**PROFESSOR:** I think you will get going. A lot of people are not here, but I think if the MRS meeting were going on across the river I would be there too if I didn't have a class to go to.

We had last time finished a discussion strain. And we introduced strain by defining it as a displacement, each component of a vector displacement U as being given by a set of coefficients, eij times x of j, which says that the displacement in a deformed body varies linearly with the position of the particular point in the body.

We could also express the same thing in terms of change of length. The change in the vector U would be given by-- we show the same set of coefficients-- eij times delta x of j. So whether you want the displacement vector or you want the fractional change of length, you get this by an expression of the same sort.

We saw though that unless we define the coefficients correctly we could have a situation where a body is not only deformed but is rotated as well. And we saw that in general unless we define these coefficients carefully we would include in this tensor a component of pure rotation, rigid body rotation. And this would not measure deformation.

However, regardless of its suitability or unsuitability, the positional vector is a vector. It transforms like a vector. The displacement U is a vector, and it will transform like a vector; ergo, the 3 by 3 array eij is a second-rank tensor and we'll transform like a tensor.

We showed though that we could take eij and get rid of the pure rotation that might be contained in those coefficients by writing it as a tensor epsilon ij plus another tensor omega ij. And that was a new wrinkle, the concept of adding two tensors together to get a third tensor. We did run into that before.

And we define the elements of the two tensors epsilon and omega; epsilon ij was given by one half of eij plus eji, and omega ij is given by one half of omega ij. And notice the order of the subscripts here in this difference. That is a matter of definition, but it defines which term is omega ij and which is omega ji minus omega ji. I'm sorry. This should be eij minus eji.

And we showed that at a tensor of this form which would have all of the diagonal terms zero and the off-diagonal terms equal to the negative of one another that a tensor of this form does indeed correspond to pure body rotation.

We showed that by looking at a point at the end of a positional vector U and looked at a displacement which would be exactly at right angles to it. And the U would be given by the tensor relation. We showed that U dot r is identically zero when the displacement vector is given by this tensor with diagonal term zero and the offdiagonal terms equal to the negative of one another.

So we have then from a general tensor of the form eij constructed in the terms epsilon ij something that is a measure of true deformation. It is a symmetric tensor by definition. And therefore in addition to all of the other properties of second-rank tensor, namely having a law of transformation and staying symmetric for any arbitrary change of coordinate systems, the radius normal property also works.

Hence, the representation surface that we construct from the tensor epsilon ij xi xj equals 1, gives us the strain quadric. And it has the property that the radius gives us the value of strain in a given direction. And the value of the radius literally is going to be the vector that's on the left hand side, the magnitude of U times the component of U that is parallel to the radial vector per unit radial vector. And this then is the tensile strain, the fractional change of length as we look in this direction.

The radius normal is going to give us the direction of the total displacement U. And the value of the property in that direction is going to be the product of that displacement with a unit vector in the direction of interest. And therefore that is the tensile strain as we said before from the general properties of the quadric.

So everything we said about second-rank tensor and in particular symmetric tensor holds for the strain tensor. We can talk about diagonalizing the strain tensor into a form epsilon 1, 1, epsilon 22, zero zero, epsilon 33. And I'll remind you that we know how to do this to set up the normal equations and solve for the eigenvalues and then look for the principal axes of a tensor.

There are special forms of the strain tensor. Something that 1 diagonal goes into this form is called plane strain. And I love the melodic nature of that, the plane strain. If this were strain induced by a Modernistic transformation, we could call it the Bain plane strain. If we diagonalized it, it would be the main Bain plane strains. And if that deformation took place in an aircraft window, we could call it the planepane main Bain strains. And we could continue on indefinitely, but I think you're finding this tiresome.

Another form of the strain tensor that doesn't look what it actually represents is epsilon 1 zero minus epsilon 1 zero zero zero zero. That looks peculiar, very special. But, again, this is analogous to what we found for stress. If we rotate this tensor 45 degrees, we would find that treat tensor was diagonally, had all the diagonal elements zero. And we would have the epsilon 11 prime-- let's just call it epsilon prime-- and this epsilon prime zero zero zero. And this is pure shear

Something that we'll show shortly, and in fact I left it to you as a problem on a problems set. The sum of the diagonal elements, epsilon 11 plus epsilon 22 plus epsilon 33 is something that's defined as the trace of the tensor. And for the strain tensor, the trace turns out to be equal to delta V over the fractional change in volume. And we'll show that in just a little bit as well.

