PROFESSOR: I think it's about five after the hour so we ought to get started. Before we forge bravely ahead, I'd like to make sure that everybody has a copy of the things that we've been handing out. There is a copy of the handwritten notes on the derivation of the 17 plane groups. Need a copy of that? There you go.

And then there is, in addition, a set of diagrams from the international tables that give very nice pictures of all of the plane groups in the arrangement of symmetry elements. That's the only other thing that was handed out up to this point.

For your continued edification and amusement, I have another problem set. And let me say something about this problem set. The first problem gives you some angles between crystal faces and asks you to deduce a possible set of lattice translations which are consistent with those angles.

And in the days before diffraction, that was what crystallography was all about. It really was mapping the geometry of crystals. And the interesting thing is, you could measure these angles very precisely with a device called a reflecting goniometer, Provided you had a crystal with nice, shiny faces on it. You had a two circle instrument, and you could adjust the crystal so that a light beam, a very finely collimated beam of light, was focused into an eyepiece. And you could measure angles to within not one minute, but one second of arc.

And from this you could deduce if you could assign Miller Indices to the faces. You could deduce not the absolute magnitudes of translations, but you could deduce the ratio of them. And along came x-ray diffraction and shook everything up. Turns out, sometimes you were right and other times you were wrong, because you had determined a self consistent set of indices, but not the ones that were correct.

So this is to give you a little look at the early days of crystallography, and to see if using the way Miller Indices are defined you can calculate the ratio of axes. Not terribly demanding, but worth doing.

And we had talked earlier about these combinations of symmetry elements as constituting the elements of a group. And in the second problem I ask you to take a not terrifically simple, but a fairly complex point group, 4mm, and show that, indeed, the operations that are present satisfy the group postulates. And that is worth doing once so that you convince yourself these really are groups.

And then the third problem is easy to state and it is diabolically tricky. So I'll let you have a go at it, but don't beat your brains against your desktop for an entire evening over it. Try it. If you don't see the solution to it, all will be revealed later on in class.

But it's based on the fact that the plane groups, which we've now derived, 17 of them, these can be viewed as the base level of a three dimensional space group. And for each of them, you could take another translation, t3, that was perpendicular to the plane of the group, and just imagine all of those rotation axes and all of those mirror planes not being two dimensional operations, but three dimensional operations.

The only one where you could pick the translation, generally, would be the oblique lattice, p1, no symmetry at all. And there you could pick the translation in any orientation you wished. But for each one of the 17 two dimensional plane groups, there is a corresponding three dimensional space group. So we got 17 three dimensional symmetries for free without really doing any additional work.

However, there's one thing that one should not gloss over. We found that a rotation point in a two dimensional plane allowed only a very limited number of lattices. But we were not thinking of things in terms of three dimensions. So what I'm inviting you to do in the third problem is to consider, now, that construction that we did where we showed that rotation angles were restricted to values of cosine of alpha equals 1 minus p over 2.

Now generalize that to a three dimensional situation, where the translation does not have to be perpendicular to the rotation axis, but can be inclined to it. Are there additional rotation axes allowed? Are their fewer? Something we ought to examine. But there's a little bit of ingenuity that you have to use in that proof. But I invite you

to have a go at it on your own.

So with that tantalizing introduction that will want to send you running home and start it as soon as we finish our class this afternoon, let me hand out, without any further blather, problem set number five. Pass that in the back corner.

Last time, without saying much about them, I handed out this extract from the international tables that summarized the 17 two dimensional plane groups and their properties. And I'd like to spend a few minutes going over the considerable information that's contained on these pages.

Each one is treated in the same way, and let me start with one that's almost trivially simple, and that's the two-fold axis in the oblique net. Across the top of the page you find, in boldface, the symbol for the plane group. And then, just counting in order of increasing symmetry, the number of that particular plane group in the set. And then a symbol that really has its full meaning only in three dimensions, but it gives the symbol for the lattice, again, 2 and then a 1 and a 1, which says that if this were a three dimensional space group, there would be a two-fold axis in one direction and no symmetry at all in the other two directions.

