

PROFESSOR: OK. Before we get started, I'd like to deal with a small matter of some unpleasantness. The class is sort of like a football game. When there's two minutes to go, you shoot off a pistol. But when there are two meetings to go until we have the quiz, we shoot off a pistol to wake you up.

We're scheduled to have a quiz on October 6. And even though October seems far away when you're still in September, that is going to be a week from this coming Thursday. So if you have problems that you're working on, try to get them to me on Thursday, or just come slide them under my office door, if I'm not in. And I'll have them back for you on this coming Tuesday.

The way the material has played out is that we're really at a nice, convenient juncture between one chunk of interconnected material moving on to another. So I think the first quiz we'll confine to two-dimensional symmetry. And beginning in about two minutes flat, we'll begin to move into-- take the first small steps, at any rate, into three-dimensional symmetries, which will be much more complicated in which we will not deal with the exhaustiveness that we have been able to afford the luxury of in two dimensions.

Before I begin, let me-- does everybody remember their spherical trigonometry? Has anybody had spherical trigonometry? OK. What I will then do is give a short primer on some of the definitions and concepts in spherical trigonometry. And then we shall immediately use this to combine rotation axes in space. Pass those back.

AUDIENCE: I had a quick question on this.

PROFESSOR: Oh, sure, please.

AUDIENCE: With the limiting possible--

PROFESSOR: Yep.

AUDIENCE: --reflections and conditions, that does say they have to be figured out?

PROFESSOR: Actually, that was a good question and something that we are not going to use at all in the symmetry tables. Somebody asked what about this notation in the far right-hand edge of all of the plane groups-- conditions limiting possible reflections. One usually doesn't put a two-dimensional crystal in an x-ray beam fairly often, although I suppose a thin film actually is almost a two-dimensional crystal.

But you've probably all heard one way or another about the magic conditions relating the Miller indices of a plane that will require that the intensity diffracted from that set of planes is identically zero. And they're linear combinations of H, K, and L. And one of the rules is that if H plus K plus L is even or not, the intensity may be zero. These are rules for systematic absences. And the corresponding information is given for you here for these not terribly realistic real two-dimensional crystals.

So, for example, if you turn to number seven, P2MG, it says conditions limiting possible reflections for the general position. For H and K, there's no condition. For H zero, H has to be even, if the reflection is to have non-zero intensity. And for the last two, for the general reflections, H, K, if there's an atom occupying the position either zero, zero or the position zero, one half, then for the general planes with indices H, K, you will see intensity only if H is even, as well-- same as the condition above.

This is something that is not generally known that everybody knows-- that if the crystal is face-centered cubic, there is a pattern of absences. But there are additional absences if the atom is in a special position. And this can very often be used to advantage because you can single out certain classes of Miller indices for which one atom in the structure will not diffract or which another atom in the structure will not diffract. And that can be of great utility in unraveling a structure.

We'll see some examples of this in useful form when we deal with three-dimensional space groups. And the corresponding sheets for the three-dimensional symmetries will be handed out to you-- some of them, not all of them.

Let me take a little bit of time to remind you, if you've forgotten them, but to inform you of certain definitions and trigonometry in spherical geometry. Spherical trigonometry differs from plane geometry in that all of the action takes place on the

surface of a sphere. And it'd be nice if I had a spherical blackboard. Actually there is one in the x-ray laboratory that I can draw things right on that spherical surface. But this is a sphere.

We'll see directly that the radius of the sphere is not important. So we'll take that as a unity, which is a nice, even number. And as my dichotomy of the afternoon, if we pass a plane through that sphere, if the plane hits the sphere, it will intersect it in a circle. If the plane passes through the center of the sphere-- and we've assigned the radius of the sphere as unity, then this is a circle that's referred to a great circle. Sounds like a value judgment, but it's simply saying that's as large as the circle is going to get is when it passes through the center of the sphere., it would have unit radius, just as the sphere does.

So if you take any other plane which intersects the sphere but doesn't pass through the center, it's going to have a smaller radius. And this is something that's called a small circle.

OK, so if all of the action is going to take place on the surface of the sphere, and we have two points on the sphere, A and B, sitting on the surface of the sphere, how do we measure the separation of A and B? Well, if you think in terms of a normal three-dimensional person, you say, zonk, connect them by a line. And that's the distance between A and B. Now, you can't do that because all the action has to take place on the surface of the sphere.

People who deal with spherical trigonometry all the time are airplane pilots. And if your pilot is going to take you from New York-- where would you like to go? Paris? That sounds like a nice place. But if you're going to go from New York to Paris, you don't plow your way through the intervening earth. You follow something that is at a constant radius out from the center the Earth, at a height of 5,000 feet above the surface of the Earth, an additional radius.

