Today, clearly, I am a noble gas.

Thanks to-- it was actually the TAs' idea.

And I was like, of course, that sounds awesome.

So I hope you guys have a fantastic Halloween.

Obviously, what you want to do is any kind of trick or treating or partying, you know the drill, you bring your periodic table, because you never know.

And that's what happened-- so on Sunday right before the exam, I got this.

And so this is Charles and Raymond.

And they're saying we wanted to celebrate the Sox victory in Boston, but because the midterm was the next day, we brought along our periodic table to study.

There were so many people moving around it felt like we were in a sea of electrons.

And of course, the only thing that could have improved on that was actually like a little dance video.

But that will probably come.

I'm sure there on that next.

But you see, they brought it not just to study for the exam, because they didn't know if it was going to be important or not at the rally.

You never know.

So make sure you have your periodic table with you.

Now, OK, oh, yeah, they mentioned the exam.

So speaking of the exam.

Here are the results.

And you can see that there is a pretty wide distribution.

You can also see the averages is 77.

And just to remind you-- that's about here-- just to remind you, these marks, 85, that's the A range.

This is the B range.

So the average was in the solid B range territory.

And so it goes.

The standard deviation was 12.

Now I could tell-- you know, the exam 1, the topics of exam 1 many of you had already seen.

And I think in this exam, some of you had not seen some of these topics, especially like the crystallography, but also even the molecular orbitals, the band structure.

And I could tell that, you know, some people had to work harder, maybe a little bit stressed, and I could sense, some of that.

But when I get stressed what I do is I need to kind of de-stress somehow.

And sometimes some people listen to music, some of the other things.

I always like comedy as a way of relaxing.

And so what I do is I'll Google like for articles about Harvard.

And so I found this one.

This is actually an article in The Crimson from a few years ago.

And the most common grade at Harvard is actually an A, a solid A, the most common grade.

Suspicion that the college employs a softer grading standard than many of its peer institutions.

You think?

I mean, if everyone's getting an A, you think?

So what I wanted to point out is there's a difference.

And it's not just about your privileged, therefore, you deserve an A, whereas we know that that actually takes work.

That's not the point I want to make.

The point I want to make is that we know also what to do when we miss things.

We know what to do when we don't get things right.

That's when you do the work.

So wherever you are on this curve, go back and figure out what didn't work.

What did you miss?

Figure that out, because that's where you learn.

Thomas Edison who said, I never failed, I just did 10,000 experiments that didn't work.

You've got to get through that.

You've got to know that it takes hard work.

And that's the thing that we know here.

That's the difference.

So please make sure you do that with exam 2.

We are all here to help you continue learning.

I'm a noble gas.

And speaking of continuing to learn, where were we?

X-rays.

On Friday, we had sort of some other things going on.

But I also was trying to teach you guys about X-rays.

And what we did is we learned how they're generated.

Remember that?

The Roentgen experiments.

And so I want to pick up here with the kinds of X-rays that we have.

There are two kinds of X-rays.

And we learned about those on Friday.

And I want to just remind you about those.

And I also want to show you a video to kind of recapture what they are.

The first kind of X-ray, remember, we plotted this as intensity.

And I'm not going to draw the cathode ray tube again and the experiment that Roentgen did and all that.

But I'm going to just jump to the two kinds of x-rays that you get.

And so if you plot the wavelength of the X-ray versus the intensity of the X-ray, then one kind is the Bremsstrahlung, which comes from that that electron getting slowed down.

And if it slows down, it emits radiation in a continuous spectrum.

And remember, we sort of drew these.

And this would be like the incident electron energy.

Let's say incident energy of the electron.

Maybe like that's, OK, I don't know, like 10 keV.

And then up here the incident energy of the electron was you know something like maybe 30 keV.

And so you see that as you hit that anode, remember what Roentgen did, he took a cathode ray tube and he upped the voltage.

So he really cranked up the voltage.

So those electrons coming off the cathode are going really fast.

And then what he did is he put a piece of metal in their way.

And what happened is those really high energy electrons, they see those metal atoms and sometimes they get inside the electron cloud and they turn.

And that's when they give off this continuous radiation.

