MITOCW | MIT3 091F18 lec19 300k

But I want to pick up where we left off on Monday.

We were talking about the three Bravais lattices.

There a couple more things that I want to say about them.

What we captured, the key essence, apart from they're being these cubic crystals and the different elements that form them, is this idea that you can go from the unit cell, once you know the unit cell, you can get the atomic radius.

So that's kind of cool.

Because you know information about things like, for example, packing.

So then we had the packing fraction, the atomic packing fraction.

Calculated that.

The maximum, the max packing fraction.

Packing fraction.

We calculated things like the closed pack direction.

Well, you can also go to things like the density.

Once you know how to go back and forth.

And so for example, if I want the density of a material, that's grams per centimeter cubed, right?

That's the density.

But you could write the density in terms of the things we talked about on Monday.

So again, you know, I want you to be able to go back and forth.

Once you know the unit cell, and you can know something about the radius of the atom, then you can get the density.

For example, here, the density could be defined as the number of atoms in the cell, times the grams per mole of that element, divided by the volume of the cell, of the unit cell, times Avogadro.

Now, you can go through the units and you can work out that this is grams per centimeter cubed.

So just as an example, if I had, let's see, the example I have is copper.

So example, copper.

So you know, everything comes from the periodic table.

Everything.

Life, class, everything comes from the periodic table.

So I go-- I say, I want to know-- I go to the periodic table.

And instead of looking up the density, I look up other things.

So I look up, for example, that it's FCC.

And then I look up that it's 63.55 grams per mole.

And I also look up the atomic radius.

So I look up these things, the atomic radius.

And that's equal to 1.3 angstroms.

So I look all this stuff up.

And the point is, I can now go back and forth.

I can use the information, because I know if it's a crystal and I know the crystal type, FCC, then I can use this information to get other aspects, right?

So other properties.

So for example, I know that the radius of the atom for an FCC, if it's close packed, if it's-- you know, FCC one element, remember it grows out until they touch.

And that got us how we get the radius of the atom.

And it's a root 2 over 4.

But I also know that there's four atoms per unit cell because it's FCC.

I also know that the volume of the cell is simply the lattice constant cubed because it's a cubic cell.
All the ones here are cubic.
So the volume of these cells are cubic.
From this information, I can compute the density.
So again, it's going back and forth.
The radius of the atoms packed in, the lattice constants, the number of atoms in the cell, these are the things we talked about on Monday.
And as you go back and forth, you can do things like this.
All right, good.
Now we talked about the we talked about the Bravais lattice there, right?
And those are three Bravais lattices that I want you to know.
Bravais lattices.
But the thing is that there's something else you need to know in order to know what crystal you have.
And so this is the FCC Bravais lattice.
There it is.
It's over there on the right.
It's the face-centered cubic.
OK, gesundheit.
And I'm going to pass this around.
All right, oh yeah, I'm starting over here because I keep on starting over there and it's not fair.
That's not right.
Yeah, all right.

Got a couple-- OK, so that's FCC, right? So we're going to write down FCC. But the thing is is that see, this is our stamp. Remember, it's a stamp of points that are equivalent. That's what the lattice vectors are. They are not the things that you put at that point. That is something else. Now, on Monday, we put the things there were atoms, spherical particles. And they're all the same. That was their introduction to crystallography. But the basis can be more than just a single atom. It can be more. So how do we think about the basis? So here's a lattice. This is a lattice of points. The way you want to think about a lattice is a stamp without putting things there yet. The basis is what you put there. Let's write that down because it's so important. So the lattice is all we're going-- oh, I'm going all caps, how to repeat. And the basis is what to repeat. So if this is my lattice and I decide that I want to get a million downloads on YouTube, I'm going to put a cap there.

And this is my crystal. It's a crystal of cats. That's OK. I have done nothing wrong. Because I have simply, according to the rules of crystallography, I've had a lattice and a basis. And I've just defined my basis as a cat. And that's the crystal you get. But see, the basis could also have been, for example, two atoms colored differently to show that they are different atoms. And then this would be my crystal. So the actual crystal that you get may be different than the lattice structure. All right, so let's take a look. So for example, over here, you know, if my basis is a single atom, nickel, copper, gold, platinum, well, I showed you these from the periodic table on Monday, right? We highlighted them when we talked about FCC. Then the crystal that you get is FCC. These are the ones we did on Monday. Those are FCC crystals. But at the same time, if my basis-- check this out. Oh, this is salt. When you guys pour salt on your food, do not see it any more except as this. This is salt. This is salt. It is-- let's see-- simple cubic. Is it, though?