And then, next comes the symbol for the point group of the crystal. And we derived this particular group by dropping point group 2 into a lattice. And then the coordinate system that is necessary to describe the features of this plane group, if you take the edges of the unit cell as the basis of a coordinate system. So this is something called a crystal system.

So for each of the plane groups, you have this information spread across the top of the page. Then underneath that is a diagram that, by means of open circles, shows the way in which that particular symmetry moves a motif where atoms, in the case of a crystal, moves atoms around. And for p2 we have the pair of motifs of the same chirality related by a two-fold axis. And that, then, is hung at every lattice point of an oblique net. And then, immediately to the right, is the arrangement of symmetry elements in the group.

Then, the way in which that particular plane group can move atoms around to generate a structure is summarized for you. And the first thing they have to state is where you're going to choose the origin. There is no unique lattice point. It's convenient to take the origin at a location of high symmetry, and in this case the smart thing to do is to take the origin at one of the two-fold axes.

That's a non trivial question, because there are some groups that have different kinds of rotation axes. P4 has a four-fold and the two-fold. Taking the origin of the coordinate system at a location of high symmetry, then, gives you the scope of picking either a two-fold or a four-fold axes. Yes,sir?

AUDIENCE: On the left hand figure, what's with the-- those aren't mirror planes [INAUDIBLE] are they?

PROFESSOR: On the--

AUDIENCE: [INAUDIBLE].

PROFESSOR: Here they have this. That's just to split things up into quadrants, so you have a feel for how the atoms hung at the lattice points split up into different quadrants. That is a very good point, though. Mirror planes are shown as bold lines. Sometimes the outlines of the cell look pretty bold themselves. So if you turn the page to pm, if you have the notes with you, can see the lines that are reference lines for the cells are lighter in their weight than the symbols for the mirror planes. But it's a very subtle difference. And when you Xerox it a couple of times it becomes almost indistinguishable

AUDIENCE: Can you just say, one more time, [INAUDIBLE]?

PROFESSOR: That means that this is the location of 0,0. And it is always assumed, but nowhere stated specifically, that the origin is in the upper left hand corner. And what is also assumed, but never stated, is that the x-coordinate in the a-axis goes down and the y-coordinate in the b-axis goes from upper left to the right. That is nowhere stated anywhere in the international tables, but that is the direction that is assumed for the reference axes.

So we'll take our origin of the two-fold axis. That's a sensible thing to do. And then there are two ways you can look at how the particular plane group generates a pattern. You can do it with little circles or little commas, or something like that. In other words, do it graphically.

But a way to communicate the atomic arrangement in a structure, which is going to be the most free of ambiguity and rigorous, is to do it analytically. And that's what the tables do for you next. They give an analytic description of the way in which the symmetry elements will move an atom around.

For this particular plane group, things are very simple. This is the direction of x, this is the direction of y. And if we plop one atom in here, it will be at a location x and y. So that's what happens when you drop one atom in it. That atom gets hung at every lattice point, and it gets rotated by the two-fold axis.

So you're going to get two of them per lattice point. Somewhat arbitrary which pair you take. The coordinates of this atom are x and y. The coordinates of this atom inside of the box is 1, minus x and 1, minus y.

That would do it, but it makes sense, esthetically, and to see that the atoms are related by symmetry, if, instead, you specify as the two atoms per cell the two that are hanging at the lattice point. And in that case, the coordinates of the first, if they are x and y, would be minus x and minus y.

If you have a pair of numbers, 0.283 and 0.456, then minus 0.233 and minus 0.456 leaves no doubt that these are positions that are related by symmetry. If you have coordinates, like 0.2, 0.3 and then 0.8, 0.7, without doing some arithmetic in your head, it's not clear that those are going to be atoms related by symmetry. So the coordinates that will be stated for you, then, will be the coordinate of the pair of atoms at the lattice point, and some of the coordinates would be negative.

