

PROFESSOR: My watch says five after 2:00, so why don't we get started? This is going to be a strange lecture. I'm expecting some wise guy in the back to say, all your lectures are rather peculiar! But I have a phone call from Europe coming in sometime around 2:15, 2:30. Somebody's coming to visit us next week, and we're going to set up a seminar.

So I don't know exactly when it's going to come in, but I have to be in my office. So what I will do is adjourn at quarter after, 20 past the hour. And then so I don't keep you here sitting restively wondering when I'm going to come back, we'll adjourn until 3 o'clock.

So you seem to have been taken longer and longer breaks during intermission. So I'll give you a full $\frac{3}{4}$ of an hour so you can get it out of your systems. And then, we'll take shorter breaks from here on in.

OK this is going to be pretty much our last lecture on symmetry. And we will begin, at least in half of the next class on Tuesday, to begin talking about physical properties, and in particular tensor properties. But I'd like to say a little bit about the derivation of space groups and take a look at how this information is tabulated for you by the kind folks who prepare the international tables.

And there are really very strict parallels between what we did in two dimensions. And that's the reason why we did it so thoroughly and systematically, except that there are three dimensions. And because we are taking 32 point groups and putting them into 14 lattices, there are a lot more combinations to be considered. And there are a lot more of them that are unique.

Also, they're a little bit more difficult to visualize and depict. So there are some new conventions in preparing a representation of three dimensional symmetries on a sheet of paper or page of a book which, of necessity, has to be two dimensional. So we'll go over some of those conventions.

But the main reason for going a little bit further is that there is another surprise lurking in there for us as soon as we begin to combine translation in three dimensions with a symmetry element. But let me go through in some detail the monoclinic space groups.

So we have at our disposal to decorate with symmetry elements two lattices. And they are a primitive monoclinic lattice with two translations, a and b , that define an oblique net, and a third translation, c , at right angles to that net. And then, either two choices for a double cell-- and I'll draw these in projection because I can do both of them with one diagram.

Either this is a and b and the extra lattice point is in the center of the cell halfway up from the base. This would be body centered. And that's represented by I for *innenzentriert*. In German, that's German for body centered. Or the alternative would be to pick a cell like this, in which case the extra lattice point gets caught in the center of one of the faces.

So this depiction here would be a side centered lattice. And it could have the extra lattice point in the middle of the face out of which b comes. And in that case, the symbol for the lattice is B . Or alternatively, without changing any of the nature of the specialness of the lattice, the extra lattice point could be in the middle of the face out of which a comes. And that would be an A lattice.

With the first, setting with the c axis unique, there is no c lattice because the oblique base of the cell would not give us anything new if it were centered. All right, so there are those two lattices. And then, there are three point groups.

And they were 2 , m , and then a combination of a twofold axis perpendicular to a mirror plane. So it looks as though in principle there are going to be 6 combinations. In point of fact, there are a lot more because of the surprise that we have in store for us.

Before proceeding further, though, let me ask rhetorically the question. Which lattice type would you pick as the standard one? And here, there's a major decision that

has to be made.

Should the labels on an axes give a unique symbol for the lattice? In other words, if you have the double cell for a monoclinic crystal, should you define the cell to make it body centered always, or to make it A centered or B centered always? Or should the labels be defined by the relative lengths of the axes?

So those are the two possibilities. And there's no right or wrong way. You pay your money and you make your choice. And on pragmatic grounds, this is the convention that's followed. And it's purely a pragmatic decision because lattice constants have been determined for literally tens of thousands of materials.

Sometimes, the lattice constants are known and the space group is not. But it would be terrible if the label that you applied to the axis could be C attached to the longest one, the shortest one, or the intermediate one. It would be impossible to calculate any database for lattice constants displayed by particular materials.

So there's all this-- this is what the decision was made. This is the decision that was made many years ago. And for monoclinic crystals, the labeling of the axes is determined by the c axis being the unique axis. That is, the axis that is along the twofold axis or perpendicular to the mirror plane.

And then, the labels b and c are defined by magnitude of b greater than the magnitude of a. So I inherently drew this in the proper fashion. So the labels are applied to monoclinic crystals in that fashion.

The price you pay for that is that the symbol for the lattice for a monoclinic crystal that has the double cell could either be A, B, or I depending on the relative lengths of the axes. If these were the two shortest, it would be a body centered lattice. On the other hand, if this and this were the shortest pair, then it would be a side centered lattice. So the symbol for the lattice type will bounce around depending on the dimensions of the translations.

