

Happy Friday.

How is everyone?

Woo!

Woo!

Woo!

Cool.

Cool.

I am excited.

We're going to keep talking about XRD today.

We're going to pick up where we left off.

So I filled in some numbers.

And then, we're going to fill out this chart and really get to a deep understanding of XRD.

I'll also talk about Moseley's law and a little bit about another type of XRD that is done.

Now, where were we?

Oh, OK.

We were here.

So on Wednesday-- and before we fill this chart out, I want to go back and make sure we, kind of, get this.

Right?

We talked about the Bragg condition.

And we talked about how the unique thing about x-rays is that their wavelengths are right in that, sort of, precious distance regime of the spacing of atoms in a crystal.

And so if I shine them on the crystal, then they can diffract.

And they can have constructive and destructive interference, but only if they line up.

And that's what the Bragg diffraction tells us.

It tells us the the Bragg condition for when they line up.

And in particular, this is a pretty nice image.

So you can see here's one x-ray coming in.

And it's a wave.

It's a wave.

So it's going to be a wave that goes like that, and then it bounces off of this surface.

Now a second one doesn't bounce off that top surface.

It bounces off of the one beneath it.

OK?

And they're separated by a distance  $D$ .

So this could be any set of planes.

Right?

So here are my planes now.

So these black atoms are one plane.

Right?

But these yellow ones are another one.

That's another plane that you could see.

Remember, one of the assumptions of the Bragg condition is that these planes are like mirrors.

So we lose a sense of where the atoms are exactly, and we just write a mirror there.

And we say it's reflecting off the mirror.

So where's the next one?

And you can take the orange ones.

That's another plane.

The red ones and so forth.

Now you have a wave on top.

OK?

You've got a wave on top.

And then, you got a wave coming down and bouncing off the one beneath it and for those to constructively interfere so that you pick up a signal in the detector.

There's only one way for that to happen.

And that's if this distance plus that distance is equal to a multiple of the wavelength.

Right?

And that is the Bragg condition.

It has to come all the way down to here, which makes that theta equal to that theta.

You see that?

Because they've gone up to this point, up to that line.

They've gone the same distance.

So they're waving together.

All right?

And it's that point where now this is the extra that the one that bounces off of this plane, that's the extra distance it goes.

That's the Bragg condition.

OK?

That's the Bragg condition.

And remember, in this class, OK, so it could be any multiple.

But here, we're just going to assume  $n$  equals 1 because it's the easiest case.

OK, good.

That's the Bragg condition.

Then, we did something beyond just that because that tells us what the wavelength has to be to get a spot, to get something the detector can see because it constructively interferes.

Everything else is destructive.

No signal.

But we did one more thing.

We also said that  $d$  for some set of planes.

Remember, this HKL is just telling me which one of these I'm talking about.

That's what HKL is.

I'm going to pick one of these planes.

And the distance between them is  $d_{HKL}$ .

OK, good.

But we know from before, from our Miller times, we know that that is equal to the square root of  $a^2$  plus  $k^2$  plus  $l^2$  for the [INAUDIBLE]

we're talking about.

All right?

So you see, it's kind of Bragg plus Miller.

Bragg plus distance Miller.

Right?

Miller cubic.

That's what we're really combining here.

The distance given by this formula when we talk about Miller planes, that combined gave us this.

$\lambda$  over  $2a$  squared equals sine squared theta HKL over  $h$  squared plus  $k$  squared plus elsewhere.

And all I've done is substitute and square.

OK?

And we did one more thing on Wednesday.

And we talked about constance.

And we said, well, if something is equal to a constant, then it's a constant.

All right?

That's some good math.

That's some good math.

And so we said, well, that's the whole beauty of these characteristic x-rays because if you take a  $k$  alpha line from copper, it's always 1.54 angstroms.

It's always  $\lambda$  equals 1.54.

That's what's so nice about it.

Doesn't depend on anything else.

Just the metal you put in there is the target.

It's called a target because you're targeting it with electrons.

So the copper target,  $k$  alpha,  $\lambda$  constant.

Lattice constant?

That's built into the name.