This is something called the general position. And that transformation of coordinates is different for every one of the plane groups. That's what makes them different. They're different in the way they move around an atom in a general location and fill

space with it. So that's the general position, and it is unique for each plane group. And there are several ways in which this information is conveyed to you. Move this over a little bit; x, y and minus x, y.

The first thing that's a characteristic of the position is the number per cell. So you get the number 2, or this is sometimes referred to as the rank of the position. Drop in 1 and you get a second one out related by symmetry.

The next is, and I'll go to the last next, this is the site symmetry. And by definition, this is always 1, no symmetry at all, for a general position.

So why make a big deal about all of these characteristics of the general position? The reason is that there are locations that are termed special positions. And let me clean up this right hand part of my diagram.

And say that, for plane group p2 you will always get two atoms per cell if you place an atom in an unspecialized location. What would be a specialized location? Suppose we would drop the atom down right smack on top of that two-fold axis? Then that two-fold axis is just going to twirl the atom around on its axis and it's not going to map it into a second location.

So following the general position is always provided to you a set of special positions. And what's special about them? They are on a symmetry element.

You can look at the characteristics of a special position in two ways, either geometrically or you can do it analytically, as I'll show you in just a moment. Imagine that the atom is to sit here, x and y migrate progressively towards the location 0,0. And then the other atom related to it by two-fold symmetry will move towards it until finally the two of them will merge into just one single motif.

So when that happens you get not two per cell, you get only one per cell. And the reason for that is the site symmetry is 2. It's on a two-fold axis.

But there are other two-fold axes as well. What if the element migrated to the position 0, 1/2? If that were the case, if the representative atom moves to here, this

one up here will migrate down and the two will merge into one atom that sits at just 0, 1/2.

So there'll be another type of special position, one per cell, also, on a two-fold axis. This one was at 0,0, and this one is at 0, 1/2.

You remember, we made a point of saying that there are four different kinds of two-fold axes within this plane group. Different in how they're positioned relative to a pattern, different in that they are not mapped into one another by some other symmetry element which is present.

So each of these four locations is a location of another general position of rank 2, sitting on a two-fold axis. x and y migrate down to 1/2, 0, and this one and this one will come together.

So there's another one, giving you one per cell, sits on a two-fold axis, and this would be at the location 1/2, 0. And finally there's another one in the center of the cell, and if you let the atom migrate to that location, again, the atoms will coalesce pair wise into a single one.

So there'll be another one, one per cell, and also on a two-fold axis, and this would sit at the location 1/2, 1/2. And those, then, are the characteristics of this particular simple plane group.

There's another symbol that's added, and this is something called the Wyckoff symbol. Wyckoff was a crystal chemist who attempted valiantly, back in the early days of the century, when there were a couple of dozen structures determined per year because it was such a grand, new adventure, and few people knew how to do it.

But Wyckoff tried to summarize, between one pair of hard covers, all of the crystal structure determinations that had been performed in a single year. And he went at this courageously for perhaps a dozen years, and then results began to accumulate so rapidly he just said, the heck with it, clapped covers on it, and that was the end of the series of books. So they don't get very far, but it was a real useful contribution at

the time.

This is just a shorthand way of referring to the position. And he starts with a for the most specialized, runs the way up through the alphabet until you've assigned a letter to each of the positions.

This is a nicety. All these special positions, for example, sit on a two-fold axis, and you don't really have to specify the coordinates, because they have to be either 0 or 1/2. So this gives us a way of saying you have an osmium atom in position 1a and you have an oxygen atom in position 1c. And it's a nice shorthand way of avoiding mentioning things which could be calculated once and for all and not stated explicitly.

So this, my friends, is the language in which you will see structural datas cited, when people have determined, using diffraction methods, the locations of all of the atoms within the units, some of a particular material. If the coordinate is variable, with today's techniques and high speed computation, you can get x as a fraction of a cell to usually at least plus or minus 1 in the fourth place. So it's data that can be determined extremely precisely. Yes sir?

