PROFESSOR: But you all knew that. That is quite a mouthful. So if you like, you can refer to it as SST. And today, we're taking off.

So my name, for those of you who don't know me, is Bernardt Wuensch. My room number is 13-4037, The office that's become a legend in its own time. And my extension number is 3-6889. And hey, just to get you sensitized and thinking about the right things, let me point out that my extension number has a point of 180 degree rotational symmetry right in the middle.

You can pick it up, turn it head over heels by 180 degrees. And it's mapped into coincidence with itself. Just happened to get it. You might think I would have had to have fought for years to get an extension number like that. But no, it just happened to come my way.

OK, some words about the formalities of the subject. First of all, the format of the class is unusual. We meet four hours a week, but because most if not all of you are graduate students anxious to get some work done in the laboratory, we do this in two two-hour chunks. So we meet Tuesday and Thursdays for two hours.

Two hours is a lot of time for anything, however good. So what we do is to take a long intermission halfway through and let you go out and enjoy what's left of the lingering summer for 10 or 12 minutes. And then, come back refreshed and we will resume.

Most graduate students like this arrangement because it gives them a chance to duck out and make a setting on a furnace or turn something off in the laboratory. And it works out better for them than having a one hour time chunk every day of the week or four of the five days of the week. In any case, nobody's complained about it. So I assume that will work satisfactorily for you as well.

The other question that one immediately asked at the beginning of the term, how many quizzes? And we're supposed to tell you that straight up. There will be three quizzes. No final examination-- do I look like the kind of Scrooge that would prevent you from getting a good flight home at Christmas time or have you working, cramming for a final examination a few days before Christmas?

And for my part, I can remember the good old days-- or not so good old days-- when I did give a final. And there I would be, lying down on my stomach under the Christmas tree grading final examinations. And every time one of my little kids would come near, I'd lash out with my foot and say, get out of here, kid! Can't you see Daddy's got papers to correct? Well, no Scrooge. No final examination. We'll have three quizzes.

The quizzes will also be a little bit unique. Since we have two hour chunks of time, I found by experience that if I give the quiz during the first hour everybody is sitting around glassy-eyed, absolutely brain dead and pay no attention to the lecture that follows. If I give the quiz in the second hour, everybody is pretending to pay attention and then sneaking surreptitious looks at their notes just so they can have everything packed away before they have to write on paper.

So my quizzes are two hour quizzes which lets you not work for two hours, but gives you all the time you could possibly want. And people start leaving after about an hour and a quarter. But you can stay for the entire two hours if you want.

Even at that, I found by experience that if I give you two hours for the quiz, after about an hour and a half, everybody's looking out the window, looking back at the ceiling, not a single pencil is moving. Then I will say, OK, you all done? Everybody starts writing again and going through their papers once more.

And even after two hours I find that in order to get the quiz papers, I have to plant one foot on the edge of your table, grab hold of your quiz with both hands and drag it out of your clutching fingers. So you can take the full two hours. But it should not be necessary for you to consume that much time.

The quizzes will come-- and this is something else we're supposed to explain to you-- they will come at one third of the way through the term, two thirds of the way through the term, and 2.983/3 of the way through the term. And if you're wondering where that number comes from, this lets me put the quiz just before the final week of the term when we're not supposed to give examinations. So there'll be three quizzes.

You will have opportunity for lots of practice with problems. We will have on the order of 15 problem sets. And for the most part, they will be very short, or modestly short, and designed to give you some practice in working with the material. Because as the nature of this subject begins to unfold, you'll see that it involves a type of mathematics that you've really perhaps not had much practice with. It involves geometrical relations. And to really master it, you have to work with the material and get some practice.

Another question that's perennially asked if not outright raised in private, what do the quizzes count? What do the problem sets count? The answer to that is that the problem sets will count a lot towards your understanding of the material.