So a characteristic of pure shear is that it does not result in any change of volume of the solid. There's deformation, but the volume stays exactly the same.

Let me then proceed to show that the trace of the strain tensor is indeed the change in volume. And want I'll do is to look at an element of volume that is oriented along the principal elements of strain. So if this as x1, this is x2, and this is x3, the strain tensor I'll assume is oriented. So we have a term epsilon 11 zero zero zero zero; epsilon 22 zero zero zero; epsilon 33.

So let's suppose that the solid originally has edges L1, L2, and L3 along x1, x2, and

x3, respectively. So the initial volume before any deformation will be simply L1 times L2 times L3.

Let's suppose now we impose the strain, and the volume then we'll increase to some value of V plus delta V. And the length L1 will change to a value L1 times 1 plus epsilon 11. That is to say it'll be L1 plus epsilon 11 times L1, which can be factored out in this fashion. L2 changes to L2 times 1 plus epsilon 22. And L3 changes to L3 plus epsilon 33 times L3, which I'll write in this fashion.

So expanding this product, it'll be L1, L2, L3. And then if I simply multiply out these terms, I'll have 1, and then I'll have epsilon 11 plus epsilon 22 plus epsilon 11 times epsilon 22. And this will be times 1 plus epsilon 33.

And if I carry out that multiplication, that will be 1 plus-- and I'll get exactly these terms again-- epsilon 11 plus epsilon 22 plus epsilon 11 times epsilon 22. And then a term epsilon 33 plus epsilon 11 epsilon 33 plus epsilon 22 times epsilon 33. And then a third-order term, epsilon 11 times epsilon 22 times epsilon 33.

Now having gone through the painful process of expanding that, I will proceed to say that the epsilons are always going to be very small. Elastic strains are typically on the order of 10 to the minus 6. So a product of two of those strains is 10 to the minus 12. And a product of three of those terms is going to be on the order of 10 to the minus 18.

So this last term is going to be minuscule. And now I use a higher order term intentionally rather than a higher rank term. This is really a term of higher order. The same is true of all the peer-wise projects of this [INAUDIBLE].

So I now have left if I turn out these higher order terms to pasture, I'll have 1 plus epsilon 11 plus epsilon 22 plus epsilon 33. And the rest is negligible. And this will be the original volume V times 1 plus epsilon 11 plus epsilon 22 plus epsilon 33.

So delta V over V, if I subtract off V on the left, delta V over V then is simply going to be equal to epsilon 11 plus epsilon 22 plus epsilon 33. So this is indeed the fractional change of volume, and it's the trace of epsilon ij.

Now, physically, you wouldn't expect the volume to change if I change my reference axes because that's a scalar quantity. So I've shown by a hand-waving, backdoor argument that in fact the trace of a tensor does stay invariant for at least this particular tensor. But it's fairly straightforward to show that for any tensor aij the trace of the tensor is invariant when you change the coordinate system. And that's not hard to do. If you're clever, it takes about three lines. So I'll invite you to the exhilaration of discovering that for yourself on a problem set.

Any questions or comments? All right. Having defined strain as a symmetric secondrank tensor when we factor out rigid body rotation, we can view strain as a physical property.

And I think I tried to hoodwink you last time by saying this is a property of material. So therefore strain tensor has to also conform to all of the symmetry restrains that we have derived very exhaustively. And you said, no, no, no, no, that can't be; I don't believe that I can only give a uniform uniaxial deformation to an orthorhombic crystal.

And I say, yeah, but to get the deformation, you have to squeeze the crystal. And that is going to be linked to the deformation by the elastic constants, and they are physical properties. And that maybe makes you think a little bit. But actually even though operationally you impose a strain by imposing a stress or by doing something else to the crystal that results in a strain, you can nevertheless pick any stimulus you wish to achieve a desired state of strain.