Because a lattice, a simple cubic remember the definition.
A simple cubic lattice would mean a stamp of a simple cube where every corner is exactly the same exactly the same.
That's what a lattice is.
So this cannot be a simple cube.
This is not simple cubic because they're different.
They're different.
At the corners, I've got two blues and then two red and then two other blues.
So they're not the same.
It cannot be a simple cubic structure.
This is an FCC lattice.
This is an FCC.
Yeah, I'm starting over here again.
I'm trying to even it out.
That's an FCC lattice, but with a basis of sodium and chlorine.
So it's an FCC.
You can call it an FCC lattice.
But the basis is a sodium chloride pair.
And this has a name.
It's called the rock salt structure.
It's called the rock salt structure.
It's an FCC lattice with this two atom basis where, look, you can see the FCC lattice here.

Look at those blue points, right?
Blue outlines an FCC lattice.
But now the basis is one atom here and one there.
So now I take that, this pair, and I put that at all the lattice points.
You see that?
You put that in all the lattice points of FCC and you've got salt. And that is how you must see table salt from now on.
Well, we talked about diamond.
This is diamond.
Diamond is the same Bravais lattice.
It doesn't look like it at first.
It doesn't look like it at first.
But see here, I have a different pair.
Here I have a carbon-carbon pair.
Or it could be, or silicon-silicon.
There are actually a number of pairs of that would form this diamond.
In fact, we specify because there are different types.
This is called cubic diamond crystal.
This is the cubic diamond crystal.
What is the lattice?
It's FCC.
It's FCC.

Now, let's take a look at that.
Look, there is my FCC.
Here, here, here.
But inside of the FCC, I've got this pair of carbon atoms.
Now they're the same type of atom.
And instead of one being kind of in the middle of this edge, as it was with sodium and chlorine, now the other atom is kind of off in a diagonal.
But it's still just a pair of atoms.
It's a pair of carbon atoms.
But if you look carefully at diamond, and this doesn't go on in this picture, but it does in real life, this is an FCC lattice of these pairs, repeating everywhere.
That's what diamond is.
It's an FCC lattice.
So the symmetry is FCC.
But the basis is a carbon-carbon dimer, right?
And that gives you cubic diamond.
OK, so there's the Bravais lattice and there's the resulting crystal structure.
Now, speaking of diamond.
And this is a graph that I showed you a while ago when we were talking about the differences between diamond and graphite.
One of the things that you can see that's so important, this is the same element, two different crystal structures.
One of the things that you can see that is so important is how direction is going to be an important

property.

You need to know how to identify direction because you know, in this case, it looks like maybe if I point in different directions, the thing would look kind of the same, or maybe have similar properties along-- but look at this.

This looks seriously directionally dependent.

It looks like if I did something like tried to carry charge or thermal energy this way, then it would be very, very different than if I carried it this way.

Well, we have a word for that.

And it's called anisotropy.

And so this is another important word, anisotropy.

If it's anisotropic, then the property, well, it could be like electrical or thermal conductivity, for example.

Thermal conductivity could be like how it breaks, the fracture.

And so on.

But whatever-- but the property is-- depends.

I'll just say it's directionally dependent.

Directionally dependent.

So the reason I'm telling you this is that I now need a way-- we've come up with sort of ways to talk about crystals.

But I now need a way to specify where I am in a crystal.

And maybe how the crystal cuts.

I need a way to talk about directionality in these crystals.

And that's what I want you to-- that's the topic for today.

So the first question-- well, to jump to the punch line is there are these things called Miller indices.

