**PROFESSOR:** All right. The end of this lecture generated so much excitement that we've continued on into the start of the next segment. So I think we'd better begin. What I told you, as several people were clever enough to observe, that the number of planes between the origin and intercept plane is equal to A times B times C, where the intercept is A T1 out plus B T2 out equals C T3 out.

That is true only if the numbers A, B, and C are mutually prime. If it's something like 4, 2, 1, you won't get that number of planes. You'll get a submultiple. And the reason for that is that some of the planes, when you generate them by these three different translations in different directions, some of them are mapped on top of existing planes.

And I'm not going to attempt to prove this, but let me just tell you the result, that if A and B contain some common factor, p, and B and C contain some common factor, q, and in the worst possible case, A and C contains some common factor, r, then the number of intervals is equal to A times B times C divided by p times q times r. And probably the best way to show that is let you show, on a problem set in the very near future, to actually map out the planes in the two-dimensional situation, for a and b that are mutually prime, and then do the same thing for a and b that contain some common factor. So this is the so-called Miller indices, the Miller-Bravais indices, and everybody hears about them, but it is not at all clear why one takes this very indirect and non-intuitive way of defining the orientation of a plane.

And the reason for this, ultimately, is that in x-ray diffraction, you want to integrate up the scattering of all atoms in a crystal. So you want to integrate over a plane that contains the atoms, and this locus has a convenient form only if you choose these indices to find the orientation of the plane. And what comes out of this, as I said to a couple of people during intermission, is that the amplitude of the scattered wave has some summation over all of the atoms.

And in that phase of that ray, that is e to the plus 2 pi i, hx plus ky plus lz. Very, very

simple form. And it has that form only because the locus, the way this plane is defined was done very, very carefully. So it's something beyond just simple geometry that forms a reason for it.

Let me say a couple more things in general about the Miller-Bravais indices. They are very, very intuitive, counter-intuitive. Let's suppose that this is a, and this is b, and this is c. And I put down here, again, the equations of the entire set of planes in the stack.

And let's look at the first planes and ask what the intercepts are. The intercepts on x, y, and z are going to be 1 over h on x, 1 over k on y, and 1 over I times z. So the first plane from the origin is going to be 1 over h of the a translation, 1 over k of the b translation, and 1 over I of the c translation. So this gives us one way of determining, given a particular rational plane, show it relative to the three translations.

From the first plane from the origin, h is going to be 1 over the intercept on T1. I'll call it a, which is what we usually do. k is going to be 1 over the intercept on b, and I is going to be 1 over the intercept on c for the first plane from the origin. So if you have a drawing of the set of planes relative to the translation, such as the one that I obliterated from just a moment ago, reciprocals of the intercepts of the first plane from the origin give you h, k, and I very easily.

The thing that is counter-intuitive is that, if you look out of context at the three indices, h, k, and I, you have the feeling that as I gets larger, the intercept of the plane on c should gradually creep up from here, to here, to here, and so on, as I gets larger. Actually, the reverse is true. As I increases, the intercept on c gets smaller and smaller and smaller and smaller, until finally, when I is infinity, the intercept is 0. So it's counter-intuitive. The intercept on the axis gets larger as the Miller index gets larger.

Let me give you a proprietary Uncle Bernie's secret method for determining Miller indices without stress and strain. This works every time. Find the intercepts of any plane. And we know from these equations what those are going to be. For the nth plane, the intercepts are going to be n over h, n over k on b, and n over l on c.

Take the reciprocals. And the reciprocals are going to be h over n, k over n, and I over n. And then find whatever integer, n, you must multiply those reciprocals by in order to convert them to mutually prime intercepts, and you've got the Miller indices in a no-brainer, automatic fashion. Another bit of jargon.

We will also use the basis vectors to define locations and to define directions in a lattice. To distinguish three integers that indicate a plane, and you all know this from previous experience, the parentheses says plane, an individual plane. There are other times when you would like to use the indices of one representative plane to indicate the entire set of planes that are related by the symmetry of the crystal.