But I'm not going to grade them. And I'm not going to factor them in along with the quizzes to decide your final eventual fortunes in this class. The problem sets, moreover, there are a lot of them. But they will be optional in the sense that if you do them, I will carefully correct them, add words of inspiration and advice, correct things where you've gone wrong and then return them to you as quickly as possible.

But if you how to do the problem, you say, ah! Why does he wants us to do this and waste our time with a silly problem like this? Don't do it. Don't do it, because if you know how to do the problem set, that's fine. And you've got better things to do with your time. And I've got better things to do with my time if the feedback is not going to be of benefit to you.

So I hope you will do them. And as I said, if you do them, I will correct them promptly and thoroughly. And if you haven't got the foggiest idea how to do the problem, do what you can. And then, write down a plea of help-- I don't understand what's going on here! OK, and then I will take the time to write out what's going on, hopefully to your benefit and use.

Will I turn out solutions? Only on an individual basis in the fashion that I've just described. I find that if I write out a solution to each of these problems, you don't do them. And you say, oh, so that's how you do that, throw it in a file, and not look at it until the night before the quiz. So there will not be solutions handed out other than correction on an individual basis on your papers.

Is that all that I wanted to say? I think that's about all for the formalities. Actually, I should add one postscript to say the problem sets don't count anything toward your final grade.

They do in one minor sense. When you have a large class and you plot up the grades and there are no lumps with gaps in between, there comes a point where you have to separate one grade from another. And if you've done well on the quizzes and you've done well on the problem sets and there's just one quiz that's a little bit, I say, OK, he or she had a bad day that afternoon. And I'll give you the benefit of the doubt.

And even though I'm not a vindictive sort, if you're right on the fence and you haven't done any of the problems, then without malice I say, gotcha! And you go down [INAUDIBLE] on the low side of the barricade. And I think that's only a natural indication because there are some cases where, with Solomonic judgement, you have to decide who gets what grade.

OK, let me say a little bit about the texts. There are a number of books that deal with crystallography. For the most part, though, they consists of an introductory chapter. Every single book on the solid state feels compelled to write some sort of half baked chapter on crystal structure or crystallography. And usually, these chapters consist of big tables.

And they say, there are 14 of these. There are 17 of these. There are 32 of these. There are like 230 of these. There are 1,170 of these.

And then, that has all the excitement and stimulation of reading the telephone directory. It's a crazy cast of characters, but it's awfully hard to see the plot. So what we will do all the way through is derive everything. So you can not only see how it turns out, but why it has to be that way. And that's the way, in my opinion, one really learns this material.

A couple of other very pedantic comments about the material. In the early part of the term, the first half in fact, we're going to use plain old geometry. Now, geometry really doesn't cut much mustard around the Institute. If you can't integrate it or take its Fourier transform, that's a mathematics you don't have to take seriously.

Well, geometry is a perfectly valid branch of mathematics. And one can do what we're going to do in more complex terms using the language of group theory. And we will, in fact, use a little bit of that later on. But for the most part, just diagrams with simple geometry are going to be one of the principle tools in the initial part of the class.

About halfway through, we'll switch over to something that is much more mathematical in the traditional sense. Here, a little bit of linear algebra and matrix algebra will help you. If you haven't had that or haven't looked at it for a while, we'll build it up from ground zero so that you'll be able to fully understand it. We'll hit a few eigenvalue problems towards the end of the term. If that doesn't get your adrenaline pumping, that will be developed in a physical context so that you're doing the sort of problem before you even know what it's called. So it's going to be a user friendly course that doesn't rely on something that you may have had two or three years ago.

OK, but the other thing that I wanted to say was that this class is not like many classes in that you talk about something for one week. And then, you put it aside and you talk about something completely different the next week. Our first half of the course will be one long process of synthesis.

We're going to start out very, very simply with little mapping transformations. This is picked up and rotated and slid over to here. And you'll say, ho-hum, let's get on with it. Come on, go faster.