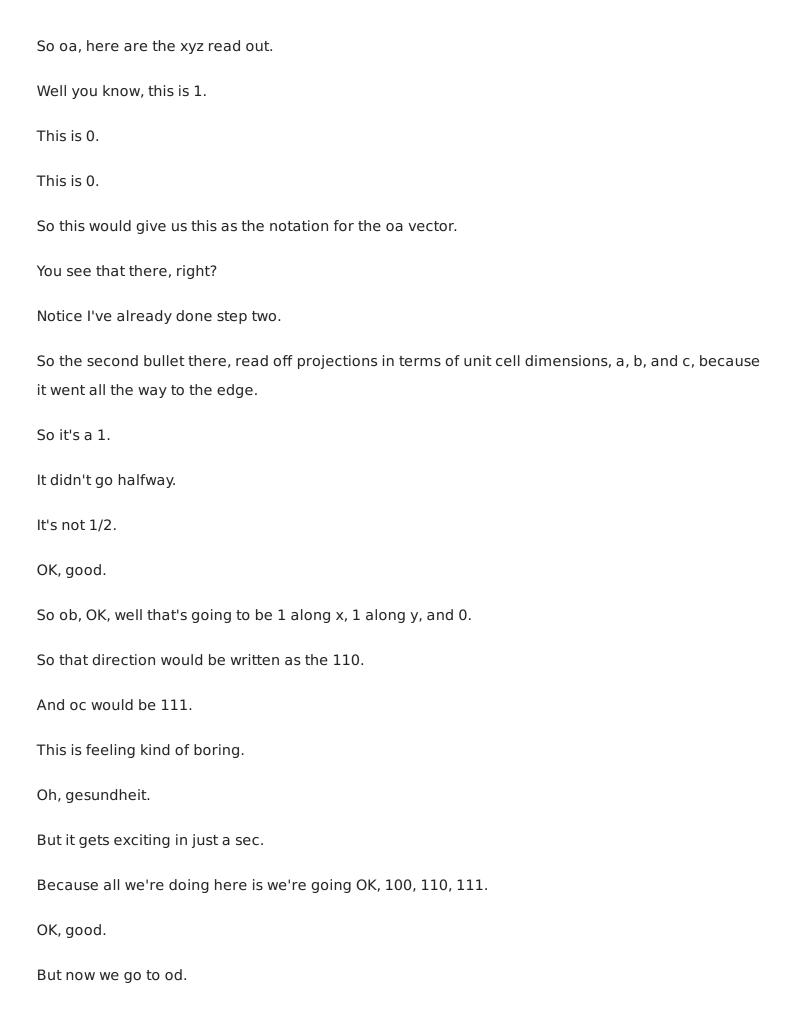
And that's what we're going to learn today. Miller indices and they describe direction and cuts, planes. OK, and the first question you can ask is, where are you? Where are you? Now it turns out that there are these people called crystallographers. And they came up with crystallography over the years. And they have very strong ideas about notation. So we'll be talking about crystallographer notation. And we'll be very careful not to do anything that would upset a crystallographer because that is not something you want to see. But the first question that you could ask is, where are you? So I'm going to draw the planes and we're going to-- the axes-- and we're always going to use the same notation, the same axis directions, just for simplicity. In this class, we're going to say that as we're talking about crystal structures, that's y, that's z, and that's x. x is coming out of the board. y is it going that way and z is going that way. Now, if I want to know where I am, then what I can do is draw the cube. Oh boy, here we go. OK, there it is. And I can just start looking at points.

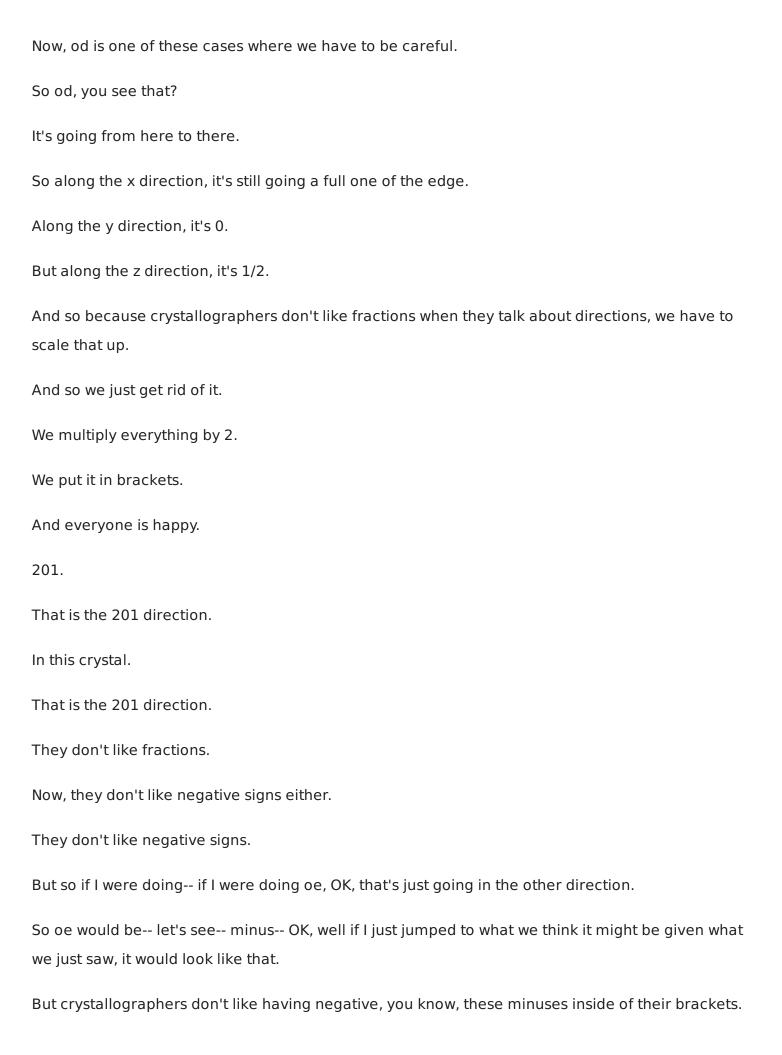
But instead of having all sorts of different numbers, crystallographers like to work with simple