So there is no symmetry constraint on the form of the strain tensor that can result. So the stain tensor then is not a property tensor. It is also a field tensor just like stress. So it can have any form we choose to create in it.

So we now have the potential of having stress as a field tensor. And we have strain as a field tensor. And within limits, we can create strains of these two field tensors of any form that we wish. And we can now regard these as things that we do to crystals and look at a whole range of properties that result when the generalized force is not a vector, a tensor of first rank, but the generalized force is a-- let's saya stress tensor. It's a generalized force which itself is not a first rank tensor. It's a second rank tensor. So we'll see a whole collection of interesting properties that fall into this category.

But first I'd like to look at one remaining second-rank tensor property, and that is thermal expansion. And this is a curious second-rank tensor property, and we couldn't discuss it until we had talked about strain. And let me introduce it by onedimensional example.

Let's suppose we have a rodlike specimen of length L. And let's suppose it is in equilibrium at some temperature T. And then we heat it up to some temperature T plus delta T.

In response to that particular change in temperature, the length of the rod will increase to a length L plus delta L. It expands. And we would find experimentally that delta L, first of all, is proportional to L. If you make the rod twice as long, the amount of expansion in an absolute sense is twice as large.

And secondly, provided you're well above very, very low temperatures, close to absolute zero, delta L will also be proportional to the change in temperature.

Thermal expansion is one of those properties which thermodynamically must go to zero as temperature goes to zero. So the thermal expansion coefficient that we've yet to define will be a function of temperature as we get down to very low temperatures on the order of a few degrees Kelvin.

So we can define then the linear thermal expansion coefficient for this rod as 1 over L, delta L over delta T. So this is something that will give us the fractional change of lengths. And what we can do now in general is to say that if we create a general strain, not a tensile strain, we have a general strain epsilon 11 plus epsilon 12, epsilon 13, and so on, has to be symmetric. So epsilon 21 is equal to epsilon 12.

We'll say that this tensor epsilon ij will be written in general for the three-dimensional case as a second-rank tensor aij times a scalar quantity delta T.

The strain is the field tensor. That's the response. The stimulus that creates this response is an incremental change in temperature. But as this is a second-rank tensor and this is a scalar, an array of coefficients in which we multiply every element of a tensor by a scalar is also a tensor.

So this is called the linear thermal expansion coefficient tensor. And it is a symmetric tensor by definition since a measure of true strain is by definition a symmetric tensor. So this is the linear thermal expansion coefficient tensor.

- **AUDIENCE:** Quick question.
- PROFESSOR: Yes.
- AUDIENCE: [INAUDIBLE] the temperature gradient [INAUDIBLE] and talk about the directionality say between here and here because of the temperature [INAUDIBLE]?
- **PROFESSOR:** Oh, yeah. Sure. Sure if you wanted to do that. That assumes that the thermal conductivity would be very small so that the temperature inside the body would not attempt to [INAUDIBLE]. Yeah. Yeah. In the same way that you could create strains that are in homogeneous as well.

We'll now for the first time start talking not in terms of abstractions but in terms of some real physical properties. What is the range of linear thermal expansion coefficient tensors? And unlike many physical properties, that's an easy one to answer, 10 to the minus 6 degree C per degree C.

Materials have a very, very small range linear thermal expansion coefficients. And let me give you some examples for real materials. They go up to maybe 10 to the minus 5 for a very soft weakly bonded materials. But the for metals-- and I'm giving you a single number now because these are averages for polycrystalline materials-- the value of A times 10 to the 6.

For lead, a low- melting metal, is 28, 2.8 times 10 to the minus 5. For copper, 18. For iron, 12. Four tungsten, a very refractory metal, 5. And for diamond, a very

strongly bonded materials, it's 0.89 times 10 minus 6.

If we look at compounds, again, the average linear thermal expansion coefficient times 10 to the 6 for polycrystalline material. For aluminum bromide, hardly a technology material of commerce, but in light of this because this has one of the largest linear thermal expansion coefficients of any material, very weakly bonded to compound.

For a more typical ionic compound, NaCL, 40 times 10 to the minus 6. For calcium fluoride, this has a bivalent cation in it, so the material is stronger, more strongly bonded, 20. For MgO, both a divalent cation and the divalent anion, as you would expect, the thermal expansion coefficient drop still more.