Constant.

Constant equals the angle and the plane it's reflecting off.

And so our job then in crystallography and doing x-ray diffraction, our job is to figure out how to keep this thing a constant.

The same constant.

All right?

That's what constant means.

OK?

That's our job.

And that's where we left off.

And we say, OK, well let's take this to the next level.

Let's do an actual experiment.

Now how do you do experiments?

Well you have equipment.

And this is what a really cool XRD machine looks like.

This is what happens when you don't have any money.

[LAUGHTER]

So this is what's in my lab.

[LAUGHTER]

It's true.

You can come see it.

But you see, the point is they knew the same thing.

We don't need fancy equipment at MIT.

No, it's the ideas that matter that you're putting into this thing.

But that's kind of cool still.

I like the way that looks.

Same thing.

Right?

Source.

Sample.

Detector.

That's hard to see.

But source, sample, detector from the 60s-ish.

OK.

[LAUGHING]

All right.

So now it's easier.

Of course, you can understand.

I mean, some of these things have different ways of doing it.

But you can understand changing the angle is going to be easier to move that sample.

Right?

And then, maybe the detector moves.

But you might keep the source x-rays fixed.

And what happens?

Well, you do this, and you generate a spectrum.

So you're changing the angle.

You're keeping this fixed.

And you're saying, what do I got?

Well here, in this case, I'm telling you what I got.

I got aluminum.

I put aluminum in there.

And I shot x-rays.

If anybody gives you an XRD pattern, they got to tell you what kind of x-rays they used.

Right?

That's really important.

At some point, you got to know this.

This is pretty important.

The lambda is from a copper target, and the k alpha lines is 1.54 angstroms.

And this is the spectrum.

And I'm being asked to get the crystal structure of aluminum and the lattice constant.

And I can get that because, look, I can simply read off peaks.

And those are the peaks, and I've kind of highlighted them there.

2 theta.



More for historical reasons, you take 2 theta measurements, even though, in the Bragg condition, it's just theta.

OK, we can divide by 2.

Right?

And so here are those first 4 peaks.

And I've just listed them here.

Peak 1, 2, 3, 4.

Sin squared of half of that.

Gesundheit.

OK, there it is.

And then, we have our recipe.

I gave you this recipe as a way to keep this constant.

All right?

It's an easier way to do it if you scale and clear fractions.

It's just easier.

So that's why I've given you that recipe.

So let's do it.

So first we normalize.

What does that mean?

Well, you have the smallest value of science course data.

I'm just going to divide everything by that.

OK?

So that's where we left off.

One because that's what I'm normalizing by.

And then, this one would be 1.33.

And this one would be 2.67.

And this one would be 3.67.

And so that's good.

But I don't want fractions.

It's going to be easier for me to think about this as integers.

And so we clear fractions.

What does clear fractions mean?

That!

Clear the fractions.

Get rid of them.

Make it integers.

How do you do that?

Find what you multiply this by so that they're all integers.

OK, I got an idea.

How about 3 times 3.

In this case, times 3 equals 3.

OK, good.

And in this case, well, I don't mean-- OK, anyway, times 3 equals 4.

Times 3.

Don't multiply it by a different number.

I'm clearing the fractions for the whole table.

I'm multiplying by the same number.

OK, good.

8.

And this is times 3 equals 11.

So I've got 3, 4, 8, 11.

And that's what I need to work with.

That's what I need to work with because now, you see, it's now-- I hope it's kind of starting to make some sense-- if I can get this to be 8 squared plus k squared plus l squared, well then I've done my job.

I've kept this constant.

That's the trick.

Right?

I've done my job.

I've just made the math easy.

If I can get h squared plus k squared plus l squared to equal these things, then I'm keeping it constant.

So let's see.

What would that be?

So this has to be h squared-- let me just write here-- plus k squared plus l squared.

OK?

I want those to be an  $h^2 + k^2$ .

So if I do that, well, this looks a whole lot like 1 1 1.

That works.

And for 4, 2 0 0.

OK, and for 8, 2 2 0.

And finally, for 11, 3 1 1.

