PROFESSOR: We are thundering rapidly to the midpoint of the term. I think a week from this coming Thursday will be exactly halfway, and the halfway point is when I usually try, give or take a day, to change gears very abruptly and start looking at the symmetry of physical properties and tensors and actual discussion of physical properties that are anisotropic. So we'll be finishing up our discussion of symmetry fairly quickly. We still have, however, some major derivations to perform, and we'll get into one of these today.

Last time we had begun the process of deriving what are called the point groups as opposed to the plane groups. The plane groups were combinations of symmetry with a lattice that extended throughout a plane in space. A point group we've seen in the form of two-dimensional point groups.

We're now going to today derive the three-dimensional point groups. And, again, the name stems from the fact that these are clusters of symmetry about a common point so that at very least that one point in space stays put. So, hence, point groups-- these are symmetries about a point.

And to put some embellishing adjectives on here, these will be the three-dimensional crystallographic point groups. Because there are an infinite number of point groups, we're considering just those symmetries that can be combined with a lattice and therefore are permissible to crystals.

I'd like to point out in case you've not been making much use of Buerger's book that we actually are getting back to Buerger's treatment. We'll do some of the derivations over the next few days with a little bit more detail and with a slightly different procedure than Buerger. But the bases covered are the same.

So let me just point out where some of this material is in Buerger's book. Buerger does Euler's Construction, and he does this in a once over lightly. I think this is not the best part of the book. This is on pages 35 to 43. In particular, he sort of leaps ahead quickly and just looks for one angle between rotation axes and doesn't get the-- do specifically the ones that are 90 degrees and are not as interesting.

Some of the combination theorems are in Chapter 6, and there you'll find the statement that two reflections at an angle mu is equivalent to a net rotation of mu, except Buerger doesn't call them sigmas. He calls them m's. He uses the same symbol for individual operations and for the symmetry of them, and I think that's a little untidy. Also, the theorem that says that if we have a mirror plane that's perpendicular to a twofold rotation axis, that gives rise to inversion center at the point of intersection.

And then he launches into a rather condensed version of the derivation of the point groups on pages 59 to 68. Then, in Chapter 7, derives the two dimensional lattices or the plane nets. This is on page 69 to 83. We've done that differently and much more exhaustively by deriving the two-dimensional plane groups and the lattices are part of the plane groups, and we've gotten them automatically.

There is a place where in the derivation of the space lattices, he's a little bit incomplete and actually does something that's wrong A-ha-- I showed Buerger was wrong at one place in his book. But anyway, this is where the material that we're covering now is mentioned in Buerger's book.

Last time, we had hit a new surprise. We had asked if we take the basic rotational symmetries and add an inversion to something like three-- so, three is a subgroup, the operation of inversion is an extender. We found that there was a new operation that came up, and this was a rotoinversion operation. And then the resulting point group, which we called 3-bar-- the symbol itself, 3-bar, is a threefold rotoinversion.

And if we were not clever enough to invent a rotoinversion operation, we would have stumbled headlong over it in adding inversion as an extender to a threefold axis. And a rotoinversion axis is something that involves in general rotating through some angle alpha to get from a first object to a second object of the same handedness and then not yet putting it down, first inverting it through axis-- through a point on the axis-- to get a second object. I shouldn't call this second because this is not rotation with inversion simultaneously but a two step operation.

So we rotate from 1 to this virtual object also of same handedness and then before putting it down, we invert it to get number two, which is left handed. And the operation of getting there in two steps but in one repetition is the operation of rotoinversion.

That operation was one of the members of the group that results when you add inversion as an extender to 3. But, really, this was not something that was a new sort of symmetry element. It was an operation that came up, but we could regard the point down that we've labeled 3-bar as simply a threefold axis with an inversion center sitting on it.

But then we looked at another one. And by anticipation, I said we ought to look at these. And we looked at what happened when we took a fourfold rotoinversion operation where we would take the first object number one, rotate it through 90 degrees, and not yet put it down. We'd first invert it through a point on an axis, and we got one that was 90 degrees away but pointing down in of opposite handedness. If we repeated that operation several times, we found that we got two objects up above a plane normal to the rotation part of the operation and passing through the point, which we inverted. So there's one right handed one up here, a second right handed one up here, and then two down below, which were of opposite chirality, number 3 and 4.