For Al2O3, a trivalent cation that goes down to 8.8, and that's really an average because this is a hexagonal material. And a second-rank property tensor for a hexagonal crystal has to have two equal diagonal elements and one independent diagonal element when you diagonalize the tensor.

Spinal, MgAl2O4 this is representative of all of the ferrites for example, 7.6. Silicon carbide, a very refractory covalent compound, 4.7.

For glasses, here's a surprise. You might think that a glass might have about the same linear expansion coefficient as the crystalline form of the same composition. But a sodium calcium silicon oxide glass, so called soda-lime silicate glass, is 9, fairly low. A borosilicate glass, like the Vicor that we love to make glass apparatus out of, 4.5. And one of the near record holder is fused silica, silicio glass, and here a measly value of 0.5.

So glasses have very low linear thermal expansion coefficients compared to crystallize materials that are predominantly ionic. And the reason lies in the nature of the structure. Something like MgO has ordered ions, and when you heat it up, it expands isotropically.

A glass is this random network of edge-shared polyhedra. So when you heat it up, yes, the dimensions of the polyhedra increase in proportion to the change of

temperature. But the framework because it's so meandering and open can buckle to accommodate the increased size of the tetrahedra that are in the linkage. So the result is the network buckles, but the overall microscopic thermal expansion is very, very slight even though the tetrahedra are changing dimensions in the same degree that they are in these crystalline inorganic nonmetallic materials.

Let me give you a handout not that it's up to date, but there was a very nice, convenient one-page article in the Journal of the American Ceramic Society a number of years ago that lists thermal expansion coefficients for low expansion oxides. So let me pass that around and let you take off for copy with that.

And that gives some examples of the value of this property for, again, for polycrystalline materials, which if you looked at a single crystal would show anisotropy. And here you'll find a few materials in the list near the top they're arranged in order of increasing linear thermal expansion, you'll find some that are just about zero when you have a polycrystalline form of the material. And you'll have some that have this very unusual behavior where the linear thermal expansion coefficient is actually negative. So let me pass this around for reference.

Now this may seem to be a curiosity that you can fine for a polycrystalline material for which the individual grains expand anisotropically a bulk linear thermal expansion coefficient of zero. Why should one care other than that being a curious result? Can anybody guess?

- AUDIENCE: Can you say that again?
- **PROFESSOR:** That these are materials which in a polycrystalline form with random grain orientation have a linear thermal expansion coefficient this is essentially zero?
- AUDIENCE: [INAUDIBLE]?
- **PROFESSOR:** Yes. Exactly. The materials out of which you build furnace linings and tanks for melting glass or smelting steel have to be made out of polycrystalline materials. You can't have a monolithic single crystal that's large enough to melt a significant amount of glass in for example.

And being polycrystalline, when the material expands, there is a great deal of stress between neighboring grains because they're randomly oriented. If the bulk microscopic thermal expansion coefficient is zero, that is going to be refractory that is very, very resistant to thermal shock. When you heat it up, you don't find intergranular cracking. So the materials that have essentially zero spatially average thermal expansion coefficients are very attractive for refractories.

You can pick up any issue of the Journal of the American Ceramics-- not the journal, but the Bulletin of the American Ceramic Society and you will find refractory companies hustling materials like Cordierite, which is a silicate material that on average has one positive thermal expansion coefficient, one negative thermal expansion coefficient. And the volume change of the individual grains is essentially zero. So that makes a dandy material for refractories.

Cordierite has another interesting property that is a really nice example of anisotropy of a physical property. If I ask you to rattle off some properties which you know to be very anisotropic, one of them that you wouldn't think of is color. Your tshirt is pink, so how can that be a function of direction? Well your t-shirt is not a single crystal.

And their single crystals which if you hold them up to light and pass through a plain polarized beam of light the crystal has a very different color for one direction of polarization then another. And these colors, interestingly, very often are strikingly different. They're crystals that are green in light polarized in one direction and red for light polarized in the opposite direction.