Aw, it's a beautiful thing.

I've gone from angles to planes.

These are planes.

H, k and l mean one of these.

It means one of those.

That's what it means, a set of those.

And I have found now, literally, which ones give me each peak.

This peak is the 1 1 1 plane.

It's x-rays bouncing off of that, reflecting off of that, and the one below it, and the one below it, and seeing where it gives you constructive interference, and gives you the Bragg condition.

And therefore, a peak.

OK.

All right.

Now hold on.

Hold on.

Now, OK, have we determined the crystal structure?

Have we determined the crystal structure?

Can anybody?

How do we get the crystal structure from this, from these peaks?

How do we get?

Well, let's see.

OK.

Let's see.

Could it be bcc?

What else did we learn on Wednesday?

Right?

What else did we learn on Wednesday?

We learned about selection rules.

You got to remember the selection rules.

Those factor in.

So let's write those down here.

Let's remind ourselves of, OK, that's important.

Right?

Now I mentioned how this came about.

I don't need you to know how to derive the selection rules.

But I did talk about why they come about because, for some of these cuts, you could have a plane in between that destroys the signal, depending on which crystal structure it is and which plane you're talking about.

And when it comes down to it, for a simple cubic, it's anything goes.

Anything.

Oh, polonium.

And for bcc, it adds to an even number.

And for FCC, no mixing.

No mixing of odd and even.

Those are the selection rules.

You don't need to know how to divide them, but I do want you to know what they are.

So now we can see, well OK, hold on.

If this were a bcc crystal and they had to add to even 1 plus 1 plus 1 is 3.

Bam!

It's not bcc.

Right?

Yeah?

OK.

Yeah, but now, hang on.

If it's no mixing on even, did I handle that one OK?

Yeah!

Odd!

Even!

Even.

Odd.

This looks like an FCC crystal to me.

Right?

This looks like an FCC crystal.

And I can go even further.

I can calculate the lattice constant.

I can calculate the lattice constant cause it's right here.

It's right here.

Right?

So that's the lattice constant.

That's a number that's a constant  $\lambda$ .

So I could take any one of those planes, any one of those, any one of these four peaks.

And if I did this right, they better give me the same lattice constant.

And that's actually the last step in the recipe.

Did I put the recipe?

Yes!

All right.

This is the recipe I gave you on Wednesday for you all to become crystallographers.

X-ray defractioners.

That's OK.

We'll make it work.

You're X-ray diffractioners.

And the thing is, you got to remember how powerful this is.

Yeah, how powerful this is because we've learned about perfect crystals.

And now, we've just gotten the single most important way to figure out which one we have.

We shine x-rays on it, and we look for diffraction peaks.

That's it.

This is a very powerful tool.

And it is used all over the place in materials chemistry, physics.

You name the field, x-ray diffraction is a starting point for characterizing the crystal.

And so, the last sanity check that you want to do here because it'll help you make sure you did these points correctly, is compute these values because, you know, this is it.

Right?

Sine squared over a squared plus k squared plus l squared better be a constant.

If it's not, then you've done something wrong in this analysis.

Right?

You could just calculate the lattice constant for each peak, and they also better agree.

So I won't do that, but it turns out we did it right.

For each one of these, that is indeed a constant.

We have achieved our goal.

With great power comes great responsibility.

How you use XRD.

How you use XRD.

Well, let's see.

Let's use it to figure out what phase of material we have.



Why does this matter, right?

Well I have a why this matters, but there's multiple reasons for why this matters.

As I think we've talked about, the properties of a material depend on the chemistry in the material, but they also depend on the structure of the material.

And we're making solids, so those structures are crystals, until next week when we destroy the crystals by putting defects in them!

But for now, they're these perfect crystals.

And they have this, kind of, repeating pattern.

Worry about hcp.

bcc, ah we're comfortable. fcc, comfortable. bcc.

Now, this is called a phase diagram.

This is called a phase diagram.

Phase diagrams will be on the quiz next week.

I'm kidding.

They're not going to be on the quiz because this isn't a class about phase diagrams.

But I want you to know what a phase diagram is.

It is a map of materials.

