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3.091SC Introduction to Solid State Chemistry, Fall 2010  
Transcript – Exam 2 Problem 1

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Hi there. Welcome. I'm Brian Spatocco. We're going to be going over exam 2 from the fall 2009 semester. The logical place to start on this exam is problem 1. And what I usually do for all the problems is discuss the things we need to know before we start it. So I would recommend reviewing these concepts before attempting the problem. And then attempt the problem and then identify your weak spots.

So here's what I personally found to be important information to know before attempting the problem. So I call it what I need, (W I N), if you want to win. There's four things. The first are Miller Indices. This is a crystallographic notation for figuring out and communicating planes and directions in crystals. So review Miller Indices

We have plane/direction notation. I'll explain a little bit more what that is in a second. Definition of planar density. And for that matter, linear and three-dimensional density as well. And 4, the concept of a crystal basis. And this is actually the concept that most students had trouble with on this particular question. So those are the things I would recommend you look at before starting. And if you haven't, check it out now.

So let's start off with part a of problem 1. And so the question asks us to draw the crystallographic feature indicated and label it clearly. It doesn't actually say if we're drawing planes or directions and that's left to the exam taker to identify. So the first thing I note on that problem, part a, is that we're asked to draw  $0, 1\bar{2}$ . And  $111\bar{2}$ .

So the first thing I notice about these two particular crystallographic features is how they're actually encapsulated. So the first one is in parentheses. The next one is in square brackets. That actually tells us some information about the problem. The first part, a part one, is  $0, 1\bar{2}$ . So you actually need to know what this implies. Parentheses mean we're looking at a particular plane orientation. Now I'm not saying a plane. I'm saying a plane orientation. Which means there are infinitely many planes in a crystal which have this orientation. OK so that's distinguishing between just one plane and a crystal.

The second part, b, we have square brackets. That implies we're either looking at a direction or a plane in a crystal. We also have things like this, which we're not seeing on the exam this time but may show up later. We have these curly brackets and we have these angled brackets. The curly brackets denote a family of planes. And the angled brackets denote a family of directions. And it's markedly different than a particular or plane orientation and a particular direction.

So let's do some visuals here to explain what we mean. So let's start off with a 1. Now we're asked for  $0\ 1\ \bar{2}$ . Now the bars indicate negative signs. So you would know that from your Miller Indices review. Now the way to do this problem-- what I find is the easiest way we reviewed in recitation-- was to not be afraid to move your origin. A lot of people are afraid to move their origin around but we have to remember in a crystal, basically what a crystal is, it's a unit lattice repeated infinitely in three dimensions. So it's OK to move your origin as long as you choose some reasonable point.

So in this problem we're looking in the back bottom left corner. That's our defined origin on the paper. But to do this problem, I would recommend choosing a new origin. I chose this one. And that's really going to facilitate doing this problem a lot more easily. So let's look at what we have to draw now.  $0\ 1\ \bar{2}$ . The 0 indicates that we're never actually intersecting the x-axis. OK, so at no point will this plane-- we know it's a plane because the parentheses-- intersect the x-axis.

The 1 bar indicates that we are intersecting the y-axis at 1 lattice parameter spacing. Miller Indices are a little tricky because they're somewhat inverted. 1 implies you are going the full distance of the unit cell. 2 implies you're going half the distance. 3 implies you are going  $1/3$  the distance and so on and so forth. So for 1, we're going to go the distance of 1. We're going to move negative 1 in y. So we're going to move negative 1. We're going to go to here. That's in our y. And when we actually make this a little clearer. I've chosen a new origin. So here's my y prime. Here's my z prime. Here's my x prime. So we're moving negative 1 and y. We're going to move half, negative  $1/2$  and z. And we're also told that this plane doesn't intersect the x-axis. So it must run parallel to that axis. Which tells me that it's going to run along the x-axis. We're going to get a plane like this. And here's our plane. That's the answer to part a 1. Pretty easy and most students got this correct.

For part a 2 we're asked to draw a direction or point to a particular place in space. I also moved my origin on this problem. And I found it easiest to redefine my origin up here. Which means that my new set of axes are going to be x prime, y prime. I'm going to keep z because z didn't move at all.

