order terms means negligible and non-important.

And when I say "second-order tensor," I don't mean to say it's not important and negligible. It's very important, so I say "rank," which has some sort of dignity to it. So I don't like the term "order," because it has another meaning.

OK, so here is a tensor that relates a vector  $p_j$  to give us the components of a vector  $q_i$ . If we change coordinate system, the components of  $p$ , representing exactly one in the same vector, wink on and off and take different values. The values for  $q$  take on different values, and therefore, of necessity, the three by three array of coefficients, which relates these different numbers, must also change its numerical values. And I hopefully convinced you at the end of last hour that there's times when you might actually want to do this when you're cutting out a particular sample from a single-crystal specimen.

How do we get the new tensor in terms of the direction cosine scheme that specifies the change of axes and the original tensor? So I am going to refer to my notes quite closely here, because I want it to come out pretty and not have to redefine variables when I'm done. So let's start with the original tensor relation,  $q_i = a_{ij} p_j$ .

Now, what we want is something of the form  $q'_i = a'_{ij} p'_j$ . And we know the relations forward and reverse in terms of the direction cosine scheme  $c_{ij}$ . So let's begin by writing  $q'_i$  in terms of  $q_j$ . And we know how that is going to transform. It's going to be elements of the direction cosine scheme  $c_{im}$  times  $q_m$ . So that will give me the  $i$ -th component of  $q$  in the new coordinate system.

I know how  $q$  arises from the applied vector  $p$ . So let me write  $q_m$  in terms of the applied  $p_j$ . And this is going to be  $a_{ij}$  times-- be careful of my variables here-- this is going to be  $a_{ml}$  times  $p_l$ . And that is going to, from my definition of a second-rank tensor, give me the  $m$ -th component of  $q$ . So far, so good. I've got two different repeated subscripts here, so this is a double summation.

Now, I'll have what I want to have, namely a  $q_{i'}$  on the left-hand side and a  $p_{j'}$  on the right-hand side if I can express the original components of  $p$  in terms of the new components of  $p$ . And I do that by the reverse transformation. So let me now write  $a_{ml}$ . And then in place of  $p_l$ , I will write  $c_{jl}$  times  $p_{j'}$ . Notice the inverted order of the subscripts. That is the reverse transformation that's going to give me  $p_l$ .

So you really have now what I'm after. This is a triple summation in  $m$ ,  $l$ , and  $j$ . I can write the terms that are in what is going to be a triple summation over a product of terms. I could write these terms in any order. So to simplify it, let me write  $q_{i'}$  is equal to  $c_{im} c_{jl}$  times  $a_{ml}$ , times  $p_{j'}$ .

And now, hotcha, I've got an expression that has  $q_{i'}$  on the left and  $p_{j'}$  on the right, and paying close attention to my notes so that the subscripts all came out the way I would like them to. So what this says is that the transform tensor  $a_{ij'}$  is going to be equal to, by definition-- or what we've shown here, it's going to be equal-- just picking off terms-- it's going to be  $c_{im} c_{jl}$  times  $a_{ml}$ . Just picking off these terms.

$m$  has no physical meaning, because  $m$  simply is an index of summation.  $l$  has no specific meaning. That is just an index of summation. But the  $i$  and the  $j$  do have meaning. They go with the  $i$  and  $j$  on the particular tensor element that we were attempting to evaluate. So in other words, to be specific, if we want the new value of the tensor element  $a_{12'}$ , it's going to be  $c_{1m}$  something,  $c_{2l}$  something, and those somethings  $m$  and  $l$  would vary from 1 to 3. So if I write this out not in the reduced subscript notation but put a summation sign in there, so  $a_{12'}$  is going to be the sum over  $m$  and the sum over  $l$  of terms  $c_{1m}$ -- the first index is always 1--

$c_2$  something-- first index is always 2-- and then  $m$  and  $l$  take on all possible values.

OK, we've got two results. We learned how to transform a vector. And a vector, if you will, is simply a tensor of first rank. And transforming the vector, we summed over all three components of the original vector. And the coefficients in that summation were one direction cosine. Now we're transforming a second-rank tensor. Again, each new element is a linear combination of all nine of the elements in the original tensor, and the coefficients are a product of two direction cosines.