But we also know that there is a limit here.

Remember that?

We talked about that?

And that this limit is set by this maximum.

It's just the maximum amount of energy that you could get out of a photon being emitted this way would be equal to the incoming electron.

The incoming electron transferred all of its energy to the photon.

So that's why there is a maximum.

And it's also why it increases-- remember, shorter wavelength, higher energy-- so it increases as you increase the energy of the instant an electron.

That is Bremsstrahlung.

Let's watch a video, because this is actually a very nicely done video that captures it with animation.

So OK, here's your CRT.

Now here they come.

Those are those electrons.

And that voltage is high.

So they're coming out.

Look at them coming out really fast.

Lots of kinetic energy.

And then they go.

And then this is what Roentgen did.

He put a little piece of metal in there.

So now those electrons are hitting the metal.

So those are the two things that he did differently.

Remember, the room lit up even when all the lights were off.

There they are.

Nice.

Good electrons.

Oh, and here they go.

And there's a metal atom.

And oh look at that.

Now what are these?

Those are x-rays coming off.

Those are the electrons hitting the metal.

And here's the metal atom.

And as the electron comes in, remember it sees the charge of the nucleus.

And it gets deflected.

And that deflection loses energy.

And that loss of energy goes into a photon.

Now, because these electrons have such high energy to start with, the energies of the photons are very high.

They're x-rays.

And so here's the wavelength.

And you can see that-- well, it's sort of a little hard to see this blue range.

But see higher energy, shorter wavelength.

Lower energy, longer wavelength.

Very nice.

So that's the animation of Bremsstrahlung.

OK.

Good.

Now the thing is what we also learned is that there is another type of X-ray.

There's another type of X-ray.

And in fact, if you crank this up high enough, you can get that other type.

So now, we go higher.

Oh, we didn't see it here.

It just looks like that and that and that.

And then all of a sudden we go up to 40 keV and we see this.

Why?

What happened here?

And what happened here is a totally different mechanism for generating X-rays.

And that was the second type that we talked about on Friday.

Those are called characteristic.

And the reason is that-- remember, we have these levels, which now that we are talking about X-rays, we give them letters, K, L, M, N.

But it's just the quantum numbers.

n equals 1.

n equals 2.

n equals 3.

n equals 4.

And what we said is that the weight characteristic X-rays are labeled is that if an electron is excited from this lower level, if an electron is knocked out of here, then there's a place for an electron from here to go down.

Maybe the electron is excited.

Maybe the electron is kicked out.

And then something here can come down.

And when that happens, just like in the Bohr model, you get radiation.

But now, unlike hydrogen 13.6 electrons, these are keV of energy.

These are very high energies.

Why?

Because it's the one S electron.

And we know that once you get down to those metals, those one s electrons, you go further down the periodic table, 1s electrons are seriously tightly bound.

And those levels have a difference down there that is pretty high in energy.

It's X-ray high in energy.

That's the point.

So now, when that cascade happens, we call that a k alpha.

And if it were to have come from here, it would be called a k beta.

And those are transitions, that unlike this continuous energy, those transitions only happen at very specific energies, delta energies.

The change in energy from L to K-- or for K beta it would be going from M to K.

It's k alpha, k beta.

We use the k because that's the final place the electron goes when it decays down.

So if I just showed you these, well, that would be like k alpha, and that would be like k beta because you know the k beta is going to be a higher energy photon because it came up from a higher level.

Well, you would also have on here some other peaks.

You would have the L peaks.

So you'd have like L alpha, L beta.

So as you crank the energy up, then you can knock out those core electrons and these cascades happen and you get these discrete peaks.

Notice, they will only come when you have enough energy in that incident electron to knock this electron out from the core.

So that's why they don't appear until you get to a certain incident electron energy.

They don't appear until you get to that certain energy.

And so we have a video on that, which also I will narrate.

Is this it?

There we go.

So there it is.

It's a metal atom.

I don't know which one.

OK, there's the incident electron.

You fired it.

And look at that.

It knocked out a core 1s electron, because it had enough energy, very high energy.

That's what Roentgen did, cranked up the voltage, higher keV.

And there it is.

A cascade down and an X-ray comes out.