OK note how, when I'm drawing these things-- we're going to draw this one now-- that the way I choose to move my origin generally tracks with the negative signs that I have. This problem I had a negative y and negative z, I moved in the negative y, negative z directions. Here I had a negative z. So I just moved up in the negative z. That kind of told me how to move my origin. It made life a little easier.

And now it's pretty easy from here. Now what we're going to do is draw 1 in the x, we'll go 1 in the y, we'll go negative 1 in z. We're pointing to this point. There we go. That's our direction. So pretty easy. Part a 1. Part a 2. So we're batting 100 right now. And just don't be afraid to move your origin. That's the take-away from this part.

The problem, of course, gets a little harder. That's something that we pride ourselves on in 3.091. If it was always this easy, everyone would pass the class and get 100s. So the second part, part b, is asking us to calculate the density of atoms in a plane. So this gets back to what I was saying before. We need to understand the definition of a planar density. OK, so I've sort of defined it here. This is  $\rho$ . Not  $\rho$ .  $\rho$  planar. And  $\rho$  planar, I define-- to help me, maybe it'll help you-- is the number of full atoms in a particular plane-- in this case we're looking at  $0\ 0\ 1$ -- divided by some

area. Because the plane is denoted by an area not a volume. Don't be afraid, I mean densities don't always have to be mass over volume. It can be some unit over some specific distance or area or volume. So that's general density.

So we're looking at the number of full items in a plane divided by the area. We're told that we're looking at Dalium, of course named after Salvador Dali. And so we're also told that we're looking at the 0 0 1 plane. I've drawn a bcc crystal here. As a scientist or an engineer, when you're given a bcc fcc, simple cubic, the first thing you put on that paper is the actual crystal structure. So I drew the Dalium up here. Not a real element, but a make-believe one. And we're going to identify our 0 0 1 plane. This is good practice. So there's our x, y and our z is right here. Our 0 0 1 plane, so we're not intersecting x. We're not intersecting y. We're only intersecting z. So here's our 0 0 1 plane.

Let me sort of bring this down for you. So we can look down on it from above. It's a square, with sides  $a$ . And here's our atoms. So now the question is, how many full atoms do we have and what's the area? The area's obviously a squared. And the number of full atoms in this area is we have four quarters of an atom. When you're in two-dimensional space an atom looks like a circle to you. When you're in three-dimensional space it looks like a sphere. So if you lived in the two-dimensional plane, you would see a quarter of an atom, a quarter of an atom, and so on. You'd have one full atom in this plane.

So this is sort of what we're looking for. And you say, oh, well I'm done. A lot people left it at that. But that's not the answer we're looking for. We want an actual numerical answer. So the question now becomes, what is  $a$ ? So we're going to digress and find  $a$  and then we'll know exactly the answer to the planar density.

So  $a$ -- this is where you have to be a little clever. How do you find  $a$ ? The lattice parameter, the lattice spacing. So the best way to do this is to think both small scale and large scale. So first let's think about a unit cell. Let me ask you, what's the three-dimensional density of a unit cell. So how many atoms do we have per unit cell? We have our bcc. We know in bcc there are two atoms. We have eight corner atoms and they're each  $1/8$ . We have one body atom. So there's two atoms. So we have 2 atoms per-- what's the volume-- well the volume is a cubed. Now we got a cubed. We didn't really make any progress here, we still have an unknown variable. But the question is, how do we get solved for a cubed.

So let's zoom out from that unit cell. Let's zoom out to a mole of material. OK, so a mole of material, how many atoms are in a mole of material? Well by definition, it's Avogadro's Number.  $6.02 \times 10^{23}$ . And then what's the volume of a mole of material? Well looking back at the problem, we're given the molar volume. Which is something that I would recommend you write down. You know all the information you're given, see what you've got. The volume of a mole is the molar volume, which we're given.