But we'll build on this and then build on what we've just done to what comes next. And unlike most of the classes in science that you take where you start with general terms and you zero in on some little nugget like f equals ma, e equals mc squared, lambda equals 2d sin (theta), a little nugget like a bullion cube that you can drop in your pocket. And then when you need it later on, you pull it out and add hot water. And then, you have a tool that you can use.

We will do something that's completely different in its structure. It will start out simple. It will grow. It will blossom like an elegant [? Filigree ?] structure that gets more and more complicated and diverges rather than converging to a nice, tight, little nugget. It's going to get very, very complicated. And the reason for doing this gradually and thoroughly is so that you can understand the complexity and where it comes from.

OK, so my moral here is keep up. It may seem easy when you start. But we're going to assume that you've got that down cold before we go on to the next step.

OK, texts. Apart from these half baked treatments which I just keep [INAUDIBLE] on, one of the very best books is by an old MIT guy, Martin Buerger, who was one of MIT's most distinguished faculty. He was the very first faculty member to be honored with the title Institute Professor, the very first one. Chairman of the Faculty, all sorts of awards from professional societies-- he has a book called *Elementary Crystallography*. This is published by Wiley.

There's some who dispute the term "elementary." But he really has a book which uses, at the outset, nothing more than geometry. He doesn't throw in comments like, "It can be shown that," or "By further work, it turns out--." He does everything for you. Everything is down there so you can see how it's done and what the results are.

To me, it is the best book on the subject. That's the good part. The bad part is that it's been out of print for about 15 years. So what I am going to do is to make-- now that I know how many of you are going to be present-- I'm going to make a Xerox copy for you of the first half of the book. What a department! What a class! You're going to get a classic text, 50% of it, without spending a nickel. And that'll be the text for the first part of the class.

We will be doing some derivation that are not in this book. And for that, I will have notes that I have written out. And you'll get Xerox copies of that. So we'll have lots and lots of handouts during the course of this semester. I'd like to call your attention, though, to two other books.

These are not textbooks. These are reference books. And you can see from the shape of this one that this is one of my favorite volumes. It's thoroughly worn out. This is something that is called The International Tables for X-ray Crystallography. And it is published by an organization called the International Union for Crystallography.

The funny sounding term, "International Union for Crystallography," sounds like an organization under which diffractionists go out and strike for higher pay. But no, this is actually a federation of all of the national societies of crystallography from all over the world. And among the useful things that they do, besides having a splendid conference every couple of years, is to publish these tables.

And volume one is called Symmetry Tables. And everything that we will derive and all of its properties-- physical and geometrical-- are tabulated in this book. It is, however, a reference book and not a textbook. You don't learn it for the first time from this book. But in terms of generating atomic arrangements from the data that's present in the literature, looking at the arrangement of symmetry elements in space, and how they move atoms around, it is the code book that tells you how to crack the arcane language in which diffraction and structural results are recorded and find out how to unravel it.

I call also to your attention, although it will not be germane to this class, there are four other volumes. Volume two is called Mathematical Tables. And this has all sorts of useful stuff. If you've ever done diffraction, you know that depending on the symmetry of the crystal, there are some planes for which h squared plus k squared plus l squared divided by 2 pi is not a reflection [INAUDIBLE] if the crystal is green, and other arcane rules like that.

All of these are summarized in these books. There are quantities that you need to calculate, things like interplanar spacings. Tables are available there. So this is a handy thing primarily for diffraction.

Volume three is called Physical Tables. And this is where you find things like absorption coefficients for x-rays and for neutrons. It's where you find the latest values of absorption coefficients, neutron scattering length. And since these things are derived experimentally, the values improve and change from time to time. So this is where you find the most up to date values of physical constants and items that are necessary for diffraction.

It never ceases to amaze me how somebody who has the good fortune of having to use the diffraction for a thesis will labor carefully over making the measurements and reducing the data. And then when it comes to using a wavelength, which is how the final numbers will be determined, goes to an appendix of a book on diffraction that was published 20 years ago. And that's not the most up to date value.