You see that?

Is that all?

Oh, yeah, and then it's going to draw-- because of those, you get these characteristic peaks.

Now, we call them characteristic, because now you see why.

So unlike the continuous radiation, these peaks depend on the atom, because they depend on the energy levels of the atom.

And so that's why like if you looked this up, you say, well, OK, let's look at the k alpha radiation.

Let's look at the k alpha peaks that come out of different atoms.

They're going to be different.

So you have very sharp lines of x-rays at very specific energies.

For copper, it's 8 keV.

For molybdenum it's 17.5.

Silver tungsten, it changes.

And you can see that it goes up, as that 1s electron is lower and lower energy because I'm adding all these protons.

So it all makes sense from the concepts we've learned.

Oh but see, now that's really useful.

That is really useful, because now I've got a way to have a source of X-rays that is super well defined.

It's super clear.

It's always this-- that's so cool.

As long as I have the same metal, it's always the same.

I can increase or decrease-- well, I can't go below the threshold.

But I can't go above it.

And that peak is characteristic of the metal.

So it doesn't change.

That's really useful because I've got now a flashlight.

I've got an X-ray flashlight where the energy that I'm sending out is always exactly what I know it to be.

I can predict what it is.

And it always will be that depending on which medal I put in there.

So that's a useful thing.

Why is that useful?

Well, that gets to the topic that is the topic of today and of Friday, which is what are we doing with these X-rays?

Well, first, we're generating them.

So that's what we've talked about so far.

But now, we're going to actually use them to determine the crystal that we have.

We're going to actually use them.

We're going to use that flashlight.

And so you can see why this would be useful, because this is the range-- we've showed this before-- of X-rays.

So they have these energies of keV.

And they have wavelengths right around a few Angstrom.

That is a little less than an Angstrom, maybe 2 Angstroms.

See where those wavelengths are?

Well, those are atomic spacings.

Those are like distances between layers.

And so if we could shine these on a crystal and somehow figure out what it is with that light-- oh, there's a way we can do that.

It's called diffraction.

Because what happens is-- and we know this from many fields.

You can think about this just as a water wave, any way.

If the wavelength is similar in size to the features, then you get constructive and destructive interference as a result of the interaction between the wave and the features.

So that's called diffraction.

And you can see it here with this very simple picture of say a water-- this could be like a water wave, a sound wave.

And there it is.

And it's interfering both constructively and destructively along these lines.

You can do this test yourself.

You can take-- I highly recommend this-- take a laser pointer.

Now if I just had a piece of metal-- I don't have a piece of metal, but if I did, then I would shine it on it.

And what you'd see is that the dot would just reflect off the piece of metal.

So I just would get the dot back.

But now I've got this thing here.

Many of you may not know what this.

This is called a CD.

But it turns out that a CD has features in it.

It's got trenches that are like a little less than a micron apart, 100 nanometers.

And this is 500 nanometer light.

So you would expect there to be diffraction.

You would expect there to be constructive and destructive interference.

And when I bounce it off of this, look at that.

There it is.

This never gets old.

I'm not getting just one reflection here.

I'm getting a whole scatter of them that have constructively interfered, because of the feature sizes being the same as the wavelength.

But now, I want to do that with X-rays.

And I want to do it onto crystals.

So how do we do that?

So let's think about that.

And we're going to think about it in terms of what the Bragg father-son pair, who won the Nobel Prize and are on a stamp.

That's what you get when you win a Nobel Prize I guess.

And what they did is they figured out how to do this.

So let's go through that just so we understand it conceptually.

So I'm going to say that I have a set of atoms.

Now, I'm not going to worry about what they are.

But I'm just going to say that there's some plane of atoms here.

And there's another plane of atoms beneath that.

So there is another one and so on and so on.

And now, these would be Miller planes.

These would be Miller planes in the crystal.

And let's just assume they're very, very simple, this plane and that plane.

And now what I'm going to do is I'm going to have some x-rays.

I'm going to have some light shining on this.

And it's going to be incident.

And it's going to be reflected.

But see, I'm going to have another wave here.

OK, let's see if I can get through this drawing, sort of, almost, kind of.

Now, here's the deal, these are waves.

