

PROFESSOR: Examine every possible means for combining the symmetry at once, but there is a seemingly paradoxical trick that we can yet pull. And let me indicate what is true here for 2mm. OK, so this is a twofold axis. Has mirror planes perpendicular to it.

If one of these is a mirror plane, the other one has to be a mirror plane as well. So there's no way we could make one a mirror plane and one a glide plane. OK, that requires a net that is exactly rectangular. So let's put in the twofold axis. And I add one to the corner of the cell.

As we well know we have to have twofold axes at all of these other locations. We want to put a mirror plane in the cell. We could pass it through the twofold axis, and that would be the same as P getting to P2mn back again. But why do we have to put the mirror plane through the twofold axis?

We have to have the twofold axis left unchanged when we add the mirror plane, because if we created a new twofold axis we create a new lattice and we'd wreck the lattice that we've constructed. But why, why, oh why couldn't we put the mirror plane in like this?

That's going to leave the twofold axis alone. It's going to leave the translations invariant. Why don't we do that? Why not? So here, trick number five, or wherever we are now. You can add the symmetry elements of a point group to a lattice, but not necessarily at the same point. You can interweave them.

But the constraint is that this addition must leave the axis invariant. Let's leave the twofold axis invariant. And vice versa. That is to say the mirror planes can't create new twofold axes, the twofold axis can't create new mirror planes. And let's make sure we understand the reason why.

If I've got a twofold axis here and a twofold axis here, I have to have a translation that's twice their separation. If this distance is δ , then I have to have a translation that's automatically created at twice δ . This is the same as saying

twofold axis with a translation gives you a twofold axis halfway along.

If I take the twofold axis, I get the translation back as a consequence. So what I'm saying is if we take the first twofold axis and repeat number one to number two, and then add another twofold axis which repeats number two to number three, you have a third one that is related by translation of twice delta.

So if you're going to interweave the symmetry elements, you have to leave the arrangement of symmetry elements at the same intervals, otherwise you would have created a translation or more that is incommensurate and incompatible with the other ones. So this is a third trick.

And we are going to need a new theorem. Let's first of all look at the possibilities. We can have the twofold axis interweave with a mirror plane. How about putting a glide plane in between the twofold axis. In other words, replace the mirror plane by a glide plane. This twofold axis hangs off here, reflect it across and slide it down to here, and you get this twofold axis here.

So that's also a self consistent compatible arrangement. How about a centered net? And that's more difficult. A centered net has twofold axis and all the places of C_2 , and then twofold axes at locations like one quarter, one quarter as well. We can't put a mirror plane in here.

That's not going to work, because it will generate a new twofold axis, and that changes the translation T_1 to half its value. We can't even put a glide plane here because this would slide down to here, reflect across, and that's not going to work. So the number of possibilities is limited, but we'll see that there's one other case as well for a fourfold axis.

OK, we need a new combination theorem that says if you have an operation a , π , and combine it with a reflection operation that's removed from it by some distance delta, what is the result? That general theorem has worked out for you on the notes, but I think what I'll do it in the interest of time is simply look at how this arrangement of symmetry elements would move things around.

And here I've taken the motif and hung it at the lattice point, and repeated it by the twofold axis. The mirror plane would take this and reflected it across to here, then take this one and reflect it across to here. And do the same thing down at the bottom of the cell. Let me now ask you what sort of plane has arisen that would be perpendicular to the mirror plane?

Could be interweaved or passed through the twofold axis. Anybody want to hazard an answer? OK. We have to have some sort of correspondence theorem that says if you've got a twofold axis, have one plane, you've got to have another plane 90 degrees away. Do I know how everything is related?

I know how this is related to this. I know this is related to this. That's by a reflection plane. I know how the twofold axes relate things. How is this pair related to this pair? And the answer is that the way they are related is by rights and lefts on here. This is right, this is right.

Reflection changes handedness to left, so I've got to have some way of getting from this pair to this pair that involves a change of handedness. And I see nobody is really jumping out of their seat, but there is a glide plane in here. Take this pair, slide it along by half of T_2 , and flip it across by reflection. And there is a glide plane right here.