And that is an entirely new beast. We have no way of describing the relation between these four objects other than saying rotate, don't put it down, first invert. Rotate, don't put it down, first invert again. So this is something entirely new. It's a two step operation. You cannot describe it any more simply than saying take two steps to do the repetition in the same sense that the glide plane that we discovered in the plane groups had a step of translation followed immediately by reflection, and that was a new sort of operation.

So here's another example of a two-step operation. The symbol for this point group is 4-bar, and the symbol for it-- if you want to indicate its locus, is, it's got a squareness to it because these objects as mutually are separated by 90 degrees, but it really has only a twofold symmetry, so the symmetry for a 4-bar axis. It's not really an axis at all. It's a 4-bar point, because only a point is left invariant. But the symbol for a 4-bar "axis" is this square with a little twofold axis inscribed in it.

Alright. We ought to really, then, step back and ask how many different rotoinversion axes there might be, and add these to our bags of tricks. And what I'm going to invite you to do is to examine this systematically on a problem set which I will pass around, along with several other problems for your consideration, as well.

And having stumbled onto that combination, another thing we might ask to broaden our bag of tricks still further is to say is there such a thing as a rotoreflection axis? And we called n-bar a rotoinversion. I wrote a reflection axis is indicated by an n with this little squiggle on top. Anyone who has studied Spanish realizes that the proper name for the squiggle is a tilde, T-I-L-D-E.

And this would be an operation where there's a locus in which we'll perform the reflection part of the operation, so this would be a 2 step operation that involves taking a first one and rotating it to a virtual object number two but not putting it down. Before putting it down, we will reflect in a planar locus. So this is number two, and it will be of opposite chirality. So that's another operation that involves rotation coupled as one part of a step that involves R, the second of our three translation free operations, namely reflection and inversion.

So are these something we should consider? What I've invited you to do is to draw out for n equals 1 to 8 the patterns produced by rotoinversion and the patterns created by rotoreflection, and then see if you regard these as new operations or whether they can be broken down into the simultaneous presence of more than one of our old friends such as 3-bar being a plain old threefold axis with an inversion sitting on it. The fact that I'm asking you take your time to do this suggests that yes, you are going to find some rotoinversion and rotoreflection axes, which are inherently 2 step operations and can't be decomposed.

What I'd like to do now, then, is to systematically look at the axial combinations. These are of the form n one, two, three, four, and six and the dihedral symmetries.

These are of the form n22, or just 32 in the case of the one with the threefold axis. And then the two cubic arrangements 23, twofold axis out of the face normal to a cube, threefold axes out of all of the body diagonals, and 432.

And what I'm going to do with you is to use these as worksheets to guide the logic of what we're doing, and we won't do every single one of them. I think once we do a few, the general principle is clear and the results there are before you. But what we'll take, then, is the axes n, the axes n22, and then the two cubic symmetries 23 and 432. Then, finally, we found 4-bar as a different rotation axis-like symmetry element, so I'll add that to the list.

Then consider what we can add to these symmetries as extenders, and these are an additional element that we can add to what is already a self-contained nice little group. We muck things up by introducing another operation, and then we'll have to take combinations of that operation with all the symmetry elements that are there in the parent subgroup and see what new symmetry elements arise.

The ground rules in these additions are fairly simple but nevertheless profound. The addition of the extender cannot create any new symmetry axes by its operation, and the reason for that should be quite clear. We obtained these combinations of rotation axes using Euler's principle, and that was thorough and orderly, systematic and complete. These are the only arrangements of crystallographic rotation axes that are possible.

So if we add an extender that creates, for example, a new twofold axis in n22, it's either going to be something that we already have in this list, and therefore not interesting, or something that just cannot constitute a group. We'll take combinations of operations and we will never find a closed finite set. So if we add a mirror operation, a reflection operation as an extender, the addition of the reflection operation sigma must be either perpendicular to the axis.

And what that's going to do is just flip the top part of the rotation axis and reflect it down to the bottom axis. Nothing new was created. And it could alternatively be parallel to the axis and passing through it. In that case, we've already seen the consequences of this addition in deriving the two-dimensional point groups, namely to 2mm, 3m, 4mm, and 6mm. No new axis is created.