So if I want to draw this as a wave, I might draw it like that.

And if these waves are constructively interfering, let's just complete that, then this wave would look like that.

If they're in phase, then that's what they would look like.

Now, this one's getting reflected off the surface.

So I'm going to do that reflection here.

And if I wanted to come back off of the surface, and this one got through the first layer, this didn't get reflected.

It's going down.

And if I want it to come back up, then this one must also look like that to be in phase.

They must be in phases they come out, or else they're not going to interfere constructively.

You see that?

So those are my X-rays.

They're waves.

They're just waves.

Oh, but this is the whole secret, because if this angle here is theta, then what that means is that this angle is theta.

And if that's true, then this distance is d sine theta, where this is d.

That's just some simple geometry.

So what you know then is, OK, now we're getting somewhere, because you know if I had a wave, this is one wavelength.

So if I had a wave come in like this and one of them is going to get reflected off of this lower surface and the other one got reflected on this, but I don't want them to interfere in any way but constructively, that's what Bragg said, Bragg and Bragg.

That's what they said.

Then the only way for that to happen is if this distance plus that distance-- so d sine theta plus d sine theta is equal to some multiple of the wavelength.

It has to be.

And so what you get is-- well, that's what they have there, n lambda, some multiple of the wavelength, equals 2d sine theta, where theta is the incident angle of that X-ray.

So this is incident-- just to be clear-- incident X-ray.

And these are reflected X-rays.

Now to keep it simple in this class, we're just going to say n equals 1 for 3.091, just to keep things simple, because I want to grasp the basic concepts here.

We're not using X-rays to get the structure of DNA.

But we're going to use X-rays to figure out cubic crystal structures.

I'm going to show how that works.

So this must be true for-- so this is in parentheses-- for constructive interference.

Those dots that you saw interface-- interface, no interference, interference.

This is true for constructive interference.

Of course, you could write any equation you want.

But if you want them to be constructively interfering when they come out, that has to be true.

And that's what the Braggs said.

But we're not there yet right, because now we've got to do experiments.

So we've got to do experiments.

So what does this mean?

Well, OK, I'm going to take X-rays of some lambda.

And I'm going to shine them on a sample.

And I'm going to measure.

So what I'm going to do-- well, I think I have a picture-- I'm going to measure-- there it is.

This is what an X-ray diffraction experiment looks like.

So I've got some sample.

And I shine x-rays.

I've got a source of x-rays.

We now know how to make that source.

And we'll just filter out one of these lines.

So I've got that source, and I can change the angle.

And then I've got a detector.

And I can measure did I get interference or not?

It's just like the dots.

So now, we know that if I do that and I say I scan-- so I've got intensity.

And now I'm plotting it with angle.

So now I'm moving the angle around and I'm changing it.

And, bam, I get interference.

And I see a spot in my detector.

So literally it would look like this.

You would get some angle where there's interference.

And the detector would say ding, ding, ding, ding, ding, I see a lot of x-rays coming off.

And now you change the angle a few degrees and I don't see anything, because it's all destructive from these crystal planes.

So it seems like then if I just vary theta, am I there yet?

The problem is that I might not know d.

A, ha, but we do know d.

We do know d, because we learned about d.

For cubic crystals, we know d.

Because for cubic systems, we know that d of hkl of any plane, the distance between those planes is equal to a over the square root of h squared plus k squared plus l squared.

And that's something that we learned.

This is distance between Miller planes in cubic crystal.

I'm saving time.

I wrote xtal.

I saved a lot of time, which I just wasted by being so proud of it.

I know d.

Well, OK, so what does that mean?

Well, let's take a look, because now I'm going to go back my equation.

And I'm going to say, OK, lambda equals 2d-- and I'm saying n equals 1.

And I'm not going to be very specific.

This is now a d that comes from the spacing between planes that are specified by the Miller indices times the sine of theta.

And I'm putting hkl on the theta as well, and you'll see why.

Because here's the thing, now I've got constants.

Now I've got constants, because look, this is fixed by the source.

So this is a constant.

If I have copper, then it's 1.54 Angstroms.

This is a constant.

This is fixed by the crystal.