It is like a treasure map, literally because you find I need iron to have a different property.

Oh!

If I go to this pressure and that temperature, aha!

It can have a different property.

Why?

Because it has a different crystal structure.

So the crystal structure of something-- in this case, it's iron-- depends on the pressure and temperature.

And the properties depend on the crystal structure.

So we've got a way now to change materials.

Same element.

I'm just changing its structure.

I love this one.

This is water.

Now don't worry about how complex this is.

Actually, the whole point is it's complex.

This is the phase diagram of water.

Now this doesn't even have them all.

There are 17 current phases of ice.

17 different crystalline structures of ice.

That is incredible.

Right?

You can actually imagine why, from your knowledge in this class already, those are hydrogen bonds.

They're kind of strong, but they're not too strong.

There's a lot of ways that those water molecules could form a solid.

And they do.

17 to date and counting.

Let's see.

And this tells you which one you have.

Now Earth's operating conditions are right around here.

And that's a really good thing because there is a liquid phase in there.

Ice 1 is here. It is ice one.

And it's a really good thing because of the fish because if you weren't ice 1, then when it freezes, it wouldn't have a different density.

And the ice wouldn't float to the top.

And the fish could still live, which they do in the winter because you don't freeze from the bottom.

You freeze from the top.

That's because it's ice 1 and not ice 8.

It would be terrible.

But yet, we know about these.

And how do we know?

We know because of crystallography.

We know because of XRD.

We can figure out.

Now if you're out and maybe it's a Friday night, so maybe this is a good idea-- it's a good time to mention it-- you might get ice in your water out at a restaurant.

How do you know which kind of ice it is?

Talk about XRD.

It's the only real way to figure out which one of these you really have.

OK.

So for example, if I were to think of other types of problems you might get, well, here's a good one.

OK, here's a good one.

So this is an X-ray diffraction spectrum.

And I give it to you, and I don't even tell you what it is.

Why is that?

Here's a pattern that I put something in there, and I measure these pics.

And I tell you the source.

It's the k alpha line of copper.

So that's the wavelength of the source.

First thing is what lattice, what symmetry, does this correspond to?

Is it simple cubic, body centered cubic, or face centered cubic?

Can we get that?

We could get that because of the exact same thing that we just talked about.

Right?

This can not be.

If it were simple cubic, you'd see the peaks.

Mm!

But know that some peaks are forbidden, so they don't show up.

Right?

And you only get peaks that look like an FCC, according to our selection rules.

No mixing odd even at work.

So this is an FCC crystal.

So I've already learned that.

And then to say, well, what's the-- OK, use the 1 1 1 peak to calculate the lattice constant.

OK.

Well, we can do that.

Right?

So the 1 1 1 peak is even labeled there.

It's 38 degrees.

38 degrees.

So to theta is 38 degrees.

So that means that theta-- OK, I can do this one-- is 19 degrees.

OK.

Oh, oh, oh, from Bragg.

Lambda equals to d sine theta.

But look, label, label the plane.

This corresponds to a plane.

So some distance between some planes corresponds to some angle that gave me constructive interference for those planes.

Let's pass it around so you guys can look at these planes.

They're beautiful things.

Now that means that if I look at the first peak, I know what  $\lambda$ -- well I labeled them here.

In the last one, I didn't.

And you want to find those.

Here, I'm giving you the planes.

So if I do that, then  $d_{111}$  equals  $\lambda$  over  $2 \sin \theta_{111}$ , which equals 2.37 angstroms.

OK.

Have I answered the question?

I haven't answered the question yet because, you see, the question says what's the lattice constant.

But I'm very close.

The lattice constant is related because of Miller.

The Miller plains equation for lattice.

Lattice constant.

Distance between any planes.

Oh, this is all just coming together.

And so  $d_{111}$  is equal to  $a$  over 3.

And so  $a$  equals 4.1 angstroms.

Oh, you could go even further.

You could figure out, now that you know it's fcc-- it's a single atom base, it's fcc crystal, you could actually figure out the atomic radius.

I got  $a$ , and I know the close pack direction.

Right?