So we've got two points. Let's draw a line through them, and we can say that, in general, any new tensor element of any rank-- and you could prove it through exactly this method by going up, now, to the third rank, fourth rank, and so on, and writing substitutions of this form-- it turns out that a new tensor element  $a_{ijkl}$  however far you want to go, is going to be given by a linear combination of direction cosine element  $c_{il}$ ,  $c_j$  capital J,  $c_k$  capital K,  $c_l$  capital L, times however far you have to go times  $a_{ijkl}$ , and so on.

So these are the true indices. These have physical meaning. These have relevance to how a particular property will behave. The capital I, capital J, capital L, and so on, are what we referred to last time as dummy indices. These are indices of summation. But the first index on the direction cosines has specific meaning. They are tied to the indices on the subscript of the term that you would like to evaluate.

So we've got now a very profound relation for a tensor of any rank. And really, it just involves substitutions using the reverse or the forward transformation until you get one element on the one side related to another element on the right-hand side. And this is a specific element in the new tensor, in our case, of the second-rank tensor,  $a_{ml}$ .

This is all very abstract. It is something that we'll have to do a couple of times for a real problem before you see how it works out. The number of elements that figure into these transformations is really astronomical. Suppose, for example, the tensor involved were something like the elastic stiffness tensor, which is represented by  $c$ . And we need four subscripts. This is a tensor of fourth rank.

If we wanted to transform a particular stiffness to a new coordinate system, we would need a summation  $c_i$  capital I,  $c_j$  capital J,  $c_k$  capital K,  $c_l$  capital L, times all of the elements in the original tensor,  $a_{ijkl}$ . A fourth-rank tensor consists of an array of 9 by 9 terms. So there are 81 of these. We'd have four direction cosines out in front, and there would be a total of 81 times 5 characters that we would have to write. So to do the complete tensor transformation, we would have to write on the order of 400 quantities to get just one of the 81 elements in the new transform tensor.

So the total number of elements we'd have to write to do this would be 81 squared times 5. That's a lot of elements. We'll do a few of these transformations directly, but let me assure you that if we do a transformation that is going to involve symmetry, a lot of the direction cosines, if we're lucky, will be 0. So it's not quite as onerous as it seems.

So we would make use of this sort of formalism if we wanted to go from one set of reference axes to a new set that might represent a special specimen that we cut out of a crystal. But there's another formal way in which we could make very profound and non-intuitive use of these relations. Crystals, except for the abominable triclinic crystals, have symmetry. If a crystal has symmetry, you can transform the solid physically by that symmetry operation. And you have to measure the same property before and after.

So suppose we have a crystal that has a twofold axis. And this crystal is something that looks like this. So this is side A, and this is side B. We could move the crystal by a 180-degree rotation. Put it down. I won't draw it, because it's going to look exactly the same, except now this thing-- I won't draw, and I do draw it-- this is face A, and this is face B. If we had electrodes on the crystal before and after that transformation, we have to measure, let's say, the same electrical conductivity for both orientations of the crystal.

Now, moving a crystal relative to some coordinate system, relative to a pair of electrodes that we're fastening onto the crystal, is exactly the same thing as doing the reverse transformation of the coordinate system. That's a vague, strange-

sounding term. So suppose we have a crystal with a fourfold axis with four faces, A, B, C, D. And here are our electrodes. To move the crystal relative to the electrodes by a 90-degree rotation would involve rotating face D up to this location. A would move to this location. C would move to this location. B would move to this location, and we'd fasten electrodes on the crystal again.

If the crystal originally had a coordinate system such that this were X1 and this is X2, moving the electrodes onto a different direction on the crystal is the same as moving the crystal in the opposite sense. So we could either envision moving the crystal relative to the electrodes like this, or we could move the electrodes relative to the crystal by the reverse transformation. And the result is the same.