And there is in the old Icelandic sagas-- few people have heard of them. The Icelandic sagas which were written in about the year 500 are one of the early forms of Western literature that is really great, enduring world-class literature. In the sagas, there's one episode where Thor is sleeping and Olaf comes along and steals his sunstone. And Thor is upset he takes his battle as and cut Olaf's head in twain. And people puzzled for hundreds of years, what is sunstone. This doesn't compute in today's age. And finally a Norwegian archaeologist came up with a hypothesis that in Iceland there are remarkably large and remarkably transparent and perfect single crystals of Cordierite. And Cordierite is strikingly pleochroic. That's color that is a function of direction.

And what this archaeologist theorized is that the Vikings would take a sunstone when they went sailing on the North Sea, which is notoriously damp and overcast and gray, and your principal means of navigation was the sun. But when the sky was overcast, you couldn't see the sun. But the sun as it comes through the cloud gives you light that's very strongly polarized.

So the theory is that the Vikings would have very perfect crystals of transparent Cordierite, would hold them up to the sky, and turn them around until the Cordierite crystal lit up a bright, golden sunny yellow. What better name for the sunstone. You found the sun from the direction of polarization of the light scattered from the cloud when you've got the crystal oriented just so. In a different orientation, it would look murkier, look sort of a bluish purple for the other principal direction of the birefringence.

So there is putting crystal anisotropy hundreds of years ago to a very useful purpose to navigate on cloudy days. Unfortunately, the Vikings used it to sail down the British coast and sacked the next village. So it shows you that even the most simple of science can be put to application in war research. Anyway, won't go there anymore. So index of refraction and color can also be a strong function of direction

The numbers that I put on the blackboard suggest that the magnitude of thermal expansion coefficients are influenced very strongly by the strength of the interatomic bonding. And this shows up in a very, very striking way if you group together classes of comparable materials.

And if you plot the value of the linear thermal expansion coefficient in units of 10 to the minus 6 per degree C as a function of the melting point in degrees Kelvin, the numbers range from about 400 K for materials like sulfur up to about 3,700 for tungsten. And the variation is so beautiful it could make you cry. It goes as the inverse of the melting point.

And way up here are materials like for sulfur and lithium. And the way out here are materials like tungsten. And their relation is given by a equals 0.020 over the melting point in degrees Kelvin. So very strong correlation between melting point and linear expansion for simple elements.

If you do the same thing for compounds, you find a similar parabolic relation except it is offset. For oxides and halides, many of them with the rock salt structure, so they are isotropic. And again, if you plot here the melting point in degrees Kelvin, the numbers here range up to 60 times 10 to the minus 6. And again, a variation with 1 over T, but offset from the origin. And the curve here is that a equals 0.038 over T, the melting point T sub m in Kelvin, minus 7.0 times 10 to the minus 6.

Finally, let me finish with some data for single crystals that provide examples of and anisotropy. These are all hexagonal materials. And I will give you the-- not all hexagonal. I take that back. But they're all uniaxial crystals. The value of the thermal expansion coefficient along C and the thermal expansion coefficient that is parallel to C, so these are the elements that would be in the diagonal isothermal expansion tensor.

So for Al2O3, which is a hexagonal rhombohedral oxide, the two expansion coefficients are 8.39 and 9.0 times 10 to the minus 6, not terribly anisotropic. But the structure of alumina is a close-packed arrangement of oxygen with aluminum filling 2/3 of the available octahedral holes. So it's hexagonal only because of the sites that are filled in the array.

For TiO2, which is [INAUDIBLE] and therefore also uniaxial, 6.8 perpendicular to C; 8.3 parallel to C. For zirconium silicate, 3.7 and 6.2, almost a 2:1 difference. For the quartz form of silica, which is hexagonal, 14 perpendicular to C; 9 parallel to C.

For carbon, the graphite form, a layer structure-- you can almost guess how this is going to turn out. It's going to be humongous perpendicular to the lawyers and very

small within the plane of these tightly bonded hexagonal nets. And that is indeed the case, 1 perpendicular to C; 27 parallel to C. So there is an anisotropy of a factor of 27.

A few more. Aluminum titanate, perpendicular to C minus 2.6; parallel to C 11.5. A very well known example of anisotropy, extreme anisotropy, where one principal coefficient is positive and two are negative is the calcite forms calcium carbonate, minus 6 and 25.

