PROFESSOR: OK. We're still on Exam 2 of the fall 2009 class. We're going to be doing problem number 2 now. This is the x-ray problem, as I like to call it. It's kind of exciting. Let's talk about what we need to know before we actually reasonably try to attempt this problem. So I would review these things again.

We want to know emission line nomenclature, how to name emission lines. We want to know Moseley's Law. We want to know Bragg's Law, and I would also emphasize, I'll get onto it later, you want to know how to derive Bragg's Law as well. We want to know, this is pronounced Bremsstrahlung, it's a German word which means breaking radiation. So Bremsstrahlung radiation. And we also want to know some reflection rules, and I'll sort of elucidate that a bit more. But let me start you off in that direction.

So getting on to part A, we are told that somebody has been horsing around with our x-ray machine. We've all had this problem before. And they've changed the target. So let me first tell you what a target is, and how the x-ray machine looks. Then we'll be able to understand what exactly it is we're trying to figure out. An x-ray machine, basically the x-ray source involves electrons being accelerated into a target material, a metal. And then that gives off a whole bunch of electromagnetic radiation, so photons. Some of those photons we'll talk a little about later, in the Bremsstrahlung spectrum, are very characteristic of the material.

So I'm going to call, you know, we have long wavelength photons, short wavelength photons. Some of the photons have a very characteristic wavelength or frequency that corresponds to a particular electron transition. We're going to talk more about this in a little bit, but I'm going to call this the K-alpha photon, OK? So that just happens to be in metals, x-ray.

We know that for particular materials, we have particular K-alpha wavelengths. And what's basically happened in this problem is that, you know, maybe we knew what this material was before, and then all of a sudden we weren't around, somebody switched it on us, and now we have to figure out what it is. Don't you hate when that happens?

So the best way to approach this problem is to understand Moseley's Law, and then have it on your equation sheet. We allow all of our students to have an equation sheet, and also a periodic table. So don't panic if you can't memorize this equation. Our students are expected to, not to memorize it, but to understand it.

So this is Moseley's Law. And Moseley's Law basically tells us, let me go through these variables. We have the wave number. We have a Rydberg constant. This is a bunch of physical constants, sort of agglomerated into one big one, to save us some time. We have the final energy level, where the electron ends, and we have the initial energy level where it begins. And then we have z, which designates our element. So it's the number of protons we have in the nucleus, for example. And then we have this sigma. OK?

So, you know, in order to solve this problem, we want to know what element. So obviously, we're looking for z. Now the question is, do we know everything else? So yeah, we definitely do. Let's just go through each individual thing that we know. So we know Rydberg constant. That's just, you know, have that on your equation sheet. It's a bunch of constants agglomerated together. We know that, for K-alpha we're told, this is K-alpha radiation. Let me draw a cartoon for you here. OK? This is our nucleus, OK? This is n equals 1, this is n equals 2. I'm going to go kind off the board. This is 3. OK? And K-alpha corresponds to an electron dropping down from n2 to n1 to here, and then giving off a photon. So I'm going to draw a photon as a squiggly line like this. OK? So this is going to be h nu. This will give you our K-alpha radiation.

So we know all of those things. We know our wave number here. So we know pretty much everything. But what is sigma? Well, sigma is the correction factor that Moseley found. Now, if you're looking at this and you're thinking, wait, this looks a lot like the Rydberg equation, it's because it's sort of is. The only difference is that the Rydberg equation is only for hydrogenic-type atoms. OK? So we're talking about hydrogen, we're talking about helium plus 1, lithium plus 2. We can't assume that our target is hydrogenic, so we can't use the Rydberg equation. So we're using Moseley's equation.

And what Moseley found, just to show you where the sigma sort of comes from, and this is actually reviewed in, I think, lecture 17 of the online postings. What Moseley found was that if you plot your wave number versus your z, you've got points like this. You've got some sort of line. OK? So this is what Moseley found. And what Moseley basically did, was he fit an equation to it. And the equation looks a lot like the Rydberg equation. And because these don't intersect the origin, we've got this fitting factor right here.

We know that for a K-alpha transition, we're looking at a sigma equals 1. OK?

So we're good. We know our sigma. We know our n's. We know n final is going to be 1. We know n initial is going to be 2. We know the Rydberg constant, and we know our wave number, because we're given our wavelength here.

So we can go ahead and actually just calculate z. And let's do that right now. So let me rewrite this equation so that it makes more sense. Rydberg constant. 1 over. our n final. That's 1 squared minus 1 over, our initial point is 2 squared. We're looking for our z, and we're going to subtract off 1, because we're dealing with a K-alpha transition. So you're expected to either remember that, or have it on your question sheet. There's no way to derive that unless you've got all this data, which you won't have.