So what I'm saying is that if a crystal has symmetry-- and let me be specific and suppose that our crystal has a twofold rotation axis along X3. Let's ask how that twofold axis would change the coordinate system relative to the crystal. That's the same as moving the crystal relative to the coordinate system. It's going to take X1 and move it to this location X1 prime. It's going to take X2 and move it through 180-degree rotation. This is going to be X2 prime. And if the twofold axis is along X3, X3 prime is the same as X3.

So what is the direction cosine scheme for this change of axes? You might immediately start working and saying, well, C11 is the cosine of the angle between X1 prime and X1. That's 180 degrees. Cosine of 180 degrees is minus 1. But let me remind you that the direction cosine scheme,  $c_{ij}$ , simply gives us the relation between the new axes  $x_{i \text{ prime}}$  and the old axes,  $x_{j \text{ prime}}$ . So let me, just by inspection, write down the relation between these two sets of coordinate systems.

So X1 prime is equal to minus X1. X2 prime is equal to minus X2. X3 prime is equal to X3. So the direction cosine scheme for this particular transformation is simply minus 1 0 0, 0 minus 1 0, 0 0 1. So I just evaluated a nine-element direction cosine scheme by inspection, if I can write the relation between the coordinate system before and after the transformation. OK? And as we examine higher symmetry, the same is going to be true for the threefold axis, let's say, along the 1, 1, 1 direction of

a cubic crystal, for a sixfold axis, and so on. So we'll be able to write the direction cosine schemes for a symmetry transformation simply by inspection.

So for a twofold axis along  $X_3$ , this is the form of the direction cosine scheme. So now let me transform the elements of a second-rank tensor term by term and see what we get. Suppose I want-- let's stick with conductivity as an example. Suppose I want the value for the conductivity element  $\sigma'_{11}$ . That's going to be  $c_{1l}$  something,  $c_{1m}$  something, because these are the elements that go in here, times every element of a conductivity tensor  $\sigma_{lm}$ .

The only element of the form  $c_{1l}$  something that is non-zero in this row  $c_{11}$ ,  $c_{12}$ ,  $c_{13}$ , is the term  $c_{11}$ . In the same way in the same row, the only term of the form  $c_{1m}$  something is  $c_{11}$ . So this is going to be simply  $c_{11}$  times  $c_{11}$  times  $\sigma_{11}$ . That's the only term that survives.  $c_{11}$  has a numerical value of minus 1, and that says that  $\sigma'_{11}$  is equal to  $\sigma_{11}$ . So is there any constraint, any restriction on  $\sigma_{11}$ ? No,  $\sigma_{11}$  could be anything it likes. So there's no constraint.

Let's do another element. Let's see what  $\sigma'_{12}$  would be. This will be  $c_{1l}$  something times  $c_{2m}$  something times  $\sigma_{lm}$ . The only element of the form  $c_{1l}$  something that is non-zero is  $c_{11}$ . So I'll put in a 1 for the  $l$ . The only direction cosine element of the form  $c_{2m}$  something which is non-zero is  $c_{22}$ . So I'll put in  $c_{22}$  and let  $n$  be equal to 2.  $c_{11}$  is minus 1,  $c_{22}$  is minus 1.

So again, this gives us something not terribly interesting.  $\sigma'_{12}$  is equal to  $\sigma_{12}$ . So there's no constraint, at which point you're probably getting very restive, say, this is not telling us anything. So let me shake you up by doing one further transformation, and that is to find the value for  $\sigma'_{13}$ . And that would be  $c_{1l}$  something,  $c_{3m}$  something times  $\sigma_{lm}$ . The only form of this term of the form  $c_{1l}$  something, that's non-zero is  $c_{11}$ , as we've seen.

So I'll put in just that single term and replace  $l$  by 1. The term of the form  $c_{3m}$  something that is non-zero is  $c_{33}$ . And I'll put in a 3 for  $m$ , and this is then  $c_{11}$  times  $c_{33}$  times  $\sigma_{13}$ .  $c_{11}$  is minus 1,  $c_{33}$  is plus 1. And that says that  $\sigma'_{13}$  is minus  $\sigma_{13}$ . But if this is a symmetry transformation, the tensor has to

remain invariant. And if we're to have  $\sigma_{13} = -\sigma_{13}$ , there's only one number that can make that claim, and that's 0. So  $\sigma_{13}$  is identically 0.