So now it's pretty easy. We know Avogadro's, we know molar volume. So we can solve for  $a$ . So not too bad. You'll find that  $a$  is about 2.8 times  $10^{-8}$  centimeters. You could give me 2.85, 2.79. We're worried about the concepts here, not the numbers. So don't go back and waste a lot of time getting the exact number.

That's our  $a$ . And now that we've got  $a$ , we've got our planar density. Very easy. I'm going to write  $\rho_{\text{plan}}$ , just to save some time. And that equals 1 over this number

squared. That's one atom, by the way. And that's all squared. And we're going to find in the end that our planar density is going to be equal to  $1.27 \times 10^{-15}$ . And the units are important. That's atoms per centimeter, squared. If you don't give us the units then we have no idea if you're right or wrong. So always include your units at the end.

So hopefully that helped. We're going to take a second and clean off the boards. And we're going to start with part c.

OK we're back. We're going to finish problem 1 now from the 2009 exam 2. We're on part c. So thus far in part a, we've talked about Miller Indices, we've talked about the plane and direction notation with the parentheses and the brackets. We've also talked about planar density. And I would invite you to review those things. Now we're going to go to part c, which is really the concept of the crystal basis. And this was the part of the problem that most students lost points on. So it's the thing that I would emphasize the most on this problem.

The problem asks us to-- and I put a sad face because that's how people felt after this part-- the problem asks us to draw a particular plane in a fcc crystal. So we're given Magnesia, MgO. They want us to draw that plane and show the atoms. And we also want you to show the relative sizes of the atoms. You know we have anions and cations. And we actually give you the sizes of those ions, so it shouldn't be too tricky on that part.

But I think the best way to start is to go over the answer that was given that was wrong. And then we're going to talk about why it was wrong and how to get the right answer. So to start off, we want you to draw this crystal. The best place to start is by actually drawing the crystal in 3-D and then we're going to take the projection after that. So people think, MgO, they see fcc, and they say, oh that's not so bad. I know what fcc looks like. Let me draw fcc.

I'm going to use for this problem, I'm going to use this red chalk to represent magnesium and the blue chalk to represent oxygen. OK so magnesium, we're going to have it as a circle like this. This is magnesium,  $2+$ . And we're going to have the oxygen-- it's going to be slightly bigger because it's an anion. This is  $O^{2-}$ . Maybe I'll color this in too.

People said, OK easy. fcc. This is a simple problem, easy points. They drew what they thought to be an fcc crystal. So they did-- let's say they put the Mgs on the corners. And they said, OK now I need my faces. So maybe the oxygen are the faces. So I'm going to put in my 6 face atoms. So here are my 1 side here, and I've got the bottom and the top. There's my 6 faces. And they said, OK, easy. I'm done. And then they took the projection of  $0\ 1\ 1$ . We also know, when you put the axes on here just to make it clear. And here's our z, You know  $0\ 1\ 1$ , we know it doesn't intersect the x but it intersects the y and the z at one lattice spacing. So x doesn't intersect. It intersects z here, intersects y here's. We've got this kind of plane going on here. We've got something like this. And they just drew this. It's a little bit of 3-D visualization But they drew that and they got 0 points. The reason that that is not a correct answer is because that is not what MgO-- it's rock salt structure-- that's not what it looks like. And the reason they got it wrong is because they didn't understand the concept of the basis.

So I'm going to make a statement right now. This is a really important statements so I urge you to think about it. A crystal equals a lattice plus a basis. Here's the difference. A lattice is a collection of points. So you have an fcc lattice, you have a bcc lattice, you have a simple cubic lattice. Those are points where atoms-- I use atoms plurally, perhaps-- can exist.

OK, a basis I like to think of as a stamp. A basis represents the most fundamental pattern that you stamp at every lattice point. So let's draw an fcc lattice. So I'm going to draw an fcc lattice on this cube right here. I'm going to put points. So I'm going to make them white. They're just points. I got all the corners. They're hard to see. But they're all the corners. I got the faces. Side, back, front and bottom.