AUDIENCE: I didn't quite get the exact definition of the general position. It's a set of points related by--

PROFESSOR: The general position, it's a set of equivalent positions that are related by symmetry. Yeah. And the general position, yeah-- Each of these is called a set of equivalent positions, equivalent in the sense of being related to one another by symmetry. And the entire set is sometimes referred to as an, singular, equipoint. Sort of a condensed jargon for a set of equivalent positions. So when one speaks about an equipoint of rank 2, in this case, or rank 1.

Let me just, even for this trivial two dimensional symmetry, give you an example of some information that falls out of this immediately. First of all, you can use these special positions only once. If you put an atom in position 1c at 1/2, 0, it's used up. You can't put another atom in there in a given structure.

Secondly, if you think more globally, not in terms of atoms, which, to a good approximation, are spherically symmetric. But think in terms of a molecule, if you're a polymer scientist or an organic chemist. and not place an individual atom, but place an entire molecule. If there's one molecule per cell in this particular symmetry, that molecule has to sit on a two-fold axis. And that means the configuration of that molecule is going to be limited to having to conform to a two-fold rotational symmetric.

So just from the density in the lattice constitute, if you find there's one molecule per cell, you know that molecule has to have two-fold rotational symmetry. So you can say something about the structure of the molecule. So there are lots of ways in which the symmetry information has something to say about the arrangement of atoms in the structure. Any further questions? Yes?

AUDIENCE: How did they decide, between b, c, and d, which was the most special form?

PROFESSOR: That is a very good question. And the way it's decided is by you getting there first before anybody else did it. So everybody follows, now, the conventions that are given in the international tables. That's sort of the dictionary of all these terms. But you're absolutely right. What is more special about this one than this one? Well, they're all locations of the same symmetry. You can turn one into another by changing the origin of the cell, where you're going to define a lattice point.

So they are thoroughly arbitrary. What is generally done is to take 0, 0 for your particular choice of origin as position a. And then what should come next, 0, 1/2 or 1/2, 0? The truly observant among you will notice I snuck a quick peek at the international tables before I wrote one of these down. I can never remember which is which.

And it is arbitrary. Usually you end up with the one that has both coordinates non-zero, but that is code that's embodied in the international tables. But that's a good question. Yes, sir?

AUDIENCE: How did you decide to make the motifs [INAUDIBLE] special decisions?

PROFESSOR: Oh, I just changed the value of x and y. Those are numbers that can be, for the representative atom, each of them can be between 0 and 1. So what I just said was, what will happen if we let x and y take on not general values, but very special values? And the special values are going to be things like 0 and 1/2, if I have picked my origin at a two-fold axis. It's another reason for picking your origin at a location of high symmetry.

AUDIENCE: But how about the other non-origins of these special decisions [INAUDIBLE]?

PROFESSOR: There are two ways you can do it. One of them we just did. We just looked at the geometry and we said, if this representative atom, this is the one we define as being at location x, y. If x and y both approach 0, this atom and the one over here are going to migrate towards the origin lattice point and eventually just coalesce.

If I let x and y and migrate, x go to 0 and y go to 1/2, then this one and this one will come together and coalesce. So that's why I did that, because I knew that the number I would generate would be smaller than the number that I would get for a set of coordinates for an atom that was off the symmetry element.

I said there's another way of doing it. For something this simple it is not really that profound, but it is a way of checking whether you've counted the same position twice. I said you can imagine these special positions arising when x and y assume special values.

So let's let, for example, x be 1/2 and y be 0 and plug those coordinates into my equation for the general positions. So I'll put in 1/2 for x, 0 for y, and then I'll put in minus 1/2 for x and minus 0 for y. But what goes on at minus 1/2 has to be the same as what goes on at plus 1/2, if the structure is based on a lattice and periodic.

So what I'm really getting is 1/2, 0, 1/2, 0 twice, which is the same as saying, if x is 1/2 and y equals 0, I'm putting two atoms together right on top of one another. So you can do it analytically. And for the more complicated symmetries, where there might be for 20 or 48 atoms, that's a good way to see if you've looked at the same position twice.