And that places a rather severe constraint on the way in which the crystal is going to relate an applied electric field to a current flow.  $\sigma_{11}$  is anything.  $\sigma_{12}$  is anything.  $\sigma_{13}$  has to be identically 0. Now, let's cut to the bottom line. The direction cosine scheme is diagonal, so we can say that for any element that we pick to transform  $\sigma_{ij}$  is going to be  $c_{ii}$ , the diagonal term which has the second subscript equal to the first, times  $c_{jj}$  times  $\sigma_{ij}$ .

And this says that if we have  $i$  or  $j$  is equal to 3, then  $\sigma_{ij}$  has to be 0, because we're going to have a minus 1 times a plus 1. If neither  $i$  or  $j$  is equal to 3, then again, we will have a minus 1 times a minus 1. There will be no constraint. And the only final possibility is that both  $i$  and  $j$  are equal to 3. That would be the single element  $\sigma_{33}$ . Then we would have plus 1 times plus 1 as the product of direction cosines, and there will be no constraint.

So for a crystal that has a twofold axis, and in which that twofold axis is along the direction of  $x_3$ , the form of the tensor will be  $\sigma_{11}$ ,  $\sigma_{12}$ , 0,  $\sigma_{21}$ ,  $\sigma_{22}$ , 0,  $\sigma_{31}$ , that's going to be equal to 0, and  $\sigma_{33}$  has no constraints. So rather than having nine elements, there are only five independent elements rather than nine.

And there is now another relation that can occur in a second-rank tensor. The off-diagonal terms  $\sigma_{12}$  and  $\sigma_{21}$  do not have to be related. But for most-- but not all-- most second-rank tensor properties happily have  $\sigma_{ij}$  identical to  $\sigma_{ji}$ . In other words, the tensor is symmetric across its principal diagonal.

That is a condition that does not arise from symmetry. That depends on the specific physical property. So let me emphasize that this depends on the tensor property. And for a great many physical properties-- conductivity, diffusivity, permeability, susceptibility-- you can show that the tensor has to be symmetric. But there are a lot of tensors, particularly for the more obscure physical properties, where to my knowledge, this proof has never been given.

And along the same lines, it is well known that there is one physical property for which this is not true. This is the thermal electricity tensor. So for at least one property, you can show for sure that the tensor does not have to be symmetric and that for a crystal of symmetry 2, this term and this term are definitely not equal.

All right, let us do another transformation for another symmetry, and we can see that it goes fast when the direction cosine scheme is relatively sparse. Let's ask the restrictions, if any, that are imposed by inversion. So what is the direction cosine scheme here? Here's  $x_1$ , here's  $x_2$ , here's  $x_3$ .

Then operation of inversion at the intersection of these axes will invert the direction of  $x_1$  prime to here. It'll invert the direction of  $x_2$  prime here. It will invert the direction of  $x_3$  prime to here. So the relation between the reference axes is that  $x_1$  prime is equal to minus  $x_1$ .  $x_2$  prime is equal to minus  $x_2$ .  $x_3$  prime is equal to minus  $x_3$ , so that the form of the direction cosine scheme  $c_{rj}$  is minus 1, 00, 0 minus 1 0, 00 minus 1.

Slightly different from that for a two-fold axis for which the first two diagonal elements were minus 1, the third one was 0. Well, let's jump right to it and see if we can generalize this. It's a diagonal direction cosine scheme once again. And this says that if we transform a particular element  $\sigma_{ij}$ , it's going to be given by  $c_{il} \sigma_{lm}$ , where  $l$  and  $m$  are variables of summation.

The only ones that survive are the ones for which  $i$  equals  $l$  and for which  $j$  equals  $m$ . So it's going to be  $c_{ii} \sigma_{ij}$ . Regardless of the values of  $i$  and  $j$ , the diagonal terms are always minus 1. And therefore,  $\sigma_{ij}$  prime is always going to turn out to be equal to  $\sigma_{ij}$ , so there's going to be no constraint on any element.