So let me give one specific example. Suppose we had a cubic crystal, where these are the three translations that form the edge of the unit cell. And let's say that this is a1, this is a2, and this is a3. I'm using a1, a2, and a3, not a, b, and c. But let's not go there.

OK, these are lattice points. And if I look at this plane that's perpendicular to a1 and cuts it at one lattice point, I, this would be the 1, 0, 0 plane. And I would indicate that that is an individual plane that we're talking about. But if this crystal is cubic, all six faces of the set, 1, 0, 0; 0, 1, 0; 0, 0, 1; and then the plane that's in the opposite direction, minus 1, 0, 0; 0, minus 1, 0; and 0, 0, minus 1. These six planes define the surfaces of the cube.

So there are times, since these are equivalent to planes and will have the same properties, the same hardness, the same [? edge ?] bits and everything else, there are times when we may want to refer to the entire symmetrical set. And we do that. We call that set a form. It is a symmetry-related set.

And you can pick any one you like. Generally, you pick one with simple indices, like the one that is perpendicular to the translation a. And then you indicate by braces, which is the symbol for set. This means the set 1, 0, 0, and that would correspond to all six of these faces. The number, if you do this in reverse, and I'm going to give you the indices, what are the separate faces? That depends on the symmetry.

So to give you an example, if I have a unit cell that has three orthogonal translations, and this is a, and this is b, and this is c, so that there is no cubic symmetry to it. This face, which would be 1, 0, 0, and the one that cuts the axes at minus a, minus 1, 0 0, those are going to be the only faces with a single 1 and a pair of 0's which are equivalent by symmetry. So in this case, for this brick shaped unit cell, 1, 0, 0 would mean this pair of two faces, rather than six.

So to go from a representative face to the set of planes, you have to know the symmetry. If you can write the planes on the basis of symmetry, take one representative and let that be the form. So it leads one to observe that crystals undergoing plastic deformation have bad form. Yeah?

- **AUDIENCE:** Is that different from when you talk about a direction?
- **PROFESSOR:** Yes, yes. You will see in just a moment that we use the same system of three integers, but in order to distinguish which one he's talking about when one's thinking about integers with a different set of numbers.

Again, if we use the lattice as the basis of a coordinate system, another thing we might want to specify is the orientation of a rational direction. And let me go to a two-dimensional case. Assume that c goes straight up. Directions of easy plastic deformation will very often involve integral number of translations.

For example, this direction here is obtained by going one translation in the a direction plus one translation in the b direction. So we could use the pair of integers 1, 1, and if we are normal to see we'd use a 0 for the third integer. But how are we going to tell whether we're talking about a direction or a plane? And the way one does that is to use square braces to indicate one particular direction.

You may want to also indicate the location of a particular atom within the unit cell. In order to do that, one could really use the location of a vector, the components of a vector, xa plus yb plus zc, the vector from the origin to that atom as coefficients which correspond to the atom location. So if that is the case, the numbers are

usually not integers.

And one simply uses the three integers in an unadorned fashion. So the lattice translations give you the basis of a coordinate system, and we use those to specify features, rational or not, of planes and directions and coordinates. OK, any questions here?

OK, we are next going to take the first small step in a process of synthesis. We have found that there are, in two dimensions, five distinct kinds of lattices. The oblique, the rectangular, the centric rectangular, the square, and the hexagonal. Five kinds of lattices.

We've shown, to this point, that each of these lattices can accommodate a certain rotational symmetry. 1 or 2 here. m and m for the rectangular and centric rectangular. 4, the fourfold axis for a square. 3 or 6 for the hexagonal lattice.

So what I would like to do next, after we make a brief direct diversion, is to combine with each of these nets one of the two symmetries which can be accommodated in that net. And what we will have determined then are the patterns' lattice and symmetry, which can exist in two dimensions. The sort of things we look at actually, like the pattern of square tiles on the floor, or the two-dimensional pattern that is on a fabric design. So we'll derive those exhaustively.