So we've got this squared. We know everything, so we can basically reduce this. This is why on the answer sheet, you see something like this. You kind of skip all these steps, and we went right to this. 3/4 z minus 1 squared. And now you can just solve for z. No problem.

OK? So that's 4 over 3 lambda Rydberg constant to the half plus 1. And that's going to give you about 23. You might get 22.9. You might get 23.1. We're talking about 23. That's going to be the vanadium. That's the answer to the first part of this problem.

OK. We're going to take a second and clean up, and come right back and finish the problem.

We're going to start part B now of problem 2 on the second exam. So we basically have used the Moseley equation to find out an element. And now we're going to switch the problem up a little bit more, and we're going to ask you to find the smallest defraction angle for a particular situation. So what's the situation? Let's go back to our x-ray machine.

The way you actually do x-ray defraction, you know, it's acronymized XRD. The way you do it, is you have to generate x-rays. So we accelerate an electron into some material. That material gives off a whole bunch of photons. You then filter all the photons, so you only pick up a certain wavelength. And we're going to use the K-alpha wavelength. And then you get these K-alpha radiation, which then probes your sample.

So here we go. This is what we're looking at for this part. We've got K-alpha radiation coming in, and it's hitting our structure, which has a crystal, hopefully. You're going to do XRD. And then you're getting off some defraction, anything that's reflecting off of the crystal in some way, like this.

So the thing you need to know to do part B, is you need to know Bragg's Law, Bragg's equation. And that's number 3 on the win list. So I drew this picture here just to define the variables, but one thing I would stress for you at home, is to please, go home and, you know, search online, Google image search even. Look for a picture like this. Search Bragg's Law and look for a picture like this. And it's actually from this. It's very easy, just using geometry, to derive Bragg's Law. Bragg's Law is just the geometric interpretation of this picture. OK?

So Bragg's Law, in its traditional format, is n lambda equals 2d sine theta. And I've defined, I drew the picture to show the variables here. We have n, which is-- we'll talk about n in a second. We have lambda, which is our incoming radiation. We have d, which is the spacing between planes. Whatever plane orientation you're looking at. 2d is the spacing, is there because you need to come in, and then come out again. So you're doing twice the distance between the planes. Theta is the angle at which you're incident on the material. And n is going to be your defraction index. We're not going to worry about that in this class. We're going to assume it's one, for this class and for this exam.

So the question is asking us to find the smallest possible angle of defraction. What that means, is that we're getting all this radiation, it's hitting our material, we're moving our material around. The question is, what's the smallest angle at which we're going to see a peak on our XRD graph?

I rearranged the equation here, so theta equals the inverse sign of lambda over 2d. And we're looking for as small a theta as possible. This question is really just mathematical manipulation. I need to know a couple important details that hopefully you've read about in advance.

So we want to find the smallest theta possible. That's the objective for this problem. I've drawn the arc sine function here. To minimize theta, we want to have the argument, which I call x here, we want the argument to be as small as possible. The smaller it is, the closer to 0 you are for y, which is theta, in our case.

So we want to minimize the term in parentheses. And the way you do that, small theta means small lambda over 2d, which means you want to have a large d. And the reason I'm not using lambda, the wavelength, as the knob, is because lambda is set. Lambda is predetermined by the target material you've chosen. So for our problem, we have titanium as our target material. Which is, we can't change the lambda K-alpha. It's set by that material. So we have lambda K-alpha-- we have k-Alpha coming off, which is characteristic of titanium. So we can't use lambda as a knob.

The only thing we can mess around with here, to figure out this problem, is we have to look at d. So we want to have a large d to minimize this, and to minimize your theta.

To get a large d, we need to know the equation for planar spacing. OK? This is your equation for planar spacing. And as we sort of talked about in problem 1, in the prior video, d planar spacing is the distance between one plane of a particular orientation, and another plane of the same exact orientation. OK? So we're looking at maybe a 011 plane in this unit cell, and a 011 plane in this unit cell. What's the distance between the two? That's what this d is. OK?

So we want to have a large d. And let's look at what we have in the equation for d. We have these hkl. These are the coefficients the Miller indices of the plane. And we have a, which is the lattice constant of the material. We're looking at-- what are we looking at here? We're looking at tantalum. We can't change the lattice constant for constant temperature and pressure. So this is nonnegotiable. We can't change what a is. The only things that we can toggle, the only switch we can toggle now, is h, k, and l. So the only thing we can do, is look at different plane orientations in the crystal.