So the way we'll define distance is to pass a great circle through A, B, pass a plane through A, B in the center of the sphere. And then we will define distance between A

and B as the smaller of the two angles subtended at the center of the sphere. So this is a more reasonable looking great circle. If this is point A and this is point B, pass a plane through the center of the sphere, O, and through A and through B. And then we'll measure the length of the arc AB in terms of the angle α subtended at the center of the sphere.

So it's a crazy notion. We're measuring distance in terms of an angle. And if that's an angle, we can take a trigonometric function of that angle, like sine or cosine. And that blows the mind that you can take trigonometric functions of a distance. But we can. We'll see it's going to be useful to us, too.

And then I emphasize again, we'll take this as the smaller distance. It'll be 360 degrees minus α . That would be the long way around from A to B.

All right. We've defined now how we will draw distances between two points.

Suppose I have three points on the surface of the sphere-- A, B, and C. I can pass a great circle through A and B. I know how to do that. I can pass a great circle through A and C. I know how to do that. And I can pass a great circle through B and C.

So now I have defined something that is referred to as a spherical triangle. We know how to measure the length of the spherical triangle. Let's call the arc opposite the point of intersection A as little a and the length of the arc opposite B as a distance and angles little b , and the distance from A to C as little c . But there's something in between these arcs that looks like an angle analogous to the angle in a planar triangle. And how can we define that?

Well, the arc AB is defined by a plane, a great circle. The arc AC is similarly defined by a plane that passes through a, c in the center of the sphere. And what we will define as the spherical angle BAC is the angle between the great circles that define the two different arcs. So if there's one great circle that defines the arc from A to B and another plane that defines the arc from A to C, we'll define as the spherical angle between those two arcs the angle between the planes that define the great circles. So we're going to call this angle in here between these two planes as angle BAC.

Another construct that is a useful one-- suppose I look at the plane that I've used to define a great circle and at the center of the sphere construct a line that is perpendicular to the great circle. And if I extend that line, sooner or later it's going to poke out through the surface of the sphere. And I will refer to this point as the pole of arc AB, or the pole of the great circle that we've used to define arc AB.

So the North Pole is actually the pole of the great circle that defines the equator. And clearly there are two poles. There's one in either direction. So there's a North Pole and a South Pole to this arc AB and to the great circle that defines it.

AUDIENCE: I have a question. Why couldn't you define the angle BAC as the angle [INAUDIBLE]?

PROFESSOR: You want to make a tangent here?

AUDIENCE: Yeah.

PROFESSOR: I don't know if that's really defined. In other words, if I'm saying I want a line that is tangent to the sphere, it doesn't fix its orientation.

AUDIENCE: In the plane of the great circle.

PROFESSOR: OK. In the plane of the great circle. Suppose you could if you wanted to. There are trigonometric qualities to defining the angle in the way that we have. And the construct really is not something confined to the surface of the sphere, and everything else that we are doing is. OK?

So it's sort of the non sequitur because we started out by saying that everything has to take place on the surface of the sphere. There's things that we would do in our three-dimensional world, like defining distances between points as the shortest straight line, that are ruled out in spherical trigonometry. And I think something similar could be levied at your proposal. And the answer is we just don't do it that way. That's the real answer.

OK. If I have not boggled your mind so far, let me go a bit further with another

useful construct. We can see how we can define a pole of a great circle or a pole on an arc that is a portion of a great circle. Let me take a spherical triangle, A, B, and C. And I've got three great circles now, which have formed those arcs that make up the sides of my triangle.

Let me now find the pole of arc CB. And that means we're going to go out 90 degrees to that plane through the center of the sphere. And that's going to define some point that I'll call A prime, that is the pole of arc BC.

And I'm going to do the same thing for the other arcs that are sides of my great circle of my spherical triangle. I'll find the pole of arc AC. And I'm going to label that point as B prime. And, finally, there'll be another pole that is the pole of arc AB. And that's going to define a point C prime. Now I've got three points, I can connect these together and make another spherical triangle.

AUDIENCE: How do you know to determine where the pole is?

PROFESSOR: If you think of it in three dimensions, I got three different arcs. And for each one of them I am drawing a perpendicular to the plane of that great circle and looking at the point where it emerges. OK. So now if there's another arc, there'll be another great circle coming around like this. And I look for the pole of it. And that would be another one of the corners.

This thing that I've constructed is bizarre. But it's given a special name. This is called the polar triangle.