The thing that results is something that is called a plane group. And I'm going to take this through in detail because there are not that many combinations that can be made. And the number is enough to count on your fingers and toes. You've got to use both, so they're a fair number, but not a staggering number.

If we were to do this exercise in three dimensions, there would be 230 distinct combinations. And that's too much for anybody to go through. I know of very few people who work professionally in this area who've actually sat down and derived every single one. If you know the principles of the derivation and know how you could go about doing it if you were forced to, that's sufficient.

The results are tabulated in an admirable compilation. We mentioned that at the

beginning. This is the International Tables for X-ray Crystallography, Volume 1. So what we should end up with is a way for you to go to this reference data and know how to interpret it and make use of it.

But this is a nice microcosm. There are not many plane groups, and to do this exhaustively, will let us see the sort of reasoning that goes into it. I have to tell you that this is not in Buerger's book. We're going to do two-dimensional crystallography first, and then extend it in a third direction.

In fact, I know of no book that does this. And so you're going to get a unique, handwritten document by none other than yours truly that will do this in detail every step of the way. And I don't know of any other place where this is done.

Now, what is the origin of this name? Plane, well, these are symmetries confined to a plane. And then there's this mysterious term, group. And the corresponding thing in 3D is something called a space group.

This is a language derived from a branch of mathematics that is called group theory, and it is exactly the language that describes things that we've mentioned conversationally, such as if you take two transformations and perform them in succession, they're going to give you a third that has to be present. If you've got two present, there must be a third. We talk about symmetries being self consistent.

If you have a rotation operation that is not an integral submultiple of 2 pi, it's not going to be self consistent because you go around, and around, and around, and you will never come exactly full circle. So group theory is a branch of mathematics that deals with concepts of this sort. So it's not very hard to develop, and it gives its ideas to the notation that is used in crystallography. So let me say a few words about group theory.

What is a group? A group is a set of elements-- And what are elements? Elements are things-- For which a law of combination is defined. And the nature of the elements can be very, very different things. They could be numbers. They could be complex numbers, and the law of combination here might be multiplication.

They could be matrices, for which the law of combination is defined as matrix multiplication. Or they could be pots of different color paint, for which the law of combination is defined as mixing the two colors 50-50. I don't know any practical application of that sort of group, but nevertheless, it follows the definition, a set of things for which a law of combination is defined. And in addition, which satisfies three so-called group postulates.

And the group postulates are the combination of any two elements is also a member of the group. The second group postulate is that the identity-- I'm going to call it just identity-- and let me define, identity is doing nothing-- Is also a member of the group. And if we define the identity operation as I, this means that for every element, I followed by a or a followed by I, is the same as a by itself. If the law of multiplication were just arithmetic multiplication, then number 1 would be the identity operation because 1 times any number gives you the number. Any number times 1 gives you the same number back again.

And the third postulate is that, for every element, an inverse exists-- let's call the elements a and a minus 1-- such that a followed by a minus 1 is equal to the identity operation, and the inverse element followed by the original element, a, is also the identity operation. So if the law of combination were defined as multiplication, you would have to find, for every number, another number, which multiplied by it, gives you the number 1.

OK, let me now illustrate with a couple of simple examples. Let's consider the set of numbers 1, n minus 1. The number of elements in the group is said to be the rank of the group, or some people like to use the term order. And I don't like that term because second order or fourth order is a term applied to quantities which are not terribly important.

So we expand this except for higher order terms, which are negligible. And I don't like that connotation. So I will not use order, although it's sometimes used to talk about the rank of a group. The rank or order of the group is simply the number of elements contained in a set.

So let's show that the numbers 1 and minus 1 constitute a group of rank two. Is the combination of any pair of elements also a member of the group? Well, to do this, it's convenient to set up an array called the group multiplication table. And what you do is you simply put the elements of the group along a row. And in this case, it's 1 and minus 1.