One of the additions that is something we mentioned last time is that in the case of the dihedral groups where we have an n-fold axis and then twofold axes arranged in some fashion-- not in some arbitrary fashion. It's going to be 2 pi over n times 1/2, depending on the n-fold axis-- we could pass the mirror operation through the twofold axis. And that's what we'll call a vertical mirror plane. But when there's more than one axis present, we could also put the reflection operation diagonally in between the twofold axes.

So we're going to refer to this as a diagonal mirror. It's snaked in between the axes that are present. So, perpendicular reflection operation as an extender, one parallel to the axis and passing through it, or one that is diagonal passing in between them.

And finally, that exhausts what we can do with reflection, but we could add inversion. And if we're not going create new axes, and we're going to get a point group-- a finite set of objects-- the inversion center has to be on one of the single axis, namely these groups n, or at the point of intersection, if there's more than one.

So there's the job laid out for us. And we've got two theorems to aid us in quickly finding the new operations that arise-- in effect, taking a shortcut to establish the group multiplication table, and the two theorems are as follows. We saw that if you take a rotation operation A pi, that takes a first object that's right handed and rotates it to a second object that is also right handed. Then follow that by reflection in a mirror plane that is perpendicular to the axis. The net effect of going from 1 to number 3, which is left handed, is to create an inversion center at the point of intersection.

So there's a theorem that we can write down once and for all and say that A pi followed by reflection in a mirror plane that's perpendicular to axis A has, as a net effect, the operation of inversion. And if this is not a twofold axis, it's something like a fourfold axis or a sixfold axis, that contains the operation A pi as part of the operations contained in that axis, and that's going to create an inversion center as well. So for any evenfold axis, add a perpendicular mirror plane, and automatically the inversion center comes up.

And we can permute the order of these operations if we rotate by 180 degrees and then invert the net effect is reflection in the perpendicular mirror plane. So this is something that you permute around into three different combinations.

Does the order of the operation make a difference? And the answer is no, the order is not important. For example, rotating and then reflecting is the same as reflecting and then rotating it. It went up at the same point, number 3. Remember a fancy word for this when we define what's meant by a group, that these groups are going to be what's called Abelian, and an Abelian group is where any combination of operations a followed by b is identical to b followed by a.

I told you that great joke among mathematicians, what is purple and commutes? And the answer is an Abelian grape. Ha, ha, ha-- I think that's stupid, but it drives mathematicians into guffaws of laughter.

A second theorem, and this is one that we've already seen in two dimensions, is that if you take an operation A alpha, pass a reflection operation sigma 1 through it, that to the effect of that is going to be another mirror plane that is alpha over 2 away from the first. Notice I'm a little bit sloppy in talking about reflection operation and mirror plane because if a reflection operation is there, that's all I need to have to say that this is the locus of a symmetry point, a mirror plane.

So this is another one. Do you think that this an Abelian combination to say that A alpha followed by sigma 1 is equal to sigma 2. Is this Abelian?

AUDIENCE: No.

PROFESSOR: No, it's not. And how do you answer that? Not through any means more profound than just drawing it out and seeing what you get. Let's take 3n as an example.

So let's do the operation. In this order, do the rotation A 2 pi over 3 to go from this one up to this one, and then let's reflect across this horizontal mirror plane. So this is 1 right handed, this is 2 right handed reflect, here's number three and it's left handed. So that's A 2 pi over 3 followed by reflection in sigma 1.

And if we do the operations in reverse order, reflect in sigma 1 to go up to here, so this would be 2 prime and then rotate by 120 degrees. We would go to here to here, and that is not the same location as this one. So this is not equal to sigma 1 followed by A 2 pi over 3.

How can you tell when is the combination of operations is going to be Abelian and when is it not? It sounds rather clumsy to state it in words, but whenever the two symmetry operations leave each other unmoved, then you can permute the order. For example, in this combination here the rotation leaves the mirror plane unchanged. It just spins around in its own plane. The mirror plane leaves the rotation unchanged, it just reflects it end to end.