So we're going to do a couple more before we move on, and this one is almost trivially simple. Any other questions before we go forward?

Let's take one that is slightly more complex. And I'll go to one of the rectangular groups. And let me look at, let's take plane group p2mm, which has a fair amount of symmetry to it.

So this is the group that we got by putting 2mm into a lattice that had to be rectangular, then. And across the top of the page, this is number six, you'll see that it is rectangular. It has to have a lattice in a rectangular shape because of the symmetry.

Next comes the short hand symbol. And I always feel a little bit apologetic when I have to point out the existence of this, and the reason is that people who work with symmetry are no more or less lazy than any other human being. And some of the symbols become really ungainly when we go to three dimensional symmetry. And something like a 2 sub 1 over a 2 over m 2 sub 1 over d is a mouthful. And actually what's done is to just specify the minimum amount of information, which defines the symmetry.

So here, two m's that intersect have to give you point group 2mm. Then comes the full symbol of the plane group, p2mm. And for those who are counting, this is number six and the shorthand symbol is pmm, where the short symbol for the point group, along with the lattice, is sufficient to tell you that this is 2mm placed at the nodes of a rectangular lattice.

Then, underneath, comes the representative pattern. Again, there's a cross in the middle of this just to split it up into quadrants. The symmetry is one that we've already encountered and was fairly easy to come to terms with. Two-fold axes at the corners of the cell, and in the center and in the midpoint of the edges.

That's just like p2, except the mirror planes that are present require that that parallelogram in p2 straighten out into a rectangle. And then we put 2mm at the lattice points so the mirror planes run down through the cell like this, up and down

and left to right. So here is all the symmetry here.

Pattern, I'll say it again. It's so easy to forget. The pattern is nothing more than the pattern that 2mm produces hung at every lattice point of a rectangular net. And all of the symmetry planes and symmetry axes that arise are just ways of defining all of the relations that exist between these things when you perform that process of addition. So this is, then, the arrangement of all of the atoms in the cell and then some.

And there's a new symbol that's introduced, and somebody asked about that last time. To me it looks like a little tadpole inside of a frog egg. Has anybody seen a frog egg? That's just what it looks like. It's a little tiny tadpole in there, waiting to hatch out.

So here is our little tadpole. This is used to indicate an enantiomorph. If this were a motif with chirality, this one would be right handed, this one would be left handed. So that indicates all of the atoms or molecules that are the same chirality.

The purists among you will notice that the dummy that produced this diagram did not show the tadpoles conforming to the two-fold symmetry. Both of the commas point in the same direction. Tsk, tsk. Little oversight.

So this, then, is the arrangement of motifs in the pattern. And now let's proceed to analyze that, according to the nature of the positions that are available of different sorts. Again, coordinates have meaning only if you define the origin. And nobody in their right mind would want to pick an origin that is off, at least, the symmetry plane. But the thing to do is to take the origin at 2mm.

Again, I'll remind you that x goes down this way, y goes this way. So if I have a representative atom at x, y, I'll have another one at minus x, plus x, another one at minus x, minus y, and one at plus x, minus y. So there are the coordinates of all the symmetry of related atoms.

So putting down the general position, I get four of them if I place one in the cell. By

definition, the general position is always at a site of symmetry 1. So this is the site symmetry. Then we just rattled of the coordinates. They're x,y, minus x, y, x, minus y, and minus x, minus y.

There are lots of special positions here, now, because we have not only two-fold axes with mirror planes intersecting at them, but they're also locations of just a mirror plane alone. And there are a total of four distinct, independent mirror planes, this one, this one, this one, and this one.

So we're going to have four positions where the atom sits at a location of symmetry 2mm. And those are going to be analogous to the positions that we found for the two-fold axes in p2. And, not surprisingly, the coordinates look very much the same. 0,0 puts us on a location of symmetry 2mm. 0, 1/2 does the same, 1/2, 0 and 1/2, 1/2. So there are four positions of symmetry to 2mm.