And this shortens the job that's facing us immeasurably. So let me write that down, because that's important. Inversion imposes no constraint on any second-rank tensor property. So if we stay with monoclinic crystals, we looked at symmetry 2. Symmetry 2 over  $m$  is equal to 2 with an inversion center put on it. But inversion doesn't require anything, so the symmetry constraints for 2 over  $m$  have to be the

same as for symmetry 2.

We look at the constraints that might be imposed by a mirror plane. A mirror plane plus inversion is  $2/m$ .  $2/m$  has to be the same as 2. So this will be the same as 2. And now we've shown that for any monoclinic crystal, regardless of whether the symmetry, the point group, is  $2m$  or  $2/m$ , the form of the tensor has to be exactly the same. So for any monoclinic crystal, namely  $2m$  or  $2/m$ , this is the form of the tensor where the twofold axis, again, is along  $x_3$ , the mirror plane would have to be perpendicular to  $x_3$ , and for  $2/m$ , both of the preceding conditions.

So how about that? Let me issue a caveat, because we're almost out of time. There are five independent elements. And that's true. But elements  $\sigma_{12}$ ,  $\sigma_{21}$ ,  $\sigma_{13}$ , and  $\sigma_{31}$  are 0 only for this arrangement of axes relative to the symmetry elements. If you wanted to take a different set of axes, you know how to get the tensor for that set of axes. Each tensor element is going to be given by a linear combination of these five non-zero elements.

And if the orientation of the axes relative to the symmetry elements is quite general, all nine elements of the tensor will be non-zero. There will be only five independent numbers, which composes each of those nine elements, and they will be given by a product of two direction cosines, sometimes each of these five non-zero elements. But there will be no zeros in this array at all for an arbitrary set of coordinate systems.

Something that I think I'll ask you to do as a problem, because it's really easy to do, if the tensor is symmetric, which most of them are, one thing that you can show quite directly is that a symmetric tensor remains symmetric for any arbitrary change of axes. And that, again, is something that's fairly easy to prove, and I'll let you have the fun and exhilaration of doing that for yourself.

OK, so this means that for everything except thermal electricity, you really have to transform, at most, only six elements if you go from one coordinate system to another. That's still a lot, but it's considerably better than transforming all nine. So if

the tensor originally is symmetric in one coordinate system, it stays symmetric in any other coordinate system.

Now, one thing that I should mention-- I passed over it rather quickly-- we said that a property of a direction cosine scheme is that it is what's called a unitary transformation. And it has the property that the determinant of the coefficients is plus 1 if the axis retains the same chirality. The determinant is minus 1 if you change the handedness. That is only true for what is called a measure-preserving transformation. That's what it's called. And when it's a measure-preserving transformation, then the direction cosine scheme is a unitary matrix.

What is measure-preserving transformation? If it's a right-handed system beforehand, there's no squishing. It doesn't go to an oblique coordinate system. Cartesian stays Cartesian. If the reference axes are of equal lengths, they don't stretch upon the transformation. You can define transformations like that if you like, where the angles between them go from orthogonal to oblique after the transformation, and the units of length along the three axes change dimension. But then the determinant of the coefficients is not unity, and a lot of the nice, convenient properties that we've seen here do not hold.

All right, that is a good place to stop, I think. Next week, no quiz. If you came in late, we're going to postpone the quiz for a week. And let's see, look at all I can ask you just after one lecture on tensors. What we will do next is explore the form of the tensors for other crystal symmetries. It goes fairly quickly.

And then having done all that, I'll show you how you can determine the symmetry constraints by inspection for a tensor of any rank. And you're going to despise me for that, but this was useful, because we can get used to manipulating the notation. But there is a method called-- appropriately enough-- the method of direct inspection where you can very quickly and very easily do the symmetry transformations. So all this and more will be revealed next time, which is going to be a lot more beneficial than taking a quiz.