Here this rotation axis and these mirror planes obviously do not leave each other unchanged because the threefold axis rotates the mirror plane to two other new locations. So whenever that's the case, if the operations do not leave each other unchanged, the order makes a difference. So that's a useful thing to keep in mind.

Let's now turn to these sheets that I passed out, and you might want to unstaple them because they're designed to go side by side, and there are three pages. What I've done across the top of the pages is to give the different combinations of crystallographic rotation axes that are possible. So going from the first sheet across to the last, there's the rotation axes by themselves-- one, two, three, four, and six. Then there are the groups of the form n22, 222, 32, 422, 622, and then the two cubic combinations 23 and 432. So there are the 11 possible combination of crystallographic rotation axes, and stuck off by itself at the end is the oddball 4-bar.

For the axes by themselves, the diagonal mirror addition is not defined. The diagonal mirror position by definition snakes in between axes that are there in the axial combination. If there's only one axis, that's not defined. But you could add a horizontal mirror plane. A horizontal mirror planes adds a onefold axis. It's just a mirror plane. So that's called m in the international notation for mirror. And it's called

C sub S, C because it's a cyclic group, and the S stands for Spiegel. That's the Schoenflies notation.

If we add a-- take two and add a horizontal mirror plane-- this is the thing that we sketched out here-- this gives a pattern of four objects, two that are up above the mirror plane of one chirality, two down below the mirror plane of opposite chirality. These projections of the patterns are down along the rotation axis, and when you see a dot in a circle, the circle represents the point that is down and the dot is one that's up on top.

So there are two pairs of objects-- two right handed ones that are up and two left-handed ones that are down. And that, in international notation, is 2/m the twofold axis is over a mirror plane. So that's the way to make sense of the symbol and remember what it means. In the Schoenflies notation at C2. You've added a horizontal mirror plane as an extender.

Going down the remaining ones in that list because they're all very, very similar-- add a mirror plane to a threefold axis, the triangle is reflected down to a triangle of motifs of opposite chirality, so that's 3 over m. For sure, it's called 6-bar, but let's forget about that. The Schoenflies notation C3H, and similarly there's a 4 over m, a square above, and a square of opposite handedness below the mirror plane.

The horizontal mirror plane in all of these cases is shown as a bold line. They've added fainter vertical lines to give you an angular reference. Don't be confused by that in the Xerox copy-- the weight of the lines is not distinguished. So the only symmetry element in 4 over m, for example, should be shown by this solid bold circle that is in the plane of the paper. The two crossed lines are lighter and those are just as mutual orientations. And finally, there's another one of this form which is 6 over m.

On all of the evenfold additions-- that is, to say everything but 3m-- if you add that horizontal mirror plane, it's going to be perpendicular to an operation A pi. Therefore, inversion pops up as one of the operations in the group, and 2 over m, 4 over m, 6 over m, those regular polyhedra of objects-- can be inverted through the point of intersection of the axis in the mirror plane, and that leaves the set unchanged.

So if we go down to the bottom of the list and say, can we add inversion to these axial arrangements, in the case of 2, 4, and 6-- no, adding inversion doesn't give you anything new, because that's already there in the groups of the form CNH, or 2/m, 4/m, 6/m. Diagonal is not defined, so the only additional one that we could pick up by adding inversion is adding inversion to a threefold axis, and that's one we did the other day.

Adding inversion to a threefold axis gives us three that are up of one handedness, three that are down of opposite handedness, and the orientation of the triangle is skewed. That is called 3-bar. But it's just nothing more than a threefold axis with an inversion center sitting on it. Schoenflies' notation is C3i.

Then the only other additions to the single axes are adding the mirror plane in a vertical fashion passing through the axis, and these we've already seen in two dimensions so we don't have to spend much time on them. There's 2 mm, which is C2V. 3m-- all the mirror planes result upon adding a single mirror plane to the threefold axis-- 4 mm, and 6 mm. These are just three-dimensional extensions parallel to the axis of the symmetry that we already derived for a plane in space in the two-dimensional point groups.

So we're almost half done. It's easy, isn't it? Any questions at this point? So the only ones that are really new that we haven't seen already in two dimensions are the rotation axis perpendicular to the mirrored plane.