And therefore of necessity there's a glide plane here. And this glide combined with the perpendicular translation will put a glide plane in here as well. And you look in your tables. This is plane group number seven. And this one has a twofold axis.

It has a primitive rectangular neck, so this is called $P2m$, and now the second plane at right angles is not an mirror plane, it's a glide plane. So this is called $P2mg$, or there's a shorthand form that leaves out the two. PMG is the shorthand symbol for it. So there's a new plane group that is based on orthogonal symmetry planes.

One a mirror, one a glide, and twofold axes. Let me ask you now what is the point group of a crystal that would have this relation between the atoms that are down in the guts of the crystal? What would be the point group of the crystal? We've got two

different point groups. We've got point M, we've got point group two.

What would be the point group of the crystal? And this is a new problem, a new concept. All of the plane groups that we looked at until this point, the symmetry elements on an atomic scale down inside the plane group were exactly the same as the point group that we had added to the lattice points.

But here we've got two different point groups that had been put into the lattice. So do we say that this crystal has symmetry two or symmetry M? Or just point group 2m. That won't work because if you have one mirror plane in a point group, you have to have another.

What this introduces is a very subtle point. The point group is inherently a macroscopic symmetry. When I say a crystal has a particular point group, what I mean is that if I look at the exterior faces of the crystal, I would say there's a twofold axis here.

And that's about all, if these spaces are pair wise distinct. I have a crystal that looks like this externally. I would say that that crystal has symmetry 2mm based on the faces. If I found that the etch pits on the surfaces were not quite the same on this face and this face, I would have to throw out the twofold axis, perhaps, which means this mirror plane would go out as well.

But also I would do things like look at the optical properties. I would measure the conductivity as a function of direction. I would look at the slip systems and yield stresses in different directions, and the assignment of a point group is an experimental observation that requires that you look at all possible properties.

Not only shape, but properties like conductivity and the magnetic susceptibility, and also perhaps the way the crystal diffracts X-Rays. That's another physical property. And then when you've done as many measurements as you choose to make, you say as far as I can tell, all behavior of this crystal is determined inconsistent with this particular point group.

But you're doing macroscopic things. You're doing macroscopic things. When you

talk about the plane group or space group, you're talking what goes on on a local atomistic scale in the unit cell. So what would be the point group of this crystal? It would have a twofold axis that would be manifested externally.

It would have a mirror plane, which makes the left hand side want to be the same as the right hand side. And if this were not a mirror plane here, but a glide plane, what you would say is that this face, if I reflect it and slide it along by one angstrom is going to become this face.

And this face here, if I reflect it and slide it back by one angstrom is going to become this face. But what will that do to the external shape? I just extend all these surfaces, and it's going to be exactly what I've drawn here. How would you distinguish a mirror plane from a glide plane?

If a crystal has a mirror plane, a face that sits here passes through some atoms. Those atoms are repeated by reflection. And being slit up by an amount τ which is on the scale of atomic dimensions, and that would give rise to a face here. But can you macroscopically assign any difference to the fact that two faces atomistically don't meet, but are separated by 3.2 angstroms?

No. What you see is one face like this, and one face inclined to it with a slope that is the same for either a glide plane or a mirror plane. So another truth about crystals is that macroscopically a glide line plane manifests itself as a mirror plane.

So paradoxically this crystal, which only has a twofold axis and one mirror plane down in its guts is going to look as though it has point group two in it, even though there is no sight, atomistically within this arrangement of atoms that has symmetry $2mm$.

AUDIENCE: I have a question.

PROFESSOR: Yeah? Sorry.

AUDIENCE: [INAUDIBLE]

PROFESSOR: That's a very good question. And actually, to answer it properly requires knowing something about diffraction. The symmetry of the diffraction pattern that you observed would look as though it had a mirror plane in it.

Which is to say if we put a beam of white radiation down along this direction of a crystal, imagine these things all extending out in a third dimension, that what we would see among the arrangement of spots is a twofold axis in the center of [INAUDIBLE] photograph we'd see a mirror plane running this way, and a mirror plane running this way.