And it has some useful properties. A property of the polar triangle is that the two triangles, A, B, and C, and A prime, B prime, and C prime are mutually polar. That is, if I use the spherical triangle ABC to define and locate the three points A prime, B prime, C prime-- now if I reverse the process and find the whole of arc A prime C prime, that turns out to be point B.

And if I take the arc of A prime B prime, that turns-- I'm sorry-- take the arc of B prime C prime, that turns out to be point A. So the two triangles are mutually polar. The polar triangle of the polar triangle is the triangle that we started with. Yeah?

AUDIENCE: I guess I missed that. So if you take B prime through C prime, then all of that is going--

PROFESSOR: Yeah, I'm saying that the pole of this arc, A prime C prime, is this point here. And the way I can show that is to say that we got B by looking at the pole-- I'm sorry-- I got C by looking at the pole of the arc AB. So B is 90 degrees away from C prime. I found point A prime by finding the pole of arc CB. So B is 90 degrees from any point on that arc. So it's 90 degrees away from A. So B is 90 degrees from A prime. B is 90 degrees C prime. And, therefore, it has to be the pole of that arc. Now that was a little too quick. That's written down in the notes. And that's why I wrote them out.

One final thing and then we can put circle trigonometry to one side, and this is something that is not all obvious. If we look at a spherical triangle and simultaneously the polar triangle-- so let's say this is ABC. And here is the polar triangle A prime, C prime, B prime.

It turns out that the spherical angle in one circle triangle and the length of the arc opposite it, namely this arc B prime C prime, are complementary-- supplementary, not complementary. And the way one would do that is to say that the measure of alpha is the length of this arc here. And this total side, B prime C prime, is equal to this arc plus this arc minus this length. And these two arcs are 90 degrees.

So let me do as I've done in the notes. Let me call this point P prime. And I'll call this point Q prime.

So my argument, it says that B prime is the pole of arc AC. And, therefore, B prime Q prime equals 90 degrees in length. And then I would say that C prime is the pole of arc AB. And, therefore, the distance C prime P prime is also exactly 90 degrees.

And that says that B prime Q prime plus C prime P prime-- if I add those two together, it has to be 180 degrees. But I can write B prime C prime as B prime P prime plus P prime Q prime plus Q prime C prime plus the side P prime Q prime.

And that's 180 degrees.

But these three things that I've lumped together here are exactly the same as the length of the spherical polar triangle A' . So what we've shown then is that A' plus α is equal to 180 degrees-- QED. So this angle plus the side of the polar triangle add up to 180 degrees. And that is not obvious at all.

One final relation-- and this I will simply hand to you on a platter. I'm not about to derive it. Sides and angles in planar geometry are related. And there's a particularly useful relation in plane geometry that's called the Law of Cosines. So this is in plane geometry.

And if you have a triangle that has sides a , b , c -- a general oblique triangle-- and it has angles A , B , and C , the Law of Cosines says that the side A is determined by c and b and the angle between them. And that's clear. If I specify this length, specify this length, specify that angle, things set up like a bowl of supercooled jello. And the triangle's completely specified. So a^2 in the Law of Cosines is b^2 plus c^2 minus $2bc$ times the cosine of angle A .

In a spherical triangle there is a similar sort of constraint. If we have a spherical triangle with sides a , b , and c , and spherical angles capital A , capital B , capital C , in the same way as specifying the spherical angle A and the lengths of the two sides c and b , specifies and fixes the spherical triangle entirely. This side must be determined by the length of side c , the length of side b , and the angle between them.

And that, since everything is in terms of angles, is something that doesn't involve squares. It involves totally trigonometric expressions. And it turns out the cosine of this missing side a is given by the product of the cosines of the two other sides.

So as I said, you can take a trigonometric function of a length, which sounds like an oxymoron. And it's the product of the cosines of the two known sides and times the sine of b sine of c times the cosine of the spherical angle A . And that is also called the Law of Cosines. And this is the corresponding case in spherical geometry.

OK. So there's some machinery-- yes, sir?

AUDIENCE: What's the difference between the sines of lowercase a and--

PROFESSOR: OK, the angles are the capital letters. This would be the angle between the great circles that defines the--

AUDIENCE: Since the radius is one, there's no difference between the angles and the--
[INAUDIBLE]?

PROFESSOR: No. This angle is something, for example, we can choose. And depending on how long we want this arc to be, we can put the arc BC anywhere we like.

AUDIENCE: Does that mean your radius [INAUDIBLE]?

PROFESSOR: No. This would be, say, two points of the spherical triangle. Now we can pick any third point on the surface of the sphere, connect that with great circles, and here is a spherical triangle. OK? So I see. I think I see what your problem is.