That brings us to roughly the middle of the second sheet, and the arrangement of axes 222 represents three mutually orthogonal twofold axes. If we add a horizontal mirror plane, that's going to put an inversion center at the point of intersection because that horizontal reflection is going to be sitting normal to a twofold axis. And then since the other twofold axes see an inversion center sitting on it, there's a mirror plane perpendicular to those other twofold axes. So adding again to go through that again, adding inversion to the point of intersection of the twofold axes creates a mirror plane perpendicular to each of those twofold axes. So it becomes 2/m 2/m 2/m-- each of the twofold axes acquires a different sort of mirror plane perpendicular to its orientation.

And 2/m 2/m 2/m, even though I love saying it, is kind of a mouthful. So that's very often abbreviated to just mmm, which really is a nice exclamation when you see what a lovely symmetry it is.

The pattern shown in the diagram to the left is just the pattern of 222 with the objects reflected up or reflected down, and you get a total of 8. That means that there are eight operations in the group, and you can add up quickly what they are. They are the three operations of rotating by pi, the operation of identity, then three mirror planes because the mirror planes all indistinct, and then the operation of inversion. So there are the eight operations that are present that generate the objects from a single one.

Add a horizontal mirror plane to 32 and you get a threefold axis perpendicular to the threefold axis, so you write that as 3m. That mirror plane now passes through the horizontal twofold axes, and a twofold axis with a mirror plane passing through it wants another mirror plane 90 degrees away, so a new mirror plane pops up passing through each of the twofold axes and perpendicular to the horizontal mirror plane.

Those mirror planes are in the same direction as the twofold axis. They're not perpendicular to it, and when symmetry elements are parallel to a common direction you write them out on the same line, so here's a case of a mixed metaphor. One mirror plane that's perpendicular to an axis, the threefold axis, so you write that as 3 over m. The other twofold axes have mirror points passing through them, so you write that as 2m and the threefold axes makes all of those 2m symmetries equivalent to one another.

Pattern, and this is true for all of these symmetries, is nothing more than the pattern of the subgroup repeated by the one operation that you've added as an extender . So if you look at the pattern of 32, object all of the same chirality, all apparently up and down, and add the horizontal mirror plane. The one that is up goes down, the one that's down goes up, and you get a set of four around each of the twofold axes.

422 behaves very similarly. The pattern is just the pattern of 422 reflected in a plane, so you have a set of 16 objects-- eight of them up of one chirality, those are the solid dots, if you will, and then another two, four, six, eight that are down of opposite chirality.

You have a mirror plane that you added as the horizontal mirror plane perpendicular to the fourfold axis. All of the horizontal twofold axes see a mirror plane passing through them. So they've got to have a mirror plane that's 90 degrees away, and those are the vertical mirror planes. Either the point is obvious now or you're not following me at all, so I'll simply say on the left-hand column of the final sheet, 622 with a horizontal mirror plane goes to 6/m, 2/m, 2/m, called D6h in Schoenflies.

I'll leave the cubic ones until last. They're not nearly as bad as they seem. But obviously they have a lot of symmetry all over the place, and we'll want to take a closer look at the patterns.

The next extender is a vertical mirror plane, and we've already got the groups of the form cnv, because they are just extensions in a third dimension of one set we've seen in two dimensions. If we try adding the vertical mirror plane, which is defined as passing through the principal axis of high symmetry and perpendicular to the twofold axes, we've already encountered those in every group except 32.

2/m, 2/m, 2/m already has the vertical mirror plane. The same is true of 3/mm2. The same is true of 4/m, 2/m, 2/m and 6/m, 2/m, 2/m. The vertical mirror plane comes in automatically when we add the horizontal mirror plane as the extender, So nothing new there at all.

And now we come to one that is interesting. This is the diagonal mirror plane. And I'll do this one slowly and then in some detail because it's another example of how we would trip over something if we were not clever enough to think of it.

Let me begin by drawing the three orthogonal axes of 222. So we have one object that's up and one object that's down. The twofold axis perpendicular to the board will take this one that's down and rotate it to here and take this one that's up and rotate it to here. So that is the pattern of 222.

We can snake a mirror plane in between the twofold axes, and a mirror plane passing through the vertical twofold axis has to be accompanied by one that's 90 degrees away, half the throw of the axis, which comes from our theorem that says A pi dot sigma vertical has to be equal to a sigma prime that's vertical and pi/2 away from the first.