Scattering powers of x-rays by the electrons on the atoms are calculated from wave functions, which constantly get better from year to year. And the value of the scattering powers of the function of angle gets better from year to year. So this is where you want to go if you need any of that physical data.

And finally, volume four is-- it's not its title, but it's essentially an update of the Physical Tables, giving later values which came out about 10 years later. OK, this series was getting out of hand. So I have to bend my knees and use two hands when I pick up this one. This is a continuation of the series, essentially. But this one is called International Tables for Crystallography, period, no x-rays because neutrons and electrons are just as important today for doing scattering experiments.

And this is International Tables for Crystallography. No x-ray in there. And there are now something like six volumes out. They're not called one, two, three, and four, but they're called A, B, and C to avoid confusion. And volume A is one called Space

Group Symmetry. And then, there are a whole series of other ones. As I say, I think there's six of them that give physical data and all sorts of useful guides.

I have mixed feelings about the new series. You will see that it is about three times as large and three times as heavy, which means it's nine times as expensive. And to me, it's almost the case for most people of a situation where if it wasn't broke, you shouldn't fix it.

And what they've done is that they've put in all sorts of esoteric theory which probably is going to be of interest and use to perhaps 5% of the readers. But nevertheless, if you wanted, you'll find it there, which is something that could not be said before. They've added a few things which are useful, but a lot of additional information which you don't really need. And you pay for that whether you want it or not. Nevertheless, it's been done. You can't buy the old volumes any longer. You have to buy the new volumes.

So anyway, this is what you'll find in the library now. Maybe they do still have the old volumes, one through four. This, we will make reference to in the course of the term. I will give you some copies of certain pages in here as handouts when we need them for purposes of illustration or for use. But I spent the last five minutes just to make you aware of the existence of these books.

And these are really the penultimate source of information and numerical quantities that will be used in diffraction, one of the principle applications of crystallography. I think I have just enough enough-- to start things off, I have a syllabus for the course that is, in very dense form, exactly what we will be covering this term. And I'd like to lead you by the hand through this.

All right, what we will be doing in the first half of the term is something that is known as crystallography. OK, the meaning of the word is almost self-explanatory. The first part is crystal. We're going to be dealing with the crystalline state of matter.

To me, amorphous materials, although they may be important, have all the interest of a piece of steak before it's been cooked. The atoms in amorphous materials are fine. But they really get interesting when they organize themselves into an ordered fashion. So the name is self-explanatory. The first part, crystal, means we're going to deal with the crystalline state.

What does the graphy mean? That means mapping or geometry. And let me give you an example of a few other words that have the same sort of structure. Geo-- the Earth-- followed by graph, geography, is the mapping of the Earth. And there are many other terms that involve these two separate parts.

Crystallography, though, is very often subdivided into different flavors. There is something well defined called x-ray crystallography. And this is the experimental determination of the crystallography of a material using diffraction, usually x-rays because they're relatively inexpensive and they're widely available. But increasingly, neutron scattering or electron scattering is used for this purpose.

And there are a number of very powerful, very exciting sources of neutrons, either from reactor sources of unprecedented intensity or from what's called a spallation source, where an entire synchrotron is built just to direct a beam of particles onto a heavy metal target. And those high energy particles split off neutrons from the nuclei of the target material. Doesn't really matter what the material is. It helps if it's a heavy metal.

The nice thing about these sources of neutron radiation is that they're so expensive they are all national facilities. And the consequence of that is that anybody with a good idea and a project worth doing can apply for beam time. And if it's a good problem, you get it.

So you're using a facility that cost $1 billion. You have people whose sole function in life is to help you do the experiment and make sure you're doing it properly. And this is a very, very exciting time to be somebody working with diffraction using these neutron sources.

There's another branch of crystallography which is called optical crystallography. And this is the characterization and study of crystalline materials using polarized light. You can identify unknowns using their optical properties if they're transparent about 10 times faster than you can do with x-ray diffraction.

It's a technique that today is little used. But it's a very powerful technique. And all it takes is a microscope, and you're off and running.