For zinc metal, a hexagonal close-packed metal, surprising degree of anisotropy, 14 and 64. And for tellurium, which is a chain structure like selenium, 27 perpendicular to C and minus 1.6 in a direction parallel to C.

Even simple hexagonal close-packed metals can do strange things at low temperatures. For zinc, the expansion coefficients perpendicular to C and parallel to C as a function of temperature go at 300 degrees C from 13 and 64. At 150, the values have dropped to 8 and 65. At 60 degrees K perpendicular to C, the thermal expansion is negative and has not dropped terribly much of at all parallel to C. So this is a hexagonal close-packed structure lot. A lot of action and strange things going on in the plane at the close-packed layers, but not very much change in a direction perpendicular to the layers.

Let me raise one more issue. If we were to look at some of these strangely anisotropic materials which had negative thermal expansion coefficients in one direction and positive in another, what would the representation quadric look like?

Suppose we looked at calcite, for example, which has a large negative thermal expansion coefficient. And if we look at the thermal expansion quadric when the tensor was referred to the principal axes, parallel to C-- well, the thermal expansion tensor aij along its principal axes would be along A1 in a direction perpendicular to C, it would be for the data given here, minus 6, zero, zero, zero, minus 6, zero, zero, zero, And A33 is 25. So that's very, very anisotropic.

But what is this going to be? This is going to be a quadric that has the shape of an

hyperboloid of two sheets. So it's going to look like this. And there'll be an asymptote like this and then asymptote like this. Along the asymptote, the radius of the quadric is infinite. So therefore along these directions the strain is equal to zero. Strain goes as 1 over the radius squared.

In this range of directions here, the radius is imaginary. But remember that the strain is given by 1 over the radius squared. So this says that the strain is negative, so the material has contracted. And finally, in this range of directions where the radius is finite and positive, if the value of strain is 1 over radius squared, this says that the maximum deformation is along the direction of the C axis, and it's positive. The material expands along C; the minimum radius of the quadric corresponds to the maximum thermal expansion.

So let me close with a question. Along the asymptote of the quadric, the strain is zero. Does this mean that this direction in a crystal of calcite does not move, no deformation at all when you heat it up? I see faint shakes of the head. I don't know if that's just in awe of what's going on here or an opinion on the question. Do you think it'll be no strain?

AUDIENCE: It would be [INAUDIBLE].

**PROFESSOR:** Good answer. Let's remember a property of the representation quadric. The direction of what happens is normal to the surface of the quadric. The thing that is happening here is the displacement; ui is given by epsilon ij times U sub j. So when we look in this direction, the displacement, which would be normal to the surface of the quadric, gives us this as a displacement.

So along the asymptotes of the quadric, you can't say that there's no deformation, but that the deformation corresponds to pure rotation and not any fractional change of length.

In these directions, the length changes, but it is a decrease in length within the asymptotes. For those directions, the strain is an extension. And again, if you want to know the direction of the displacement, you find the normal to the surface of the

quadric in the direction of interest, and that's the direction in which the radius vector points.

All right. That's I think a good place to quit. I think I'll say a little bit more after the break about the atomistic reason for increases in interionic separations, which we can get some insight into from a simple model.

But before we disperse, I don't know if everybody got a copy of problem set 13. If anybody didn't, there's some extra copies up here. But I will with great pleasure pass out to you problems set number 14, which has served two purposes. One is to have you show for yourself that the trace of a second-rank tensor-- I called it second-order tensor-- second-rank tensor the sum of the diagonal elements is invariant for a change of reference axes for a general direction cosine scheme for the change of axes.

And then the other two questions are to give you some practice in diagonalizing a second-rank property tensor which is not in diagonal form. And I asked you to do this in two ways. One is by direct solution of the secular equation and finding the eigenvectors.

And then the third example, which is for a completely general tensor, to do this by the method of successive approximations. And you'll find after a couple of iterations you get fairly close to convergence.

So I shall pass this around. And again, I think there's something to be learned from that. Let's take our stretch then. I'm sure that lecture involved a lot of stress and strain. Ha, ha. Let's resume in 10 minutes. And we'll then move on to some additional higher rank tensor properties, which will be very, very interesting. Go for it.