And then there are four positions just on a mirror plane, but not on a two-fold axis. And we could do that for the mirror plane that runs along the x-axis, or the mirror plane that runs along the direction of x at y equals 2. And the order in which you pick them is rather arbitrary, but there will be a pair of positions at x, 0 and minus x, 0 that would happen if the y-coordinate was exactly-- let me draw what the position is, just off here to the right in a small diagram.

This would be where you put the atom on the mirror plane running through the origin, then these things would give you only a pair. The next one is at a position x, 1/2, and that's where the mirror plane would be the mirror plane that is along the position y equals 1/2. And here we would get atoms coalescing like this. x is general, but y is exactly 1/2.

So we'd have x, 1/2, minus x, 1/2, and I better put these off to the right, here. The remaining two are 0, y and 0, minus y.

That is also a position of site symmetry m. And that would be a pair of objects that has x equal to 0. y is anything, so that's this mirror plane here. And in that case we'd have a pair of atoms, left to right, reflected by the mirror plane that goes through the

origin.

And then last one, thank goodness, is one at a location 1/2, y and 1/2, minus y. And this would be the mirror plane exactly at 1/2. y can be anything. x is 1/2. So that would be a pair that sits somewhere on either side of the mirror plane running through the center of the cell. That's also a site of symmetry m.

Now we assign the Wyckoff symbol by working our way up the alphabet. So this is a, this is b, this is c, this is d, this is e, f, this is g, this is h, and finally we end up at position i.

For all of these, we get two atoms per cell. These have rank 2. For each of these we get just a single atom.

AUDIENCE: Can you explain the two atom per cell thing? How do you [INAUDIBLE]?

PROFESSOR: Which one would you like me to do, that last one? 1/2, y?

AUDIENCE: [INAUDIBLE].

PROFESSOR: So if x is 1/2 and y is anything, that's this locus here. And that is a mirror plane. And if we let this atom move from its location, x,y, down to this location, the one in the lower part of the cell is going to move up and these two will coalesce to a blob that sits there.

AUDIENCE: That would be 2m?

PROFESSOR: So this would be site symmetry m. And instead of getting four per cell I would get two per cell; this one and the one that's reflected across.

Now the other way of doing it is to not think about it all. Say here is x,y, minus x, y, x, minus y, minus x, minus y. And then let's make one of the coordinates specialized. Let's let x be exactly 1/2. So I'll get 1/2, y, minus 1/2, y, and then I'll get 1/2, minus y and minus 1/2, minus y.

Looks like four atoms, except if I have one at plus 1/2, the one in the neighbor unit

cell is at minus 1/2. So actually I've had the atoms coalesce pairwise, because these coordinates are actually identical to saying 1/2, y plus 1/2, y, 1/2, minus y, and minus 1/2 is the same as plus 1/2, minus y.

So you can do it that way. Just put in a special value for x or y, turn the crank on the general position, and you'll find you're going to get the same thing twice.

And if we look at position a, which is 0,0. put in 0 for x, 0 for y, then put 0,0 for all these other four positions, you're going to get 0,0 four different times.

I'm going to do just one more, and the results are here for all of the remaining 14. So I don't think there's any need to do them all. One of the things I would like to examine with you is a group that has a glide point in it, and see how that changes things. Any other questions on this?

AUDIENCE: Can you just go over the rank of fours? Four--

PROFESSOR: Four means four per cell.

AUDIENCE: Four per cell.

PROFESSOR: And if you count them around the origin as 1, 2, 3, 4. If you count the number that's caught within the box it's 1, 2, 3, 4.

AUDIENCE: And site symmetry of 1?

PROFESSOR: That's site symmetry 1 because 1 is no symmetry at all, and that is what's general about it. It's not sitting on a symmetry element which would then fail to reproduce it.

And again, if the motif was not an atom but was a molecule, if you find only one molecule per cell from the density in the cell dimensions, that molecule has to have symmetry 2mm, because it has to sit. If there's only one per cell, that set of atoms has to sit at a location that conforms to symmetry 2mm.