You're saying to yourself, that's like the same thing you just drew. It's really not. What I drew the first time, I put atoms in. That's a crystal I drew. I just a lattice right now. This isn't a crystal, this is a lattice. So to actually answer the question, we want to figure out, we want to draw the 2-D projection of a crystal. So we've got to draw the crystal eventually. Now we're dealing with MgO. We're told MgO is face-centered cubic. Which means that our basis must have 1 Mg and 1 O atom. So I'm going to do that right now. I'm going to draw what I'm going to call to be my stamp. You can use whatever method you think is best. But I call this my stamp. I'm going to draw it like this.

So here's an oxygen atom. Here's a Magnesium atom. And this little white dot is the point that's going to get stamped. And here's my stamp. And the idea is I'm going to take the stamp, this basis-- that's what it is, it's a basis-- and I'm going to stamp it at every lattice point. OK so note I have 8 corner lattice points and I have 6 face lattice points so I'm going to be stamping 14 times. So I'll do the first couple very slowly. I'll take my stamp and I'll stamp here. Here is my O. Here's my Mg. I'll stamp over at this corner. Here's my O, here's my Mg. I'll stamp in the face. Here's the face, the front face one. Here's my O, here's my Mg. So you can see what's happening. Let me just circle it for you. I'll circle one of them. Here's my stamp.

I'm going to go ahead, I'm going to finish drawing this in. It's going to get a little messy for a board. But I hope that you can go home and do it on some graph paper as well. All four corners. The face is here. I have a tendency to leave off faces sometimes. Let me make sure I've got them all. I already did that one. Yep that's right. Is that right? No. OK, now let me finish with the magnesiums. The magnesiums-- it's going to be hard to see-- exist at the center of every edge.

So it's a little tricky but let me explain what we're looking at. What you should be looking at. We have what looks to be oxygen in the face center cubic arrangement. And we have magnesium at all the edges. So you're thinking, this is weird this isn't face center cubic. Look at the magnesium, this doesn't look face center cubic. Well the thing I would challenge you to do at home is actually draw this unit cell out 4 more times. And then you will actually be able to find face center cubic magnesium lattic cell in that larger unit cell.

So this is actually the answer. This is what a rock salt structure looks like. This is MgO. You have oxygen, looks like your traditional face center cubic. And you've got these magnesium stuck on all the edges. So now we're just going to take our projection. Let me use white chalk for that. Or rather we're going to take our plane. We're looking at the 0 1 1 plane. Here's our axes again. Remember it's always right-handed. We're going to do 0 1 1. Not intersecting the x and were going to intersect z

and y. So we're going to come down across the face. We've got this. This is pretty terrible looking. But this is one of the tricks of the problem. You have to be able to visualize these in 3-D space.

So let's slowly transcribe what this plane here looks like projected out on the board. We know that at our corners and also at the faces of this cube, we've got oxygen. So here's a corner. These are our corners. At the faces, two faces, we've got oxygen. What else do we have? We know we must be hitting some magnesium. Well we know that at all the edges-- here's an edge, here's an edge-- we've got some magnesium. What about the center? Well the center we do too because we know that when we made this stamp, the bottom face with this oxygen, we also stamped halfway up a magnesium. So there's actually a magnesium right here. It's there. It's right there. Believe me. There's our magnesium.

And this is what we've got. This is the answer to the problem. Notice how I've giving my oxygens larger than my magnesiums and I've got it looking like this. In fact let me let me emphasize this even more. The fact that you could actually have drawn this differently. You could have drawn it like this. And it would have been exactly the same thing. You would have gotten full credit. You could have drawn this. This is the thing that I would recommend you try at home to prove that this is true. These two are equivalent It's the same thing. It all depends on what you choose as your stamp point. So I could have chosen to put my red at every point, my magnesium.

So this is the answer to part c. This part, most people did not get correct. Less than half the class got this correct. So think about a little bit. Identify crystal as lattice plus basis. And then think about the full scope of the problem. What do we go over? when went over Miller Indices, went over designation and crystallographic notation, so plane and direction notation. We went over the definition of planar density. Think about what linear density means, think about what three-dimensional density means. Don't be afraid to not use mass. And the last thing we just covered was the crystal basis. So review those and hopefully you did well. Thanks.

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