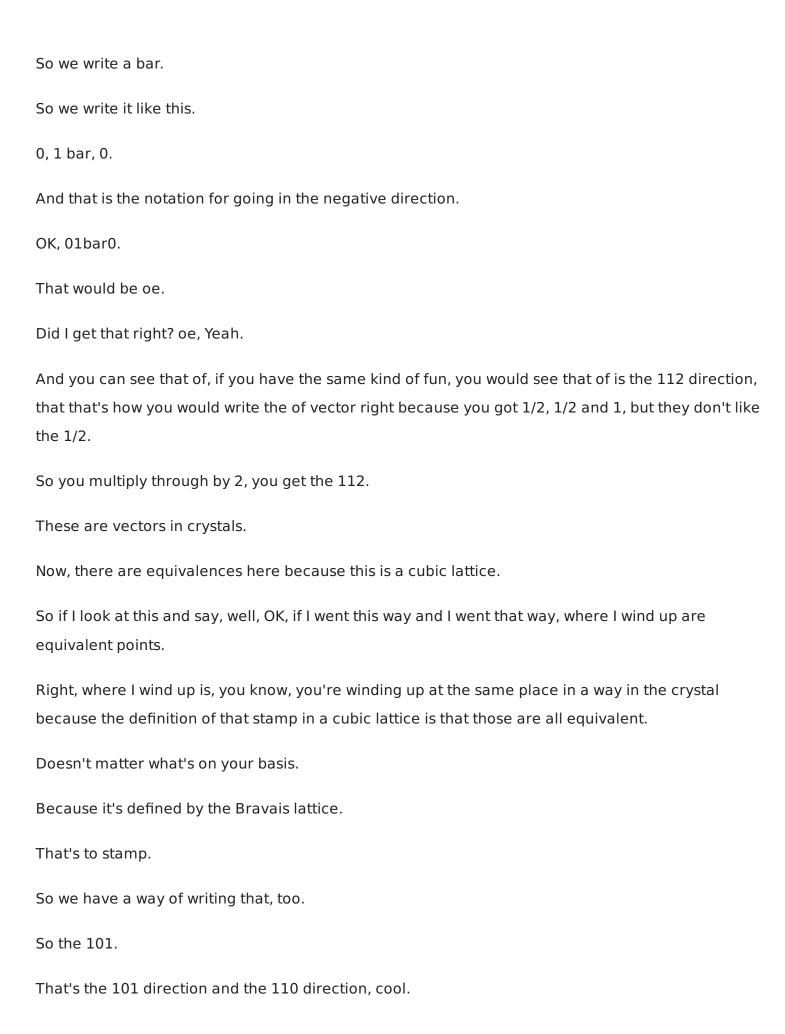
numbers.