So we would see spots on the [INAUDIBLE] pattern, which would look like this. So the glide plane would also behave it were a mirrored plane. And, maybe, if you think of what goes on with the fraction. If you ask yourself, if I brought in x-rays this way and diffracted them off a layer of atoms related by this glide plane, and then I can't do this actually to the crystal.

But, suppose I then inverted the direction of the incoming beam, and slitted along by five angstroms. Doesn't make any sense. The diffraction from these planes is going to look the same whether I bring in from one side or the other. So a glide plane, in diffraction symmetry, manifests itself as a mirror plane.

So how can you determine the presence of glide planes using diffraction? And you can. And the answer is, that the glide plane causes the intensity diffracted it from planes with certain indices to be identically zero. You've probably heard of these magical extinction rules they're called. And it says that if h plus k , plus three times L is two pi plus four, and the crystal is green, then you've got such and such, the reflection being absent.

Actually it is-- I'm getting distracted-- but, it turns out that glide planes affect just a sheet of reflections in reciprocal space. And the reason some reflections are absent is that that sheet of reflections corresponds to what the projection of the structure onto that plane would do.

And, if you project a structure that has a glide operation onto the plane of the glide

plane, the structure looks like the lattice translation is half as big. And, if that's the case, the diffraction spots are twice as widely separated. And it turns out that all of the reflections that have an index corresponding to the direction of tau are absent if that index is odd.

So, if you knew a little bit about it to begin with, that perhaps answers the question. So yes, you can determine the presence of glide planes. And later on, we'll talk about screw axes. You can determine their presence unambiguously, but you do that not the symmetry of the diffraction effects, but from systematic absences.

OK, another thing I suggested we could do is to put a glide plane in between the two-fold axes instead of a mirror plane. And this says that I have a pair of atoms repeated by the two-fold axis, the glide plane would take that pair, shift them down by half of the cell, and reflect them over. So this would be the pattern of objects.

This is not a lattice point, because if these are right handed, that's a right-handed pair, this is a left-handed pair. Now let me try you again. I know how these guys left and right to this glide plane are related. How about these ones that are up, to the ones that are down here in the middle of the cell?

There's got to be, from our correspondence principle, some plane going in this direction. Anybody want to hazard a guess at what it is? The answer to that question resoundingly is, no, not at this hour the afternoon, thank you. Yeah?

AUDIENCE: Left one.

PROFESSOR: Yeah, very good. Right ones have to go left ones, and they're going to go left and right about these planes here. And, if I combine this glide plane with t_2 , there has to be another glide plane in here. If I combine this glide plane with t_1 , there'll have to be another glide plane in here. OK, and that turns out to be plane group number eight, $P2gg$, not $P2mm$, both mirror planes have become glide.

All right, we're almost there. If you look at the hexagonal symmetries, there is just no way that you can interweave things, and an attempt is made in the notes that I handed out. You just cannot do it. But with $P4M$, $P4$, there is one final possibility.

And I'll just set that up and not carry them out.

OK, I'm going to put on just P4 with twofold axes in here. Now we have planes that go in orientations like this. And then there is another plane 45 degrees away that is a symmetry independent plane.

And the question now, I'll let you have a crack at it, is there any way in which I could take planes in the diagonal orientation or parallel to the cell edge and interweave them in between the rotation axes in such a fashion that the rotation axes were left invariant?

Again, conversely if they're not left invariant, we will have created new translations and wreck the lattice. So how could we slip in planes, either reflection or glide, and leave the axes invariant?

AUDIENCE: One quarter and three quarters?

PROFESSOR: Yeah. Do you want parallel to the cell edge?

AUDIENCE: Horizontal.

PROFESSOR: Horizontal? Yeah. This [INAUDIBLE] here has a fourfold axis up, a fourfold axis down, a fourfold axis up. Twofold axis down, twofold axis up, twofold axis down. So this would be a lovely location for a glide plane. So that's one.