Let us go to one more. And I'm going to take p2mg, because it's one that has a glide plane in it. This is pmg for short. This is number seven. P2mg is the proper

symbol, and that's point group 2mm. And, again, the coordinate system is rectangular.

This is one that we derived last time. The arrangements of elements in this is, once again, a rectangular lattice, two-fold axes. If we take the origin at 2, would be at the corner of the cell and in the midpoint of the edges. Then there's a glide plane passing through the two-fold axes. And there is a mirror plane passing in between the two-fold axes.

And here's a good example of an arrangement of symmetry elements that has a mirror plane in it, and then a line that just indicates the edges of the unit cell. And can you distinguish the bold line from the light line? Barely. But the bold line is the mirror plane.

And what does the arrangement of atoms look like? This is a tricky one, because there are two different symmetry elements; a two-fold axis, and that's going to take an atom at x, y and repeat it to minus x, minus y. But here, now, is a case where there's another symmetry element that does not intersect the first one. So that mirror plane is going to reflect this atom down here to an enantiomorph and reflect this atom down here to another enantiomorph.

So if this is x then this is y, this one sits at minus x and minus y. For this atom here, y is the same as before. But if this distance is x, the distance up from the center line will be x, so this second coordinate is 1/2, minus x. I'll do that again since this is pretty small and tight.

This distance is x. We reflect the atom across a mirror line at 1/4, and therefore the one towards the center of the cell sits up above the location 1/2 by the same number, x. So this is 1/2 minus x, y.

And by the same argument, this one here is at minus y, and it sticks out beyond the position x equals 1/2 by the same amount, x. So this one is 1/2 plus x minus y. Nontrivial.

So if I began to tabulate these-- We've picked the origin at 2. Didn't have to do that.

If you wanted to, you could take the origin at m if you wanted to, and just switch everything by 1/4 of the coordinate x.

We found four per cell. The site symmetry is 1, and the atom locations were at x, y, minus x, minus y. And then we had 1/2, minus x, y and 1/2, plus x, minus y. So the coordinates are getting permuted around in a very more complex fashion than just changing sign.

Special positions. Just as before, any of these two-fold axes is going to be a site for a special position.

Let x and y go to 0. This pair at the origin will coalesce and this pair will coalesce at a point that's halfway along the cell. So there will be two of those, one at the origin, one in the middle of this edge, and their locations would be 0,0 and 1/2, 0. And this is a site on a two-fold axis and we have only two per cell.

Would this be a location for a special position, this two-fold axis? It was before. Is it now? Key point is independent sites of symmetry. There's a mirror plane here. What goes on here has to be exactly the same as what goes on here. So this is not an independent special position.

In the same way, there's a mirror plane. And if I let the atom migrate down to the mirror plane I will have the mirror plane at a location 1/4, y. And these will be on a mirror plane. 1/4, y would be a first, 3/4, minus y would be the second one that I get, and they would coalesce pairwise.

Is this is another mirror plane that could be regarded as an independent position? This mirror plane, again, is not independent, because it's related to the one we just considered by the two-fold rotation about the center of the cell. So there's only one kind of mirror plane in the structure. But, going back to the two-fold axes, there is a two-fold axis here. There's another one that is halfway along y.

So there's another two-fold axis that is independent at 0, 1/2, 1/2, 1/2. And this is the entire set. So there are three special positions of rank 2, two atoms per cell. We make the most specialized one be named a, work our way up to c, and the general

position, then, is referred to as d.

Again, so what I did was to say that this mirror plane is related to this one by symmetry, and if there's something on this mirror plane as a special position, I'm automatically going to get it on the lower mirror plane.

This two-fold axis is the same as this one. So whatever is going on as a result of specializing the location on this two-fold axis is going to be provided for me automatically at x equals 1/2 by the action of this mirror plane. There's nothing that throws this two-fold axis into this one, though, so they're both independent.

Now, one of the symmetry elements that I steadfastly ignored was the glide plane. What happens if I place an atom right on the glide plane?