I could actually figure out the atomic radius.

And I could go into my periodic table and figure out what I have just from the atomic radii listed in the periodic table and the crystal structures.

FCC.

Atomic radius.

Which one is it?

It's gold.

It's gold.

So this is the kind of thing that you guys now have the power to do.

You have the power to do this.

You can go back and forth between-- based on your knowledge of crystals and now your knowledge of x-rays and how x-rays interact with crystals you can do this.

Oh, that went too far.

OK, so now I'm going to get to the why this matters.

So there's two different sources, two different targets.

Remember, we can call them sources or targets.

And notice they both have this continuous radiation.

And I will talk about that.

The [INAUDIBLE] will end with a discussion a little bit on what you can do with that.

But for now, let's keep focused on these lines, these discrete characteristic lines.

So there's the k alpha from molybdenum.

There's the k alpha for copper.

OK, now Moseley, Henry Moseley, was a brilliant scientist.

And he was working with Rutherford and others.

And he was really interested in looking at the trends.

So he took all of these elements.

So from calcium all the way to zinc.

20 to 30.

And he said I want to look at the k alpha lines of all of these.

I want to look at the K alpha lines of all of these.

And what he found was extraordinary.

He did more.

38 in total.

But I'm just going to show you his data for these.

OK?

And what he did was absolutely profound because what he noticed-- there are the lines.

These are actually his measurements.

OK?

These are his k alpha lines.

And what he noticed in going from calcium down to-- ohh-- brass?

OK, we'll talk about that in a minute.

It's supposed to be zinc, isn't it?

Why is it zinc?

Well, why is it not zinc?

Let's think about that later.

For now he noticed that this has a square root relationship to the energy.

So Moseley came up with-- he was working on this in 1912.

OK?



You got to remember 1913.

1912 was when Rutherford did the gold foil experiments.

It had been 44 years since Mendeleev put his periodic table to paper and published that.

So for 44 years, we had a periodic table.

But see, the thing is, there was a huge problem with the periodic table because Mendeleev had this, sort of, brilliant realization that periodicity-- periodicity-- was related to, both, the atomic mass-- and remember, we talked about this-- and the properties, the chemical properties.

That chemical properties.

That allowed him to create in ordering of the elements.

In ordering of the elements.

That is still the ordering, essentially, that we have today.

But the problem is why did they have that ordering?

I didn't really tell you why, sometimes, he was like, well, the properties win.

OK, maybe the mass-- no, no.

Properties win.

Properties need to be aligned in this column, so I'm I'm going to move those over.

Like, that's what he did.

But he didn't know why, except that it made sense to him.

Moseley's experiments told us.

They gave us the why.

Aw, it was so important.

And Moseley's law-- Moseley's law-- was, essentially, him thinking about the Bohr model for these characteristic x-rays.

So he said that  $h\nu$ -- so that's the frequency for some  $k\alpha$  line-- is equal to 13.6 eV.

All that looks familiar.

Times  $z$  minus 1 squared.

And then, he did the difference in energy, just like we've done now a number of times in this class.

That's what he did.

And this is  $3/4$ .

Why this?

Well, let's talk about that in a second.

So 13.6 eV times  $3/4$  times  $z$  minus 1 squared.

Two things about this, right?

One is why is it  $1$  over  $1$  squared minus  $1$  over  $2$  squared?

Well that's because they knew, or at least they were pretty confident, that you had this positive charge in the middle here.

That's the protons and the nucleus.

And then, you had these electrons.

Right?

So you had, like, the  $1s$  electrons.

And then, you had another shell out here.

And so they knew, OK,  $2s$ .

Maybe that's combined with  $2p$ , so it goes on.

So what happens in the x-ray experiment?

Well what happens is you shoot an electron in.

Rank and just crank the voltage up so high that an electron could come and knock that out.

Right?

And so that's what did it.

And so now one of these can cascade down there and give off a k alpha photon.

Right?

This is nothing new.

We've talked about this.

But you see it here in the equation.

You see it in two ways.

First, we're going from 2 to 1.

$1^2$  minus  $(1/2)^2$ .