From the fact that I am placing the same diagram on the board yet again suggests that there's another way. That's a perfectly good suggestion, and that's one of the things we would have to examine. Is there any other way I could put in a mirror plane or a glide plane and leave the axes invariant? Yeah?

AUDIENCE: [INAUDIBLE] 45 degrees?

PROFESSOR: 45 degrees. Through here. I don't want to do it through here because the fourfold axes sit on the same side, but you want to put it in like this? I don't think you can do that. Glide plane won't work here. How about a mirror plane?

There's no mirror plane that goes through these twofold axes for P4mm. What we had there were mirror planes here, and then going this way were glide planes. We've already got that. How about putting in a mirror plane like that? This goes into this. Halfway along there would have to be another mirror plane in that orientation.

Here's a twofold axis that demands that there has to be another one if it has a mirror plane passing through it. So there's another way. One final one, and I will not keep you guessing anymore, sneaking a peak at the answer. There is another way you could do it, and that would be to put the glide plane down diagonally through the cell.

That is put the glide plane here. That and take this twofold axis, reflect it across to here, and slide it down to here. So this twofold axis would be related to this one by glide. So those three possibilities are available for point group 4mm and a square net.

If you try them, and the simple way of doing it without any general theorem would be to draw in the way the symmetry elements repeat the motifs, and then ask what they require for the remaining symmetry elements. All of these give the final result. So they yield the same result.

You can develop a general theorem for what you obtain if you have an operation a , α combined with a plane, and make it a general plane, a glide plane that is removed from the axis by some distance δ . And that theorem is written out for you in the notes on the very first page.

You take a glide plane, and this is a specific example, a , π , if you have a glide plane that misses a twofold axis by some distance δ , then the effect of those two successive operations is a glide plane at 90 degrees to the first, and it's removed from the twofold axis by two δ . It has a glide component, excuse me, has a glide component two δ .

So there's a general theorem for the twofold rotation. The general theorem for a fourfold or a threefold rotation is considerably more complex to derive, but that's

contained for you in the notes as well. All right, we've come to the end of one other major part of our story of symmetry.

These are the periodic patterns in a two dimensional space. And these are then the 17 crystallographic plane groups. Crystallographic is rather redundant because they are groups that have [? in ?] translation and therefore these are the symmetries, the two dimensional symmetries that are suitable for the atomic arrangements in crystals.

As a little bonus, we also have, as a result, 17 of the three dimensional space groups. Just imagine each of these plane groups with a translation perpendicular to the plane of the plane group, and that would leave all the symmetry elements coincidence.

So you could pick a third translation at right angles to the blackboard of any arbitrary length, and you would have a three dimensional lattice that contain the symmetries of a plane group.

I think I mentioned earlier that the way you distinguish a plane group with a twofold axis in it from a space group with a twofold axis is that a lowercase letter for the lattice type implies plane group, and an uppercase symbol, capital P stands for a primitive lattice in a space group.

So something like lowercase p4mm is a plane group, capital P4mm is a space group with a third translation of arbitrary length at right angles to the plane group. We talked about plane groups and space groups, let's take a giant leap backwards. How about the one dimensional space groups?

Bet you were wondering about them all along and were afraid to ask. So what would be the story for one dimension? It's nontrivial. A one dimensional space group would be a lattice row. You have just one dimension to play with, and you can make that space periodic by translation. So there's one lattice type.

Just the lattice row. And what sort of symmetries could you place in that lattice? Now you have to define your ground rules. In our two dimensional symmetries, we

did not permit any operation which would pick the two dimensional space up and rotate it and flip it over and put it down again, because that is a transformation that takes you out of that space and pops you back into it.

And we will not in our discussion of three dimensional crystallography consider symmetries operations that take something, suck it up into a fourth dimension that we can't comprehend, and then all of a sudden pop it down in again, and suddenly it appears. I mean, that sounds bizarre. We wouldn't want to do that.

So for plane groups, we did not allow for any operation, say a twofold axis that would flip the object over and turn it upside down. But why not? I mean this, is mathematics. If it's your ballgame, you can make up the rules. So why couldn't we have a twofold axis in the plane or the plane group? It would have to leave the net invariant.