That's also a constant.

Fixed by the crystal, because that's also a constants, because it's the lattice constant.

We're not changing that.

So for a given set of planes that these waves are bouncing off of and maybe constructively interfering with, that depending on the theta, then these are constants.

So if I regroup then-- so I'm going to regroup them.

And so I'm going to say that-- let's see, d-- so I'm going to substitute in that expression up there down here.

And I'm going to use a copper source.

So I'm going to say-- well, let me go through this one step at a time.

So d equals 1.54 Angstroms over-- let's see-- 2 sine theta hkl.

Now what have I done here?

This is for a copper source.

So I'm fixing in the constant.

So that's the Bragg condition.

But I also know that d is equal to-- I don't want to write it again.

It's also equal to that.

OK, good.

OK, so let's put that together.

We'll do a little division.

And what we get is 1.54 Angstroms over 2a squared, the whole thing squared.

I'm squaring it-- I don't want the square root-- equals sine squared theta hkl over h squared plus k squared plus l squared for-- let's be very specific-- for constructive interference and a copper source.

So now, I'm getting specific because this is how experiments with X-ray diffraction are done.

But now the last time I checked, if you got something equal to a constant, then that something also is a constant.

And this is a constant.

And so what I need to do now is figure out I'm going to measure these data is where I get a signal.

Remember, I'm going to now change theta so that I see where I get signals.

Now, those thetas divided by the hkl that they are bouncing off of must be a constant.

They must not change.

That is at the heart of X-ray diffraction.

That is at the heart of it.

And so we're going to do that with a specific example today and Friday.

But before we do that, there's another thing that we can observe.

There's another thing that we can observe.

Oh, this is what it would look like.

So here it is.

So now I I've changed-- now, why do we do 2 theta?

It's kind of historical.

You plot X-ray diffraction spectra.

So this is an XRD, X-ray diffraction spectrum.

This is the intensity of the peaks.

And these are the peaks.

This is a beautiful thing.

I'm seeing a crystal here.

I'm seeing a crystal.

And by Friday, you will be seeing a crystal.

Those aren't just peaks.

Those are planes in a crystal.

Those are planes in a crystal, which tells me not only that I have these planes, but it tells me what crystal I have.

But that's not how we start.

The way we start is we do these measurements and we just read off angles.

So we got to get from there to there, to crystal structure.

So what I want to determine is the crystal structure and the lattice constant.

That's my goal.

What I have is a spectrum that looks like this where all I've done here is put these specific angles here.

And you have to be given-- so this is the aluminum XRD spectrum.

So if you shine X-rays on aluminum, this is what you get if you know also that those X-rays are from copper, which means that lambda is fixed.

So this should be like the information you get to start.

You'd be given this spectrum, given these peaks.

And you've be giving this information here.

It's a copper target.

And from that, we can determine the crystal structure in the lattice constant.

Now, there's something-- oh, why do we do 2 theta?

Well, it's historical.

It could have been theta to make all those dividing by 2s go away.

But instead, you can see that as I rotate this, this changes by theta.

The detector changes by 2 theta.

So that's why extra spectra are given in 2 theta.

There's no other real good reason for it, even though in the Bragg condition, it's not 2 theta, it's theta.

This comes from geometry of the planes.

And this just comes from historical setups and how you move the detector.

So what's measured and plotted is the 2 theta.

But before we go, before we do this transformation, where we take an X-ray spectrum like this and we get the information we want, there's one more thing.

And that is not all reflections are allowed.

Not all reflections are allowed.

And so let's talk about that, and then we'll come back to the spectrum.

Now, you can kind of understand this by looking at just a simple kind of comparison here.

So these are the hkl's.

Remember, that's the hkl for a Miller plane.

This is h squared plus k squared plus l squared.

Why do we put that?

Because we know we're going to need it.

There it is right there.

So we know we're going to need it.

But if you look at the simple cubic, that's simple cubic.

Any combination of hkl is OK.

There is no combination that would give you interference along those plains stacking.

You may say, well, OK, yeah, what are you talking about?

Why are you even bringing this up?

Well, when you see the other two crystal structures you'll see what I mean.

So now we have the case of BCC-- when you see this, you see BCC and FCC.