$3/4$ .

Right?

But second-- and this was critical-- the z minus.

The z minus told us that all these positive charges in here, all these positive charges, are screened perfectly by one electron, this one that was left.

And it works.

He assumed perfect [INAUDIBLE].

So what do all these see?

They see z minus 1.

They see z minus 1 if z is related to the atomic number.

Now here's where this was so powerful because when you-- and if you can't read this, don't worry about that.

I just want to show you that it is a perfectly straight line.

When you plot the K alpha transitions, these are different elements.

These are his different elements.

And if you plot the square root of the frequency versus element, it is a perfect line that holds.

And so what Moseley wrote in the paper is we have your proof in 1930 that there is, in the atom, a fundamental quantity.

A fundamental quantity, which increases by regular steps as one passes from one element to the next.

This quantity can only be-- only be-- the charge on the central positive nucleus, of the existence of which we already have definite proof.

Now we know about that.

We know from experiments that Rutherford did that that nucleus had the positive charge.

But they didn't know that it was connected to the position in the periodic table.

In fact, years later, people talking about those experiences-- I mean, people didn't even take Rutherford's experiments as seriously until Moseley's work came along.

44 years had come since Mendeleev.

But Moseley gave it the foundation that it needed.

Periodicity is because of atomic number.

Periodicity is atomic number.

That was not known.

That  $z$  gives you the periodicity.

Right?

And that gives you, also, the number of protons.

This was a time when they didn't know what was going on.

Why did the mass change so much the neutron wasn't discovered till 1932, 20 years later?

But this gave the grounding that was needed to the chemistry of the periodic table.

It was a very important discovery.

Very, very important discovery.

So that's my why this matters.

And it's really tragic because he died, tragically, in World War I at age 27.

And the Nobel Prize was not given in 1916 for either physics or chemistry.

He died in 1915.

And most people, at the time, believe that he would have won it at age 28.

That's how important that discovery was.

OK, let's go back to brass.

I got to go to brass.

What's going on here?

What is going on with brass?

Right?

Any ideas?

Why didn't he just put zinc there?

It looked so good until brass!

What is going on?

Well, ha, here, I'll give you a hint.

OK, the melting temperature.

Let's see.

Ah, brass.

OK, zinc melts around 420 C. Brass, which equals zinc and copper, melts at around 900 C or more.

Greater than 900 C.

That's a hint because if we go back to the video-- let's go back.

Oh, the sound is on.

Those are the electrons!

A small portion of the time.

Let me set that up because I'm doing in the middle.

The electrons are coming off of a cathode because Rankin has cranked the voltage way up, and pumped all the air out.

So those electrons are coming off with thousands and thousands of KEV.

OK?

They're coming out.

And that's what's on the right here.

There they are.

The cathode is shaped to focus the electrons onto a small portion of the target, which increases the intensity of the x-rays produced.

The target is, typically, a piece of tungsten or molybdenum, which may be embedded in a stationary water or oil coiled rod, or on a rotating disk.

The high speed electrons collide with the target and rapidly lose energy.

There are two x-ray producing interactions between the incident electrons and the atom.

Ah!

Look at the power!

You can feel the power coming into that tiny little piece of metal.

Now some of the time, you get the transition that we talked about.

You knock an electron out, and you emit a photon-- a k alpha photon-- or maybe an L beta photon.

Right?

And sometimes you slow the electron down so you get the Brahm's fraulein.

But there's so much energy being pumped into this material.

And a lot of times, those electrons just collide and heat up the metal.

That metal is getting extremely hot.

And in these experiments, either you cooled it, or you might rotate it quickly so that it gets to cool down.

It gets a little break.

Or you do both.

Or you just throw up your hands and you say, you know what, I'm just going to go for an alloy that's got some zinc in it, but won't melt every time.

Yeah, that was a good idea.

So you put brass in, OK, you're going to get the copper lines.

But you'll get the zinc lines.

You'll get the zinc lines.

And that was why he used brass.

And that's why you can see you get extra lines in the case of brass.

Al right.

Good!

All right.

Now I am very excited about Moseley.