So that's a complication in the space groups. In the two dimensional plane group, that issue never came up. We just took B greater than A for the rectangular and the

oblique nets. OK, so let me do quickly a couple of the monoclinic space groups. Let's take a twofold axis and put it into a primitive monoclinic net. And this is exactly the same as our plane group, P2, with the twofold axes extended parallel to the c translation.

So we would have twofold axes in all of these orientations. And that's simply P2, little p in two dimensions, with the twofold axes extended normal to the plane of the plane group. So this is p2. This is capital P2. And that is way we distinguish plane groups from space groups. So the symbol for the lattice is a capital symbol for the space groups.

So I didn't have to use any new combinations theorems. I simply say there's a third translation perpendicular to the net. So everything protrudes out of the plane group into a third dimension.

Let me now combine a twofold axis this a and this b and this c with a lattice that is not the primitive lattice but one of the double cells. And I'll take it, for convenience, to be the body centered flavor because it's easier to draw. And the operation that we've added to the lattice, if this is a combination of a twofold axis, is the symbol A pi.

And I know what happens if I combine A pi with a translation that is perpendicular to the rotation axis. I get a new rotation axis, B pi, that's halfway along the perpendicular part of the translation. And that's where all of these additional twofold axes came in.

But if a lattice is a body centered lattice, there is now a translation that goes up to the centered lattice point. So what's that going to be? What is T followed by A pi followed by T, where T is $\frac{1}{2}A + \frac{1}{2}B$? And that is a part that is perpendicular to the axis, and then a third component, c, which is parallel to the axis.

As with all these theorems, what you do is you draw it out once and for all and see what it turns out to be. So let's do that. Let's say that this is the translation that goes up to the point $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$. Here is the parallel part-- the perpendicular part, rather.

This is $1/2$ of A plus $1/2$ of B.

And then, we have a part that's parallel to the rotation operation, $A\pi$. And that is $1/2$ of c. So let's just do it. Here's my first object number one. It's right handed. I'll rotate 180 degrees to get a second one that's right handed.

And then, I will translate it up to here. And here sits the third one. It's also right handed. How do I get from one to three?

It's not really clear how I do that. And again, I'll draw it in projection because this is looking pretty messy in three dimensions. So here's my first one. I rotate 180 degrees to get a second one. The chirality is all the same. And then, I translate up to this point. So if this one is at z and this one is at z, this one here will sit at z plus $1/2$. And this is the third one. Anybody got any idea?

Can't be reflection. They're of the same chirality. It can't be translation because the orientation is different. Yes, sir?

AUDIENCE: Then it has to be some form of rotation.

PROFESSOR: Right, has to be. But how do we get the object up to a different elevation? Well, we've stumbled headlong over a new type of operation, just as we discovered the glide plane when we started putting mirror planes into a lattice in combination with translation. The only way I can get from the first to the third is to rotate 180 degrees about exactly the same point that I would have before, namely at $1/2$ of the part of the translation that is perpendicular to the operation.

But then before putting it down, I've got to take a second step. I've got to slide it up by a translation component that is parallel to the axis about which I've rotated. So to complete my theorem, $A\alpha$ followed by a translation that has a perpendicular part plus a parallel part is a new type of operation that involves rotating through 180 degrees. And this is located at $1/2$ of T perpendicular.

But it has a translation component which I'll call generically tau. And tau is equal to the parallel part of the translation. So if I separate out this new sort of operation in

all of its grandeur, what it does is it takes a first object, rotates us 180 degrees, does not yet put it down, first slides up by the amount τ . Doing the operation, again rotates it 180 degrees, doesn't yet put it down, slides it up by τ . Doing it again moves us to another one up here.

So what we've generated is a helical spiral of objects about the central axis about which we're rotating. And this is a new two step operation that's called a screw axis. There is a persistent rumor that it derives its name from the effect that it has on 360 quizzes. But that is just an ugly rumor. There's nothing to that at all. So this is a new two step operation that we'll call, in general, $A \alpha \tau$. And what it will do is to generate a screw like distribution of objects.

For those of you who have come in late, since you've been demonstrating a predilection towards longer and longer breaks, we're going to adjourn now and have a 40 minute break so you can get it out of your system. And we will resume at exactly 3 o'clock sharp. And we will launch into an elucidation of the nature of screw axes.

And again, for those of you who were not here at the very start of class, the reason is that I have a phone call that had to come in about this time of day and no other time. So rather than keep you shifting, wondering whether I'm coming back, we'll start at three when I should be done with my business. OK, so that's it. You missed all the important discussion of what's going to be on the next quiz, and nobody will tell you because they want to keep class average down. All right, so sorry for the longer than usual interlude, but we'll start again promptly at 3:00.