So this is the logic I used to go through the problem. So you want to have as small an h, k, and l as possible, because the smaller these are, the larger d is, et cetera. So the final piece of information where we have to be clever is knowing how to get the smallest h, k, and l. We're told that we're looking at tantalum. And the students in this class have access to a periodic table, which has a vast quantity of information about all the elements in it. One of the things it has is the crystal structure of pure elements. So for tantalum, we're looking at a bcc structure.

So we're looking at bcc. bcc, from your reflection rules, which is the number 5 on the things we need to know to do this problem-- for bcc, you have to have your h plus your k plus your l-- let me write it over here-- h plus k plus l-- must be even. That's a rule, OK? Proving that is a little bit beyond the scope of this class, but that's a rule that we went over in class, and it's in the lectures as well.

So we have a couple things now. We want to minimize h, k, and l, and they have to be even. So basically, what that means is, we have to go through a couple permutations. So let's think about it. 0 0 0. That's even, but that doesn't really correspond to a plane. That doesn't make, you know, that's not going to help us. 1 0 0, or 0 1 0. So let me write some of those down. Let's look at, you know, 1 0 0. Well, that's not even, so we can't look at that.

So what's the next smallest thing we could go? How about 1 1 0? Those are the smallest coefficients we can have for a plane which has the rule that the h plus k plus l must be even. So this could be 1 1 0, this could be 1 0 1, this could be 0 1 1. But what we're basically talking about, if you remember from the first problem, is the family of 1 1 0 planes.

So I plugged in just 1 1 0 for h, k, and l. You get a d of 3.31 over the square root of 2. And then with that d, you know that you've just maximized the size of your d, which means we've minimize the size of lambda over 2d, and that means we've minimized our theta. And now for theta, we can easily calculate that we're looking at an angle, if we plug in for d, which is 3.31 over the square root of 2, here. And if we plug in for lambda, which is given to us as 2.75 angstroms, we get an answer of 36 degrees. Put that right in the middle.

And I put in the middle to emphasize that this is sort of the logic you have to go through, sort of a, you know, circular logic, to get to that answer. So that's the answer to part B. And remember, this is pretty much math. Just manipulation until the very end, where we discussed the reflection rules for bcc.

I want to go on to the last part now, and I'm just going to erase this. We only need a little bit of room.

This last question was actually my favorite question in the entire class. And actually, we only had 3 students get it right, out of 480. So this was a great question, and if you get it right, then you're doing really well in the class.

So let's look at C. It's really a chatty question. We're not looking for a number. The question basically asks us, we want you to talk about, to sketch the emission spectrum of an x-ray target that's bombarded by photons instead of electrons.

So let's go back over to what we said in the beginning. When we generate x-rays, generally the way we do it, is we accelerate an electron into a target material. In part B, the target material was titanium, but it could be anything. A very common target material is copper. copper K-alpha is a very standard target material, or wavelength to use. You accelerate your electron, and you generate the spectrum of electromagnetic radiation. OK? So this is our spectrum. We have large wavelength, we have small wavelength, we have some wavelengths in the middle.

And generally, what we would see, coming back over here, I'm going to draw it like this. This is what you'd normally see, if you're using electrons. Professor Sadoway refers to this as the whale-shaped curve, probably because we're in New England. But this is what you would normally see. Now, this y-axis is the intensity. That's basically the number of photons you count at some specific wavelength. And you see these spikes. And these spikes correspond to K-alpha. This is K-beta. We'll talk about what they are in a second. L-alpha and L-beta. And et cetera. You'd have M-alpha, N-beta. You go all the way down. But they have very low intensity.

So this is what we would normally see if we use electrons to hit our sample. But we're not using electrons. And this is actually the answer we got for probably 90% of the solutions from students. They just drew the Bremsstrahlung radiation, Bremsstrahlung, breaking radiation. And they walked away, and thought they had full credit. But in reality, this is not the correct answer, because you think about what's actually causing this whale shape. Once you understand where the whale shape comes from, then you understand what happens if we're using photons instead of electrons.

So let's actually understand where these characteristics come from. There's two things to pick up from this plot. We have a whale shape. We've also got these spikes. So first, let's talk about where the whale shape comes from. Let me just do it with blue. We'll talk about the spikes in a second, because they're actually a different phenomenon.