You know, it allowed us to actually understand this not just because.

Look at this.

Mendeleev was like, you know what, cobalt and nickel can't be swapped.

Hey, all you people who just think about mass, you're not going to put them in the order you think.

I'm changing that.

I'm changing it because properties matter.

Moseley said, no, you're changing it because it's the right order because of the blue numbers.

You're changing it because there is an actual count here that matters.

And that is why your periodic table is what it is.

Absolutely critical.

It put the lanthanides in the right place.

It allowed the prediction of elements-- like [INAUDIBLE] and a number of others that hadn't been discovered yet-- and it set it all on this much more solid grounding.

So that is the contribution of Moseley.

I can't help it!

I'm very excited so I brought t-shirts.

I knew I was talking about Moseley.

Now-- Woo!

I'm going.



OK.

All right.

There.

And in the middle.

And over there.

[CHEERING]

And over there.

[CHEERING]

And over there.

This way!

And, oh!

That's a bad arm.

[CHEERING]

And up there.

[CHEERING]

Hold on.

Hold on now.

OK, there.

There.

And this is all for Moseley.

Ah!

This is all for Mosley!

[CHEERING]

All right.

Now, OK.

[SIDE CONVERSATION]

Now apart from me showing off-- I don't have much of an arm-- one thing I'd like to say is, if you did already get a t-shirt, please, just hand it off to a friend or somebody.

You know, let's share.

Sharing is always caring.

Now here's another type of x-ray I want to talk about.

And z, actually, this is much less used today.

I hope you've gotten a sense of how powerful these characteristic x-rays are.

You know exactly what the wavelength is.

But in the very earliest XRD experiments, it was the Bremsstrahlung radiation that was used.

And that was by Van Laway.

So I want to just tell you about that.

And so here's an example of an Mo target.

Now let's remind ourselves what we're looking at.

These are x-rays.

These are x-ray intensities versus wavelength.

And this corresponds as 5, 10, 15, 20.

That corresponds to the [INAUDIBLE]..

Electrons.

That's thousands of electron volts of the incoming electron.

That electron that came in here and knocked this out from the cathode.

Right?

OK.

Now that electron-- if it comes in, and we talked about this already, but let me remind you-- if it comes in at, kind of, a low energy, well, you're still going to get this continuous spectrum.

This continuous spectrum.

Oh!

Why does it look like that?

Beyond the scope of what we need to know.

But in case you're wondering, it has to do with very complicated effects that happen when x-rays come off and then are reabsorbed by the same material.

You can imagine that that could lead to all sorts of interesting cascades of absorption and emission.

That's what leads to this shape.

But we don't need to know those details.

What we need to know is that as you increase the power of those incident electrons, you're going to get more and more intensity of x-rays.

And this goes down.

The minimum wavelength or maximum energy of the continuous spectrum-- the maximum energy goes up because the maximum energy you can get in the continuous spectrum is equal to the incident electron itself.

So it's set.

Right?

Remember the Duane something limit?

Duane Hunt?

OK, we talked about that already, how to get that value.

Yeah, but then you get to this certain point!

And look, all of a sudden, the characteristic lines appear.

And those are the K alpha lines for molybdenum.

Why all of a sudden?

Well because you got over the amount of energy needed to kick out a 1s electron from molybdenum.

That's exactly why.

Before that, you had enough energy to produce x-rays, but not enough to kick out the 1s electron.

It's kicking out the 1s electron that gives you characteristic peaks.

OK, good.

This is all reminder stuff, but I want to get back on that page.

But see now, OK, this continuous part is also used.

And it was used, like I said, by Von Laue.

And Von Laue was, again, a really, really smart cookie.

And he used the Bragg condition to prove that the x-rays and the space light of structure of crystals can be interfered with each other to make this diffraction.

But what he did was different.

OK, so the Nobel Prize was given for this epoch making discovery.

And I'm actually very happy that the people that worked with him also shared the Nobel Prize.

Walter and Paul.

What they did was different though.

They took this continuous spectrum.

And instead of fixing the angle and the lambda-- I'm sorry, instead of varying the angle but having a fixed lambda, they did the opposite because the continuous spectrum has all lambdas.