A glide plane, if you use a motif that has some handedness to it, we repeat the atom by translating half of a translation, not yet putting it down, first reflecting it across. This is an enantiomorph. Doing it again gives me an atom that's related to the first by a translation.

What happens if I let the atom migrate onto the glide plane? Let this atom move down to here. Now it sits here. This one, repeated from it by glide, will migrate up to here. Nothing happens. It's just that the amount that the atom is displaced from the locus of the glide plane is different in the two cases. But there is no coalescence of the atoms, because of this translation component to the glide plane.

So a conclusion, then, is that glide is never a candidate location for a special position.

This is a good example of a case where I can check what I've done, and to see if I counted the same position twice. I said that both of these locations are not special position. The mirror planes are related by symmetry.

Suppose I were not clever enough to notice that, and I said, OK, there's going to be a special position, 1/4, x, 3/4, minus y. That's what happened if I use this mirror plane as a special position.

What would I get if I took 3/4, y and 1/4, minus y? Looks like a different specialized position. But let me put this number into my expression that is the formula for the general position. If x is 1/4 and y is y, then this position here would be minus 1/4 and plus y, 1/2, minus x would be 1/4, and y is y. Over here, I got the same thing back again.

And 1/2, plus x would be 3/4, and minus y is minus y, minus 1/2 and 3/4, plus 3/4 are the same thing. So what I've gotten is the position 1/4, y, and 3/4, minus y twice.

So what this is telling me, analytically, if I just plug in the coordinates of what seem to be a distinct, special position is, I get the same atom on top of itself twice. And it looks exactly like choosing the first mirror plane.

So that's a good way of checking, particularly in a very high symmetry where there are all sorts of sites of possible point groups that could cause coalescence, to just crank out the coordinates and see if, in fact, you have exactly the same pair with the same coordinates that correspond exactly to the x and y of some previous location that you identified.

I think, hopefully, you have a feeling for how it works. If you look at some of the higher symmetries, the number of atoms that constitute the full equipoint set of equivalent positions. For p6mm there are 12 locations in the general position, and because the coordinate system is oblique, x and y get permuted into linear combinations of one another. So that's really, extremely complicated.

If you look at some of the square symmetries, the number of the special positions is very, very high. There are two positions in p4mm, there are two positions of rank 1. There is a position of rank 2 that sits on 2mm. Three different mirror planes, and the general position with rank 8 requires working your way all the way through g in the alphabet. Yes?

AUDIENCE: I had a question about the p2gg [INAUDIBLE] whether they're at the entrance of the [INAUDIBLE]?

PROFESSOR: For p2gg, the only site of point symmetry is a two-fold axis. So the only thing that you could use for a special position in p2gg is a two-fold axis. And there are two different two-fold axes. They relate in a curious way because of a glide plane. And this is a case where the site of a special position is not related by rotation or reflection, but by a glide. P2gg looks like this. Two-fold axes in the old familiar places, 0, 1/2. The glide planes are here, here, here, and here.

So which two-fold axes are equivalent? The glide would take this two-fold axis, reflect it down, and slide it over to here. So whatever goes on here goes on at this two-fold axis.

AUDIENCE: Sorry. I guess my question was, can you put the glide planes at any edges of this sites? [INAUDIBLE], or--

PROFESSOR: You could. You could, but you would lose, then, the apparent similarity in coordinates in that, if you put the glide plane at the two-fold axis, if this is x, y, this one over here is at minus x, minus y. And then if you repeat it by glide, that would slide over to here and then be reflected down here. So there'd be one pair up here and one pair down here of opposite handedness, so you would not see the similarity.

No, that's right. If you took the origin at the glide plane, you would not see the simple relation between the numbers that you do when there is that a rotation axis of a mirror plane. But you can take the origin anywhere you want. And the advantage of doing it at a symmetry element is then the numbers that describe where the atoms sit are simple permutations of sign, or adding 1/2 to the number of the preceding atom that was just mapped to a new location.

I think you're more than ready for a break. Let's resume in 10 minutes, and we'll move on to something completely different.