And then you put the same elements along a column, and then you combine them. 1 times 1 is 1. Minus 1 times 1 is minus 1. 1 times minus 1 is minus 1. Minus 1 times minus 1 is plus 1. Sometimes, as I'm giving this part of the lecture, somebody passes down the hallway, and they hear 1 times 1 is 1. 1 times minus 1-- and they go in reverse to see what in the world could be going on in this high-powered mathematical lecture. That's why I close the door.

OK, so any combination of elements is also a member of the group. Is the identity operation present? Yes because minus 1 times plus 1 or plus 1 times minus 1 gives you the same element back again. So for every element in the group, the combination of any two elements is present. For each operation, we've shown that an inverse exists and for every element there's an identity operation, and the inverse exists.

So the pair of numbers, not terribly exciting, 1 and minus 1 where the law of combination is defined is a group of rank 2. I'll give you another example. I won't bother to carry out all the terms, but the numbers 1, minus 1, i, and minus i, where i is equal to the square root of minus 1, and where the law of combination is defined as multiplication, constitute a group of rank 4.

With this simple introduction, I think one can see that symmetry transformations can be regarded as operations that are elements in a group. And let me give you a simple example. Let's look at a combination. We still haven't considered the mindboggling possibility of having more than one symmetry element present in a space at the same time. But let's suppose we have two mirror planes that are completely orthogonal, and see what sort of pattern they would generate. Here's a first motif. If I call this mirror plane m1, and this mirror plane m2. m1 is going to take this object and reflect it across to here. m2 will take this object and reflect it down to here. Take this one, and reflect it down to here.

And now I know how this is related to this, how this is related to this, how this is related to this. But this one and this one are exactly the same thing. And those two objects are not related by reflection. If this is a right-handed one, this is a left-handed one, and this is a right-handed one.

So if something relates these two, it has to be something that does not produce an enantiomorph. The only thing that's possible then would be translation. And these two guys are not parallel to one another. You can't get this one by just sliding this parallel to itself. The only thing that's left is rotation. And, lo and behold, we can get from this one to this one by a 180-degree rotation. And we can get from this one to this one by a 180-degree rotation.

So here's an example of a way in which we've combined without showing why this is possible, or how I got there. Here's a combination of symmetry elements that gives us a possible arrangement of objects in space. It's going to be convenient to have a notation to indicate such combinations.

And we call them Harry, George, and Sam, or some popular, affectionate name. Or call them number 1, number 2, number 3. But a nice notation is going to be a descriptive one which tells you what you have. And what is done in crystallography is to indicate these possible combinations by a running list of the different kinds of symmetry elements that are present.

And here, we've got a twofold axis, for which the symbol is 2, and two mirror planes that are different and function in different ways in the pattern. So this combination is called 2mm. OK, that's getting ahead of our story. But what I wanted to do now is to show you that this set of symmetry elements contains four operations that constitute a group.

There's the operation of a one-fold axis. That's the identity operation. There is a

reflection across the first type of mirror plane. And notice, now, the utility of having a symbol that indicates a specific operation rather than a symmetry element. There's a second reflection operation, sigma 2, and there is a rotation operation through a 180 degrees, A pi.

So I'd like to show that these four operations constitute a group of rank 4. So how do we show this? We first set up the group multiplication table. And then we simply combine these four operations pairwise.

Put the same 1, sigma 1, sigma 2, and A pi down this side of the array. Doing nothing, doing nothing, is the same as a one-fold axis doing nothing. Doing a reflection sigma 1 followed by doing nothing gives you sigma 1 back again. Doing a reflection sigma 2 followed by doing nothing gives you sigma 2 back again.

And similarly, rotating A pi followed by doing nothing is the same. If I go along the columns, doing nothing followed by sigma 1 is sigma 1. Sigma 1 and 1 combined is sigma 2. A pi combined with sigma 1 is A pi. So far so good, but not surprising. Doing sigma 1 and following it by sigma 1 is reflecting left to right across mirror plane 1, and then reflecting right back again.