Right?

And so you can imagine how this works.

Right?

You can imagine how this works.

So in the Laue version of XRD, you shoot the x-rays, which have all the wavelengths in them, at a crystal that's fixed.

I'm not changing the angle.

OK?

I'm not changing the angle.

And what you get are still diffraction peaks.

You get spots.

So In Laue XRD, you have a single crystal.

It's got to be the same everywhere, in this case.

You have a single crystal.

Theta is fixed.

You don't move it around.

But lambda varies continuously.

OK.

And the pattern that you get reflects the symmetry.

Pattern reflects the crystal symmetry.

How is that possible?

Well, you can actually see this by thinking about the-- do I have another picture?

I just have his one.

You can see this by thinking about that model, which is somewhere out there in the sea.

Where is the model?

I don't see it.

Ah!

All the way in the back waving around.

Let's see if I can draw this.

Let's see.

Ah, I'm not going to try.

If I shoot x-rays that have a fixed  $\lambda$  in, but I vary the angle, then as we've been talking about, there's going to be certain angles where you get constructive interference.

Now if I keep the thing fixed and I shoot all  $\lambda$ s into it, well, take a look at the crystal.

Imagine that I'm holding that structure right now.

OK?

Well I'm going to see this set of planes here.

So I'm to see this set of planes.

Maybe they're [INAUDIBLE] planes.

I don't know.

Right?

And I'm going to bounce off of that and constructively interfere, maybe, if I've got the right lambda.

But see, if I'm looking at the crystal and it's fixed, I'm going to see also there's another set of planes like that.

Do you see?

There's another set of planes like that.

And if I'm a different wavelength-- not the same one, but a different one-- I might constructively interfere with those.

But you can see that the angle that I make will be different.

And so I'll put a spot in a different place.

You see?

So I've got all the wavelengths there.

And as they constructively interfere with different planes that they see, they make different spots.

They make different spots.

And that's what those are.

In those spots, it's more complicated to get crystal structure from those spots.

It's more complicated.

You can get symmetry fairly easily.

But getting the structure itself is a little bit more complicated.

It can be tricky.

And for that, another reason most work today is done with characteristic peaks, XRD.

But this happened before.

And so I wanted to show it to you.

And this resolved, actually, in one of Laue's very famous papers.

It resolved the structure of zinc sulfide.

It was very important work.

And those are the spots.

Look at that pattern there.

See, the thing that you could get is the symmetry.

Oh, by the way, by the way, I'm not going to test you on Laue.

I'm only talking about it for five minutes here.

So in this class, I want you to know about using characteristic peaks, and all the things we've been talking about.

Laue is just on the side for knowledge.

We won't test on this.

But I want to end by telling you a story.

This tells you something about crystal symmetry.

What is symmetry?

Well it just means, if I rotate it, is it the same?

Or if I translate it, is it the same?

Give me just one minute because this is actually a really interesting story.

That's translational symmetry.

We looked at this picture already.

There's no rotational symmetry.

To get back to this picture, I'd have to rotate the whole thing by 360 degrees.

But see, there are crystals that actually have only rotational symmetry and no translational



symmetry.

And Dan Shechtman was the one who discovered these in the 1980s.

Nobody believed him.

His advisor told him to go back and read the book.

And you know who wrote the book?

Linus Pauling.

Linus Pauling wrote the book on chemical bonds.

Literally, the book was called The Chemical Bond.

And Linus Pauling took the lead.

He won two Nobel prizes, not one.

He took the lead in attacking Shechtman.

Shechtman had discovered quasi crystals.

Shechtman had discovered quasi crystals, but nobody-- he was fired his papers.

His papers weren't published.

And for 10 years, nobody believed him.

Linus Pauling said famously, "There are no such things as quasi crystals, only quasi scientists." That's how bad it was.

Oh!

But Shechtman had his day.

He won the Nobel Prize.

And he had his day.

And he was proven right.

And these quasi crystals are absolutely fascinating.

Rotational, but no translational symmetry.

Have a great weekend!