And what I'm showing you here isn't the 100 plane.

It's the 200 plane.

So this is the family-- remember, the family-- of 200 planes.

There they are.

But now you see that what happens-- and I have a picture here to show you, but I'll tell you first-- what happens is the light comes in.

So there's those squiggly X-rays.

It comes in.

And there is, OK, d, which depends on the lattice constant, is related to the lattice constant.

But look.

Now there's another plane in between.

There's another plane in between.

And in fact, with the 200 planes, that plane in between exactly cancels out the constructive interference.

Here it is.

So there's what I would have had.

If you want to think about this as the 100, there's the 200s.

But notice when I go from 100 to 200s, I add this plane in here.

And because that plane has atoms in it, because that plane has atoms in it, it acts like a mirror, and it can also reflect.

And so what happens is I would have had this nice-- there it is.

There's a picture I drew.

There's that first X-ray bouncing off.

There's the second one bouncing off.

And those are nicely in phase.

So I would see that.

If that's the angle that gave that to me, I'd see that in the detector.

But now, for BCC or FCC, I've got something in the middle.

And that something in the middle is exactly canceling out.

You see that?

So now, it cancels that out.

In fact, that's called forbidden.

You won't see a signal.

And so these are called selection rules.

And for a simple cubic, you can see there's nothing inside.

So there's nothing in this unit cell that could do this.

So everything's allowed.

Whether there's a plane in there or not, it doesn't matter.

The selection rule is whether it's ever allowed.

And for a simple cubic, everything's fine, because nothing would cancel out.

But in here, you see in this 200 case, you can see very clearly from that picture how it cancels out.

But there's many other kinds of angles or planes that might also do that.

And so I'm going to just give you what the selection rules are.

We won't go through and derive them all.

But let's see, they are actually quite simple.

And so I'm going to write them down.

So if we look at allowed reflections, and then we look at forbidden reflections-- so this is what the selection rules tell us-- so if it's simple cubic, then it's any h, k, and l.

And there's no forbidden reflections.

But if we go through BCC and FCC, then what we find is that for BCC the selection rule is that h plus k plus l equals even.

If that is even-- and we won't derive these, but it comes from the same very simple picture I just showed you.

If something is in there that can cancel out the constructive interference, it's going to be forbidden.

Otherwise, it can constructively interfere.

And that's what this tells us.

For BCC, it turns out to be h plus k plus l.

And so here, what's forbidden for BCC is h plus k plus l is odd.

And for FCC it's h, k, l, all odd or all even.

And the forbidden FCC is h, k, l, mixed odd/even.

These are the selection rules.

So if I were to give you the planes that you see, then right away from an X-ray spectrum, you could just use these selection rules right away to know something, to know something about it.

And if you work this out and you look at, OK, so we have simple cubic.

So h squared plus k squared plus 1, 100, BCC, FCC, you're not going to see it.

That doesn't mean that there is no 100 plane in those crystals.

It just means that if you shine X-rays on it, you will not see it.

OK, so the 110, though, now here, OK, so we see our-- by the way, mixed, even, odd, and it adds to odd.

That's why neither one of these works.

Here we go, adds to even, BCC OK, but it's still mixed even odd, won't be FCC.

3, it's not mixed, so it can be a allowable reflection for FCC, but not for BBC.

Because if you add them up, it's on odd, and so forth and so forth.

And look it, 7 doesn't exist, because you can't do it.

No matter how hard you try, you can't get 7.

That's OK.

And there's 8 and 9 and so forth.

So 9 also-- so here it's allowed, but it's not allowed in either of these, because you can't get either of these to be satisfied.

This is what selection rules give us.

And it comes, again, from simple-- oh, OK, well, that that's another thing.

I said a simple, I have to tell you something, because the Bragg condition, it relies on an assumption that's mostly true.

But the Bragg condition requires that the reflection is independent-- some of you may be thinking I did I draw it onto the atom or did I draw it in between atoms?

Where did that thing-- does it have to reflect off an atom?

We're not going there.

With the Bragg condition, it's independent of the atom positions in a plane.

And the second thing which is what I've been sort of alluding to is that the atomic planes are mirror like.