Well actually such entities do exist, and they have been derived. They're called the two sided plane groups. And if you want to allow that when you make up the game, you can actually do that if you wish to allow it. And also there could be a mirror plane in the plane of the space that would take the top side and relate it to the bottom side.

So you can do that, you can permit that. That's a different beast entirely, but you can allow that to be one of the transformations. So for our one dimensional space, I would submit to be consistent with what we've done and just finished in two dimensions.

And what we will do in three, we will not allow for any operation that will take the space and transform it into a second or third dimension, and then put it down again. So that being the case, the only operation that is possible is a mirror point that would reflect things left to right.

And let me illustrate now with some patterns. There's the lattice point. So let me put in some motifs. and I have to make a one dimensional motif, but to distinguish the ends I'll take a little artistic license and make one end of the motif a little fatter than

the other. Or alternatively, I could put a little one dimensional headlight on this thing that would shine just in one direction.

So here's a motif hung on every lattice point, and so this is no symmetry at all. So the symmetry part of the symbol would be one, and the lattice is primitive, and what do you think people use? We've used lowercase symbols, we used uppercase symbols, what's left? Yes?

AUDIENCE: Greek?

PROFESSOR: Good try. Gothic. Actually, what you do is you use a Gothic symbol with all these nice little shaded angular shapes. That's a Gothic P, isn't it? Yeah, that's a Gothic P. It is. It actually has thick and thin parts, curved parts [INAUDIBLE]. So that's P1.

What about another symmetry? Well if we have a mirror point in there, another possibility would be to have these motifs point alternately left and right. So I'll take some non one dimensional license and say that there would be mirror points at these locations.

Really nice symmetry, but actually it would be totally wasted on these poor denizens in a one dimensional world. Life would be dull and uninteresting because they couldn't see anything except the motif on either side of them, because everything is constrained to one dimension.

There's an old saying about sled dogs that says if you are not the lead dog, the scenery is not very interesting. And the same is true for these poor people in a one dimensional world. They could never see the elegance and beauty of that. But in any case, that would be Gothic P, no snickers, please, and that would be m. And those are the only two possibilities and a one dimensional space.

We have a couple minutes to go, but I think this is a good place to pause. And I'll give just a brief indication of coming attractions. We're now going to look at point groups in three dimensions, and a good way of entering this much more complex situation is to go back to something analogous to what we did for two dimensional symmetries.

And I'm going to first consider the arrangement of rotation axes in three dimensions. We do not have the constraint that all the rotation axes be perpendicular to the plane of a two dimensional space, being therefore more properly rotation points.

We've got three dimensions we have to view a rotation axis as extending infinitely in a direction, and there's no reason why we can't have another rotation axis at an angle to it. But you know that already. Everybody's heard about cubic crystals. Even if you think all crystals are either body centered cubic, primitive cubic, face centered cubic, or complex, four kinds of lattices.

But you've heard of cubic crystals, in the cubic crystals clearly the rotation axes are inclined to one another and arranged spacially. So we're going to ask the nontrivial question, how can we combine more than one rotation axis at a time about a common point in space?

And the constraint is going to be that a rotation about the first axis followed by a rotation about the second axis, wherever it is, is going to have to turn out to be something that is crystallographically compatible with a lattice. So that's the constraint. It's not an easy question.

And just to make you feel proud of yourself when we get through this, this uses a geometry that is due to one of the great mathematicians of all time, Leonhard Euler. Probably the most remarkable thing about Euler was that he's Swiss. How many world class scientists have you heard of that come from Switzerland?

Not very many, and the reason is it's such a small country, and if genius occurs as a certain fraction of the population, that's not going to happen very often in a country like Lichtenstein or Switzerland. Have you ever heard of anybody prominent in science who came from Lichtenstein?

No, probably not. OK, this then is going to be a nontrivial piece of mathematics for us, largely because it involves spherical trigonometry. Which I'm sure if you've ever heard of, you've forgotten, and probably don't see any utility in it. OK, with that exciting prospect in hand, I look forward to seeing you on Thursday.