Some other flavors of crystallography, well, I'll mention the one that we're going to use. What we're going to talk about is something called geometrical crystallography, to distinguish it from these other branches. And this is synonymous with symmetry theory. So that's what we'll do for the first month and a half or so.

All right, let me introduce now some basic concepts. Geometrical crystallography is the study of patterns and their symmetry. So let me give you an example of some very simple patterns that extent in one dimension. And let me put in a figure. The thing that is in the pattern is something that's called the motif. And let me use a plump, little fat comma. And I'll make a chain of these things extending in one dimension.

The nice thing about this fat little comma is that it is a figure which, in itself, has no inherent symmetry. So it is asymmetric, without symmetry. And imagine this is being repeated without limit in both directions, both to the left and to the right.

We then draw another pattern with a different sort of motif. And let me use a rectangle with one concave side. OK, and I think you get the picture of this one. And imagine that as extending without limit indefinitely to the left and to the right. Then, I'm getting tired of inventing new motifs. So let me use the same motif the second time, but arrange it in a slightly different way. And again, imagine that as extended indefinitely.

OK, having now generated these three patterns in two dimensions but extending periodically in two dimensions. Let me ask the question now. And even if you have not the foggiest idea, you have a 50% chance of being right. Are any of these patterns the same? Or are they all different? Are any of the patterns the same? Or are they different?

Well, that's a-- yeah?

AUDIENCE: [INAUDIBLE].

PROFESSOR: OK, that is an answer that's right because the bottom two involve the same sort of figure. They have the same sort of the motif. They both have the same rectangle with one concave side. And that's a valid answer. Do you have a different answer?

AUDIENCE: The first and third are the same.

PROFESSOR: First and third are the same. Why do you say that?

AUDIENCE: They both have [? rotational symmetry. ?]

PROFESSOR: OK. This is the point I was trying to introduce. And that is your choice of answering the question, one is the nature the motif. And you're absolutely correct. This pattern and this pattern are both based on the same motif.

But in patterns, we are less concerned with the motif that is in the pattern than we are with the relations between one motif and all of the others. And in that context, the first and the third pattern, although they look entirely different, are really exactly the same sort of pattern.

So let's begin to analyze what sort of operations are in these patterns that take one motif-- and obviously, they're all the same-- and relate it to all of the others. First of all, there is an operation which I'll call translation for obvious reasons. And I'll represent that by a vector, T, since a translation has magnitude and direction but no unique origin.

I could take this pair of objects sitting nose to nose, pick them up, slide them over by T, put them down again. And I have the relation that gives me this neighboring pair. Pick it up again, move it to the right by the same translation in the same direction, put it down again. And I've got this pair.

So that is one operation that can exist in patterns. This is the operation of translation. So let me call that by a vector relation. And it has magnitude. It has direction, but no unique origin, just like a plain old vector. So in other words, I can't say that the translation moves us from here to here or from here to here. It's all the same thing-- magnitude and direction, no unique origin.

In fact, all of these patterns have translational periodicity. There's a translation in this bottom pattern and another translation from here to here in the middle pattern. The thing that makes a crystal a crystal is that it is an arrangement of atoms or molecules which is related one part to another by the operation of translation.

If you don't have translational periodicity, you do not have a crystal. So that comes to the essence of what crystallography is about. You can imagine, in one sense, the generation of this pattern by a rubber stamp sort of operation.

Suppose I have a rubber stamp. And I put on the rubber stamp the pair of motifs like this. Pick it up, move it over, chunk. Pick it up, move it over, chunk. And I can stamp out the pattern in that fashion.

Notice that my statement about no unique origin in these terms can be stated that it doesn't matter where the two motifs are on the stamp. they could be up in the upper left hand corner, right in the middle, down in the bottom. As long as I move the stamp through the same distance and the same direction, I get the same pattern.

Now, that's not bad for an introduction. But I want to be more general than this because when I deal in terms of a rubber stamp operation, that is a transformation that involves taking one little chunk of a two dimensional space, picking it up, and putting it down in another location to another unique location in space.