I mean, this is sort of an obvious assumption since I've been assuming they've been mirrors.

But if you start thinking about atom position, you might go back to that selection rule picture and say, well, wait a second, does it always have to hit the atom?

What if this one was over or something like that?

No, no, we assume it's just one continuous plane if there are atoms in it.

If there's no atom in it, then it's not a reflective plane.

But it's continuous in the assumption of the Bragg condition.

Now we go back to our picture.

So what we want to do is, again, our goal, should we choose, our goal is to go from this spectrum knowing this information-- it's a copper target and being able to read off the peak-- our goal is to determine the crystal structure and the lattice constant.

That's our goal.

And let me let me just write this again, because it's extremely important.

So maybe I'll keep that one.

I'm going to erase this and put it right in the middle, because this is what drives XRD.

This is what drives XRD, which is that our goal is figure out what makes this constant always.

Now, you say what is this constant always?

This is the expression, which I'm going to write again.

So what I have if it's a copper source is 1.54 Angstroms divided by 2 a squared.

That's a constant.

That equals sine squared of the theta for some plane divided by h squared plus k squared plus l squared.

So I'm just kind of repeating what I've said and what I've written elsewhere, but that is really it.

That is what we do in X-ray diffraction.

What makes this?

Well, by this what I mean is this term on the right.

How do I make sure that this never changes its value?

Because the thing on the left never changes its value.

And just making sure that you've got that concept, that is this, oh, yeah.

And it turns out I got a recipe for you to follow to do this.

And it's on the previous slide.

And so we'll start thinking about it now.

And we've got five more minutes.

And then on Friday, we will finish this and then talk about what to do with those continuous X-rays.

So what do I do?

Well, the way you do this is systematically.

And the first thing you do is you read off the 2 theta values that generate a set of sine squared value.

So that the X-ray spectrum measures 2 theta.

But you know from here that I need sine squared.

So I'm going to write down the sine squared values.

So that's a first step.

So for the first one, I've got the first peak.

So I would start to log my data.

The first peak and the 2 theta is 38.43.

And the sine squared theta is-- and I'm just going to do that math-- 0.1083.

OK, good.

And the next one, the next peak is 44.67.

And the sine square of that is 0.1444 so on.

So you read off all the peaks and you make those columns.

So I've gone through.

Now the second one, normalize the sine squared theta values by the smallest value.

You say, so why am I doing that?

Trust me, this will achieve our goal.

This will get us there.

This is a nice simple recipe to achieve our goal.

So the next column would simply be sine squared theta divided by sine squared theta min.

Well, I ran out of room there, but that's going to be obviously 1.

And this would be 1.333 and so on.

So that's the next one.

So I'm just setting that the top row to 1.

I'm setting the top row to 1.

Good.

Now, I'm going to clear fractions.

So I've normalized, and now I'm going to clear fractions.

And if I do that, I clear fractions.

Well, you say, what does clearing fractions mean?

It means just what it implies.

I don't want fractions anymore.

It means I just need to multiply the whole set of numbers by something that gets rid of the fractions.

And it turns out that in this case it is 3.

So 3 times sine squared theta over sine squared theta min, and that is going to be 3.

And that is going to be 4 and so on.

We're almost there.

We're almost there.

And we're not going to finish today, but we're getting real close.

That's good.

It leaves us with a sense of anticipation and excitement.

So, OK, I got clear fractions.

What values of h, k, l, if I have this h squared plus k squared plus l squared, would give me the sequence of clear fractions?

What values of h squared?

Now, remember, you say, why am I doing this?

Again, go back to this.

This is why.

I have a simple recipe for you to accomplish this goal.

That's where we're going with this.

So I'm now going to see with those clear fractions, now it's very easy to see what h, k, l's would give me-- h squared plus k squared plus l squared equals that clear fraction value.

So for example, here, well, if this is h squared plus k squared plus l squared, maybe this is 111.

And This might be 200, for example.

So we're almost there.

We're so close.

What we're going to do is I'm going to start on Friday I'll put this up on the board and we'll finish filling it out and going from this matrix to the crystal structure and the lattice constant.

OK, have a great Halloween.