So what we do is we define the position as the fraction of the cell edge. OK, so what that means is if, you know, OK first of all, the origin is 0, 0, 0. So that's 0, 0, 0. But it also means that if I had this point here, that's going to be 1, 0, 0. Doesn't matter what a is. Remember, a is the lattice constant. It's the edge of the cube, which has a real value in different crystals. There's copper. There's a in copper, which we could compute. But no, when we specify positions in crystal, we do it as a fraction of that length. OK, so that-- so this point, for example, would be 1, 1, 1 out there. All right. And let's do one more. This point here. All right, well that's going to be-- gesundheit-- that's going to be over a half now. So it's a half and then 1, 0. It went over a half, over 1, up 0. So it's a 1/2. OK, good. This is just where we are. We're just getting warmed up. But really what we need to know is where we're going.

And that goes from a point to a vector. OK, now again, there are some fairly straightforward rules that we follow not that we don't know what vectors are. We know what vectors are. The point is, do we know how to specify a vector in a way that a crystallographer would be happy with? That's what we have to learn. Because again, we don't want to make them upset. So there is a set of very simple rules that you can follow. And I've got this for the direction and I've got this for the planes. So here are the rules for the direction. Here's a vector in a crystal. Origin o and here are different vectors. And what we do is we, OK, we position it to start at the origin. And then we read off the projections in terms of the unit cell dimensions. a is x. b is y and c is z. Now, we know that those of the same length in a cubic crystal. Adjust to the smallest integer values, that's really important. And enclose in square brackets. No commas. So let's do a few.







If I make it a little simpler, you know, I can say that the 100 and the 010 and the 001, oh, let's do them all.

And the 1bar00 and the 01bar0, and the 001bar all get me to equivalent places.

And we can call this a family, just because we don't want to keep writing them.

If they're all equivalent, we can say this is a family of directions.

And you've got to be careful here because you can't use a bracket anymore because it would just be one of the directions.

Instead, we use-- sorry, you can't use the square brackets.

Instead, we use this kind of bracket and we say it's the 100 family.

So if you see a direction written with brackets like that, then it means all of these directions, this family of directions.

But if you see it written with a bracket like this, it means that one vector.

Crystallographers, you've got to keep them happy.

You've got to keep them happy.

All right, now, that is directions.

That is direction.

But what about cuts?

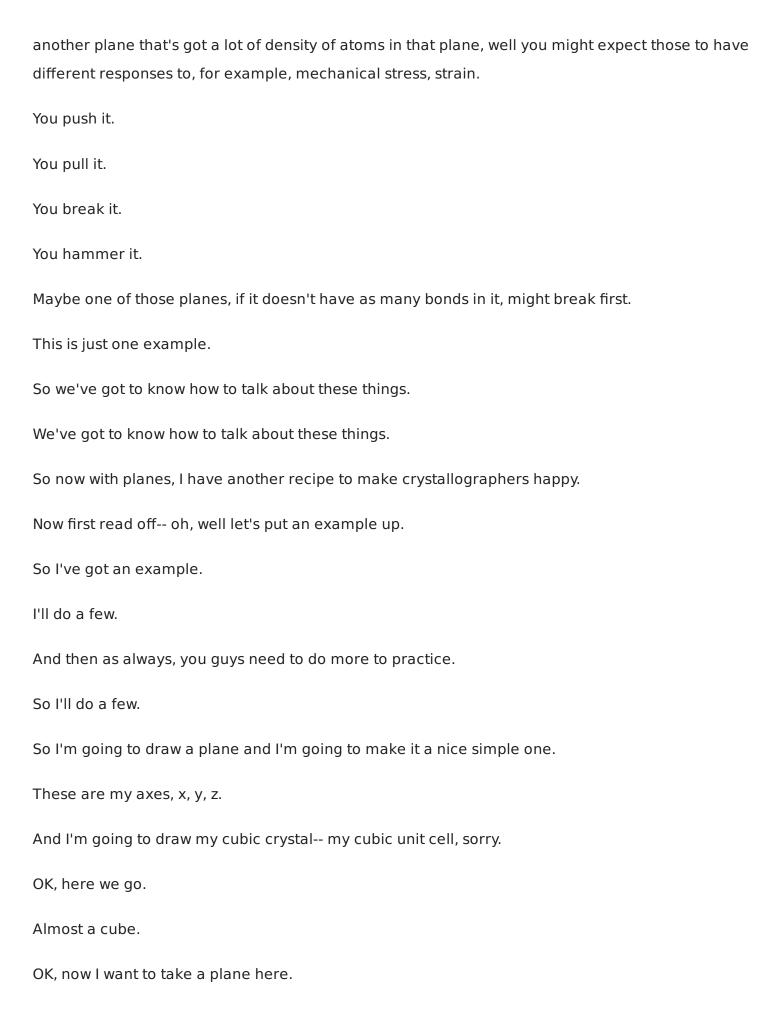
What about planes?