So that is going to be a one-fold axis doing nothing. Doing sigma 1 following up by sigma 2 would reflect across, and then follow up by reflection in the second mirror plane. I get from the first one to the final one by the rotation A pi. So this is A pi. And if I do the first reflection, sigma 1, and follow that by A pi, that gets me from number 1 to number 2 to number 3. And I get from number 1 to number 3 directly by the reflection operation, sigma 2.

OK, you notice what's happening? I get the same four elements back again in every column or row. Sigma 1, 1, A pi, sigma 2. And if I rattle these off quickly, this as A pi. This is identity, and this is sigma 1. And this will be sigma 2. This will be sigma 1. And this will be the identity operation. So the first group postulate is satisfied.

These four elements combined pairwise always give you nothing but one of these elements back. An identity operation is present because the one-fold rotation axis is

the same as leaving the thing alone. And we've seen that for every operation, an inverse exists because 1 occurs once in each row and column.

So sigma 2 is its own inverse, and for sigma 1, sigma 1 is its own inverse. For A pi, A pi is its own inverse. So an inverse exists. So we've got a group. And this is another way of saying, in general terms, if we put two mirror planes and a twofold axis together in this specific fashion, these operations, when they go to work on an initial motif, reproduce a finite set of objects and not a clutter that just fills space and never closes upon itself. Yes, sir?

- AUDIENCE: I see why you have sigma 1, sigma 2, A pi in that group, but why do you have the 1, which is a conversion?
- **PROFESSOR:** OK. If I didn't put it in-- no, that's the identity operation. This is a one-fold axis. Just this 2 was a twofold axis. So one-fold axis is a nice symbol for identity because it doesn't do anything. It picks something up and puts it right back down where it came from. OK. Yeah. That's deceptive because 1, when we're talking about multiplication of numbers, also functions as the identity operation. Yeah?
- AUDIENCE: If all these symmetries are commutative, [? that is, ?] if they all commute, do you really [INAUDIBLE] bottom diagonal [INAUDIBLE]?
- **PROFESSOR:** In general, yes.
- AUDIENCE: Generally?

**PROFESSOR:** Yeah. Actually, this is a special group because if I have two elements, a, and take b and follow it by a, that is the same result as a followed by b. And a group that has this character is said to be abelian.

There's a standing rotten joke in mathematics that asks rhetorically, what is purple and commutes? The answer is an abelian grape. I don't think it's terribly funny either, but if you had a gaggle of mathematicians here, they would chortle and double over in laughter. Ha, ha, ha, abelian grape. Well, I don't feel badly. You react about the same way to some of my funny things, too. But you get used to that sort of thing.

All right. The feeling I want to leave you with at this point is the idea that group theory and some of its concepts are exactly what we're meaning when we grope for a definition of the fact that a certain collection of symmetry operation should be finite. That is to say, it's finite. The operations combined on each other have to give a finite number, must constitute a group. And the main reason for being familiar with this is that group theory forms the basis of a lot of the words that are used to describe the combinations of symmetry elements.

For example, what we have derived here, the symmetry that's called 2mm, is something that's called a point group. Point because there is at least one point in space that's left unchanged, and that's this point of intersection of all three symmetry elements. And it's called a group because the individual operations of these symmetry elements, when combined according to group theory, can be shown to constitute a group.

The patterns that we get when we add symmetry elements to a lattice are groups in the sense, if you regard the pattern as extending infinitely in all directions, that the combination of any two elements gives you something that's also in the group. But the number of elements is infinite.

For example, in the lattice, here's T1. Here's T2. Every other lattice point can be described as some combination of T1 followed by T2. But the numbers in front of those translations can be infinite. If we put a symmetry element in this lattice, like a twofold axis, for example, the translations reproduce this twofold axis to an infinite number of locations. But yet, all of the group postulates are satisfied.