The whale shape comes from-- let me draw it for you. Let's zoom in. Let's zoom in on our target here. So here's our target material. We have an electron hitting it. It's just a metal. And we've got photons coming up. Let's zoom in really close to the surface of that target material. Let's go back over here. So we've got-- looks something like this-- we've got an electron, which I'll draw in yellow, coming in. So here's our electron. It's about to hit our material. Notice I've drawn it with some crystal structure, because that's what we're going to talk about, really zoomed in, the atomic level. Now this electron, we've talked about this in class. What can happen is that this electron could come in-- here's its path, normally, if it wasn't going to get deflected-- it can come in, and it can be deflected. OK? So it can get deflected off-- let me draw the following path in blue. So it can go off like this, like this. It could actually go straight through, without being deflected at all. It could actually be reflected back, like this.

And these different reflections correspond to the electron being accelerated. It's getting accelerated. If we define our system like this, so here's our x and our y, the electron's getting accelerated in the y-direction. This is just a simple location, but what happens, is when you accelerate a charge, you generate radiation. You generate electromagnetic radiation. Accelerating charge.

So, you know, here in the first path, where it comes through, and it gets deflected only by a little bit, you generate low energy radiation, low energy photons. So what we're talking about here is a very large wavelength photons coming out.

So we have an electron. It gets deflected. It's accelerated. And from that point, we're also generating a photon.

Same thing for all these other paths, but for the larger angle deflection. So this one here. And as you actually start deflecting back, you're generating very high energy electromagnetic radiation. And this is all because the electron is basically, you know, is getting accelerated. You can actually have, you know, the maximum energy photon you can give off here is a photon that corresponds to this electron coming in and getting stopped completely by the atom. Think electrostatic repulsion. So it comes in, and it gets stopped dead in it's tracks.

So you have some energy, it was moving some kinetic energy, and now has 0 kinetic energy. The energy of your photon that gets given off is basically the difference in the two. And that's what we call here, on this plot, the short wavelength limit. We're going to write SWL. Because this is lambda, which means that energy moves in the other direction. Lambda goes up, energy goes down. Lambda goes down, energy goes up.

So this is our short wavelength limit, which means that is the maximum, the highest energy we can generate from this setup here. So all I'm saying is that you can get deflections in any angle across this way, you can get deflections in angle and generate any number of wavelengths of photons with the minimum wavelength being this one, that's generated from this situation. So I'll just make it very, very small for you. So you generate all these wavelengths, you create all this energy of photons, and that's what basically corresponds to the whale-shaped curve. You're more likely to get deflections that correspond to something around here, because you have higher intensity, and over here, you're less likely to see those happening. So that's our whale shape.

And now, let's return to the problem. Let's ask, when we use photons, what's the situation? Well, photon means we're no longer looking at an electron. Our photon is coming in. And the thing about photons, is that they're not going to get deflected like that. They don't have a charge. There's no electrostatic propulsion, for example. So a photon will either only be absorbed and re-emitted, or it will go through the material.

So what that means is that there's no process now that will accelerate a charge to create Bremsstrahlung radiation. And if there's no process to accelerate a charge, then there's no way to get Bremsstrahlung radiation.

So the first thing you need to do to get most the points on this problem is to say, look! There's no Bremsstrahlung radiation anymore. There's no charge being accelerated.

So that's sort of the first answer. The second thing to realize is that these spikes still exist. Because the reason for these spikes is a different mechanism than it is for the Bremsstrahlung. These characteristic peaks correspond to the movement of an electron to a different energy level, and then a dropping back down. So it's very characteristic of the material itself.

So a photon can still come in. It could still liberate or move an electron. It could just knock an electron out of its shell. Perhaps n equals 1. And then the n equals 2 electron will drop down and fill in the n equals 1 shell corresponding to K-alpha radiation. If you had n equals 3 electron dropping down to n equals 1, you'd have your K-beta radiation. And likewise from, you know, 3 to 2, 4 to 2, L-alpha, L-beta.

So that's the key take-home message here. The message is that your Bremsstrahlung, the thing that you see in the notes in the class all the time, the whale shape with the spikes, that's two specific mechanisms. The whale, the Bremsstrahlung, corresponds to the breaking of an electron. These peaks correspond to the ejection of an electron, and an electron's moving around energy levels within the atom. OK?

So our learning objectives for this problem, the things that we've taken home from the problem overall, is that we know, for example, Rydberg equation is only for hydrogenic-type atoms, and we know how to use the Moseley's equation now. That was part 1. Part 2, we know Bragg's Law, and how to use it, and what all the variables mean. That's something you should learn and take home. And I really highly recommend that you derive Bragg's Law from the geometric interpretation. And part C, we really wanted to probe and understand who conceptually understood what was happening. And part C tells us, the thing that we learned from it is that this Bremsstrahlung radiation with the peaks that we saw in class, that's two separate mechanisms occurring.

So that's problem number 2, and I hope you did well.