In terms of the pattern, this second mirror plane that comes up is going to reflect this one across to here, it's going to reflect this one across to here, it's going to take this one and reflect it over to here, and take this one and reflect it to the right, as well. So now we've got a total of eight objects. This one is right handed, and this one is also right handed because we repeated it by rotation. Then we reflected that pair, so these two are left handed, and reflect it across the other diagonal mirror plane. They're back to right handed again, and these have to be left handed as well, so there's the pattern.

Is there an inversion center in this pattern? The answer is no, because there is no mirror plane that is perpendicular to a twofold axis, so this point group has no inversion in it. It's said to be acentric, without a inversion center.

Do we know how everything is related to everything else? We know how this one is related to this one by twofold rotation. We know how this one is related to this one, and that's by reflection across the mirror plane. How is the first one related to this one? How do you get it through 90 degrees and then pop it down and change the chirality?

AUDIENCE: [INAUDIBLE]?

PROFESSOR: You can't do that in one step. You've got to do just what I said in words. Rotate it 90 degrees, don't put it down yet, and reflect it down in a horizontal mirror plane. This horizontal mirror plane is not a symmetry element, it's part of the operation that's necessary to get us from this guy over to this guy of opposite chirality.

So this is an example a new type of operation, a 2 step operation. This is a 90-degree rotoreflection axis. And again, I feel compelled to put the axis in quotation marks, because really it's a pair of operations that leaves only a point unmoved, so it's really a point symmetry element.

There's another way of describing the same thing, and that would be rotoinversion. We could rotate by 90 degrees in the reverse sense, not yet put it down, and invert, and we get, again, the relation between-- what did I do? Rotate it here, yes-- rotate to here and then invert, and we got that one. So that's another way of defining the relation. A 90-degree rotoreflection is a minus 90-degree rotoinversion.

So you pays your money and you takes your choice, and what the groundbreakers who went before us did was to take rotoinversion. as the operation to survive. So here is, if we were not smart enough to invent it, our 4-bar rotoinversion axis.

So if we hadn't been clever enough-- and it would take a pretty clever, devious mind to invent a 2 step rotoinversion operation-- as soon as we added this sort of extender, a diagonal mirror plane to a group of the form n22, we would have found that there was a new sort of transformation that could not be described any more simply than to say take two steps to do it. Rotate 90 degrees and then invert. So we have to add the operation of A pi over 2-bar to our basic bag of tricks for generating patterns.

The group 32 is also a group to which we can add a diagonal mirror plane. And if you do that, again, the bold lines that are mirror planes in that group and the axes that are faint lines are easy to mix up. But if we examine that group without the confusing lines, here are the twofold axes.

And remember that they are all equivalent to one another by the threefold axis. So this axial group is the group 32. If we put down a mirror plane interleaved between the twofold axes, notice that each of those mirror is perpendicular to a twofold axis.

So we can write this as 2/m. 2/m means there's an inversion center at the intersection of the twofold axes with the mirror planes. And a inversion center sitting on a threefold axis makes it a 3-bar axis, so this group is called 3-bar 2/m.

And the pattern is what a twofold axis would do. These would be up-down-right ones. Reflect those and you get an up-down pair of left ones. Reflect again and you get an up-down pair of right-handed ones.

Reflect yet again, and you get an up-down pair of left-handed ones. Reflect still once more, and you get a down-up pair of right-handed ones. One more time, up-down left-handed ones. So you get a total of 2, 4, 6, 8, 10, 12 points.

So this is 3-bar 2/m in Schoenflies notation D3-- that's the symbol 32-- with a diagonal mirror plane added. You indicate that by a d in the subscript.

OK. I think that's probably a point where you're more than ready for a break. We've got very few yet to do.

One surprise is that if you add diagonal mirror planes to 422 and 622, you get perfectly lovely exquisite groups but they're not crystallographic, so we don't include them in our list. But we'll discuss them when we come back, and then take a look also at the cubic symmetries. Impossible to draw, but really not all that difficult to understand.

So let's stop at this point and take a stretch. People are stretching already. They need it. We'll resume in 10 minutes' time.