Here are the two planes. We define the angle of the spherical triangle as the angle subtended by the great circle. So this is the definition of A.

But now the other two points on the spherical triangle can be any point on these great circles. So this can be point B, and this can be point C. And my spherical triangle can be something like this. So the arc that defines the spherical angle A is a value that is independent from the length of the arc AC. That would be what is subtended at the center of the sphere.

I'm going to have time just to set the stage for how we're going to use these relations. And the problem that I would like to raise and then apply spherical trigonometry to is the question if I go into three-dimensional space, there is no longer any requirement that rotation axes be all parallel to the same direction. In two dimensions the rotation points were really-- could be viewed as axes that were always perpendicular to the plane of the blackboard, the plane of the plane group.

But now when I'm dealing with three-dimensional spaces, this could be the

operation A_α . And there is no reason whatsoever why we should not try to combine with this first operation a second rotation B_β -- a rotation through an angle β about this axis B and a rotation of angle α through this axis A. If we're going to come up with a crystallographic combination, the angles α and β have to be restricted to the angular rotations of either a onefold, a twofold, a threefold, a fourfold, or a sixfold axis, if the combination is going to be crystallographic. Yes, sir?

AUDIENCE: You're just rotating around those lines?

PROFESSOR: I'm rotating around those lines, yeah. So I'm saying that we're going to rotate an angle α about axis A.

And now what I'm going to raise as a rhetorical question-- what is the rotation A_α followed by B_β ? So I rotate through the angle α about A. So here's my first motif, right-handed. Then I'll rotate α degrees. And this here's number two. And that will stay right-handed.

Now, I will place on axis B the two constraints. These have to be crystallographic rotation angles, namely 360, 180, 120, 90, or 60. And I'll also, since I would like to obtain point group symmetries initially, I will require that axis A and axis B intersect at some point. And one of the variables in the combination will be this angle between the two rotation axes.

So let's complete our combination of operations. I'll rotate from one to two by A_α . If the first one is right-handed, the second motif is right-handed, as well. And then I will rotate β degrees about B. And here will sit number three. And it will stay right-handed.

So, again, the \$64 question that we raise periodically-- what operation is the net effect of two successive rotations about a point of intersection?

[INTERPOSING VOICES]

PROFESSOR: Lots of opinions. Let's sort them out. I heard translation. Well, let's put down what it

could be. We know that only translation and rotation leaves the chirality of the motif unchanged. So it's got to be one or the other.

AUDIENCE: Since there's no reason for the general orientation of the two to say it has to be rotation around the third axis, so the question is what angle and what--

PROFESSOR: OK. That is exactly the problem. Now that we know the problem, we can go home early because we know what we're going to do next time. Well, let me expand a little bit.

It can't be translation because clearly the separation of number one and number three depend on exactly where I place the first one. If I place it a little further out from A, then it's going to rotate to here. And then B is going to swing it off to some different location. So it can't be translation.

And I don't think these guys, if I rotate this way and then I rotate this way, are going to be parallel to one another. I doubt that very much. So it's got to be a rotation. So without knowing how to find it, let's say that we can get from number one to number three in one shot through rotation of an angle γ about some third axis, C. So the answer, in general, without being specific, is A α followed B β has got to be equal to a third rotation, C, about a direction that has the same point of intersection with the first two axes.

Now we've got some really, really tough constraints. Alpha is restricted to one of five values. Beta is restricted to one of five values. The third rotation, gamma, jolly well better be a crystallographic rotation and not something that is not a sub-multiple of 2π . And even if it is a sub-multiple of 2π , it has to be either 0 degrees, 120, so on. It has to be one of the crystallographic rotation angles.

So what sort of relation can we get that would give us, first, the value of gamma in terms of alpha, beta, and the angle at which we combine them? So taking A and B as the five crystallographic rotation axes two at a time, we want to put them together, if we can, such that the angle makes the third rotation axis also be crystallographic. And then we would have to find its location.

It looks like an impossible constraint . It looks absolutely impossible to do. We've got to put this first in quantitative form and then simply put in the values for alpha, beta, and gamma and find the angle that they have to be combined on to make this, if possible, be one of the crystallographics sub-multiples.

That is not an easy problem to formulate. And, as I said a couple of times ago, the geometry that is the basis of this derivation was originally proposed by Euler. And it's known as Euler's Construction.

I will have for you next time my own set of notes on this. We have finished with two-dimensional crystallography. So we are back to Buerger's book again. We had that little interlude.

Buerger deals with Euler's Construction. But I don't think he's at his best in this particular section. So we'll take it a little more slowly. And next time we'll get around to deriving Euler's Construction.