So I'm going to now make another generalization that operations, which we've begun to define, act on all of space. So I don't want you to think of this repetition in terms of a rubber stamp, although we could get the pattern that way and it's conceptually appealing. But I'm going to say now that this string of motifs has translational periodicity if, when I pick it up, move it by T in a particular direction, and drop the whole infinite chain back down again, it is mapped into congruence with itself.

Which leads me to another definition-- an object or a space possesses symmetry when there is an operation or a set of operations that maps it into congruence with itself. In other words, in plain words, you can't tell that it's been moved.

OK, is there anything else that is a transformation which leaves the set invariant? OK, if we look at the first pattern, there are [? rho ?] sides such as this one here, or this one here, or this one here, about which I can rotate one motif into its neighbor or, for that matter, pick up the entire chain and flip it end over elbow through 180 degrees. And it will be mapped into coincidence with itself.

And that is an operation, and another sort of distinct operation of transformation. And this is one that I could call rotation for obvious reasons. And there are two things I have to tell you about a rotation operation. The first one is the point about which the rotation takes place, and that's going to be some point. And let me call this point here A. So this will be some labelled point that is the location of the rotation axis.

But then, the other thing that I have to tell you is the angle through which I'm going to rotate. And I'll append to the A as a subscript the angle of rotation. So this particular operation, called a twofold rotation because it rotates through half of a circle, would be the operation A pi. This point is A. We rotate through an angle pi.

This pattern here has also rotational symmetry. In addition to the translation, there is a rotation operation, A pi, in the lower pattern. So the follow who is unfortunate enough not to have a seat-- and I should have given you this one a long time ago. I'll give that to you as your reward for giving the best answer. And you get a seat wherever you would like to place it.

The first and the final pattern are the same in the sense that they contain two operations, translation and rotation. This pattern is a much more interesting one. This also has a rotational symmetry, A pi. It also is based on a translation.

But now, there's another operation that we can do to leave the pattern invariant. There exists [? rho sides ?] that pass through the center of this rectangular figure across which I could flip an individual motif, or for that matter the entire pattern, from left to right. It's a reflection sort of operation.

So this is a new type of transformation. So we'll add that to our list. And the symbol that's usually used to indicate the locus of this operation is m, standing from mirror.

And that does it for these particular patterns. Three sorts of operations-- translation, rotation, and reflection. And in fact, that is all you can have in a two dimensional space-- not necessarily a rotation that's restricted to 180 degrees. If these patterns are translational periodic in more than one direction, you can have higher symmetries.

One of the things I would like to suggest to you is that you look around you in everyday life at the sort of patterns that enrich your environment. I see a one dimensionally periodic pattern there, the black and white stripes. It's translationally periodic, going up and down. It also has mirror planes running through the black stripes and the white stripes.

I see another two dimensional pattern back there. That has translation. But you could rotate-- no, you can't do anything. That just has translation, nothing else. Get a new shirt. That's not terribly interesting.

There's another one there that's so complex I don't think I can look at it without climbing all over him and drawing some translational vectors and things like that. But that's a nice periodic pattern. That's a good one.

But there's lots of stuff like that. Look at the grills in the ventilators. They have mirror planes. They are translationally periodic in one direction.

We've got floor tiles. These are lovely because these have examples of 90 degree rotational symmetry. Same is true of the tiles up in the ceiling, same sort of pattern. And there's another pattern with four-fold symmetry in the grills that are underneath the fluorescent fixtures.

So symmetry is everywhere. It surrounds us. We wear it. We walk on it. We sit on it.

And think how much richer your life will be when you can understand this part of your environment. Hey, that's a good, chauvinistic note, overstated, on which to end.

So why don't we take our break? I'll hang around if you have any questions or get you a copy of anything that came around that you missed getting one of. And it is now, according to my Timex watch, about three minutes before the hour. So let's take a break and stretch for 10 minutes. Ya'll come back because I've got your name's on a list.