The number of elements in the group does, however, not have to be finite. So that is another distinction that's worth making, that there are infinite groups and there are finite groups. And the number of elements can be infinite. Collection of symmetry elements that leave one point in space unmoved is called a point group. If we do something like this, put a twofold axis in combination with a pair of translations, that is an infinite set of operations that acts on all of space. This is something that's called a space group.

Another designation, distinction, that's sometimes useful to make are crystallographic point groups, such as this one, 2mm, as opposed to combinations of symmetry elements, which are perfectly lovely and which are valid groups, such as a combination of rotations of 2 pi over 5, or a combination of a fivefold axis with a mirror plane. Perfectly lovely symbols, constitute groups, but these are noncrystallographic

These would be non-crystallographic point groups. Satisfy all the requirements of the group, but if it's to be in a crystal, the fivefold axis must be combined with translation, and that's impossible. So you can have non-crystallographic point groups. There are no non-crystallographic space groups because they are, by definition, something that involve translation yet constitute groups. All right.

Set the stage for next time, so you all come back excited. We have shown that there are a limited number of symmetry elements that are possible in a lattice, rotation 1, 2, 3, 4, and 6 in a mirror plane. And these are now examples of what we would call crystallographic point groups. These would be the sort of symmetry elements that are candidates for two-dimensional patterns.

But are these the only symmetries that can be added to lattices? Could we not combine a mirror plane with a twofold axis? The answer I say to that is, sure. You bet you can. You just did it for us.

But could you combine a mirror plane with a threefold axis, a mirror plane with a fourfold axis, a mirror plane with a sixfold axis? The answer to all of those questions are yes. So there are going to be spaces here, where there will be additional groups. And when we're done, we will have the two-dimensional crystallographic point groups.

But now I have to be able to complete something. If I take A pi and combine it with a mirror operation sigma 1, what do I get? If I take A 2 pi over 3, a threefold rotation, combine that with a mirror plane that passes through it, what do I get? Again, a

characteristic of symmetry theory is that whenever I take a motif and repeat it by operation number 1 to get a second motif, and then I repeat that by operation number 2, I have three things that are identical.

And there must be some way, some operation, that automatically arises that tells me how number 1 is related to number 2. Number 1 is related to number 3. Tied in with group theory, this says that if you combine operation 1 in a space, if it's to be a group, if operation number 2 is present, you must combine those two steps, and whatever pops up must be a member of the set of operations that are present.

So we're going to have to come up with something that I call combination theorems. And this is simply expressing the result of a combination of two elements in a group multiplication table. It goes with a caveat. If you're so excited about this stuff, you're going to run home and start reading Buerger's book as soon as you get there.

You can regard these symmetry transformations as operators. And you're familiar with other sorts of operators like d by dx, d by dy. And when you apply them in succession, you actually write it as a product. d by dy followed by d by dx you write as d squared dxdy. Or you write it as d squared dx squared when you differentiate twice.

You don't mean you take the differential of the function with respect to x and then square it. You mean you do this operation twice. So these are all operators.

And what we usually understand is that if you do d by dy first and then follow that with d by dx, the sequence of operation goes from right to left. And I think that will come right quite naturally to you. You do that with differentials and other sort of operators. That is what we'll do.

Not Martin Buerger. A very strong-minded person, and he did what he thought was sensible. And he said we read things from left to right. We read everything from left to right. So I will be damned if I'm going to write d by dx, d by dy to be a sequence of operations that goes from right to left.

So all throughout Buerger's book-- and it's easy to get adjusted to, if he writes A dot

B, he means B followed by A. Whereas normally, in the calculus of operations, we will use, as the rest of the world does, this is A followed by B. Trivial point, but one that can throw you for a loop the first time you see it in Buerger's book if you follow it.

Distinction does not matter if the group is abelian. So that the order of operations doesn't make any difference. OK, that's enough for one day.

Beginning next time, know we will start to begin this process of synthesis. And the first thing we'll ask is, how do you combine a rotation operation with a reflection operation? See you next week.