So we've got our vectors, now we need our cuts.

We've got to be able to specify these things.

And you know, as we'll see, as we'll see, the properties of materials, of crystals, especially the more anisotropic they are, depend very heavily on what's in what direction.

So for example, if I have a plane in a crystal that doesn't have a high density of atoms, and then I got



I'm going to take this top one.

So I'm going to take this and I'm going to go through those-- I want to know, how do I describe that plane that cuts that way?

OK, one, these correspond to those, crystal plane algorithm.

I hear a few of you like algorithms and computing in course six.

We got one whistle.

So here's the thing, if I have a plane like this and I ask you, where does it intercept?

Where does it intercept the axis?

Right, well, it's never going to intercept the x and y axes, never.

It's never going to intercept them, no matter what I do.

But you say, but what if I put it in the xy plane, then it's always intercept-- no, that's not what we mean by intercept.

What I mean by intercept is, it has to reach them eventually no matter where it is, no matter where I position it.

But this never does.

This never does.

And so the intercepts, you know, for the ABC intercepts, so we can write those here.

OK, I'll write the same way, x, y, z intercepts, it's infinite.

And it's infinite.

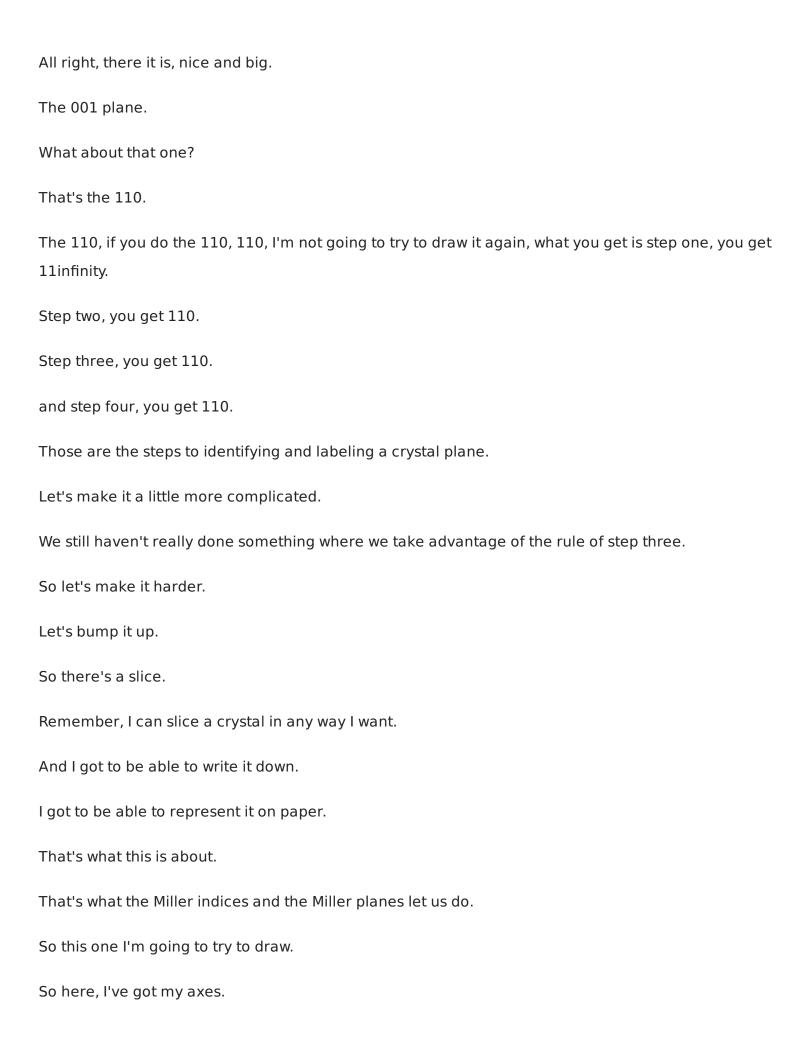
All right, and then for the z, OK here, I'm intercepting at this part of z.

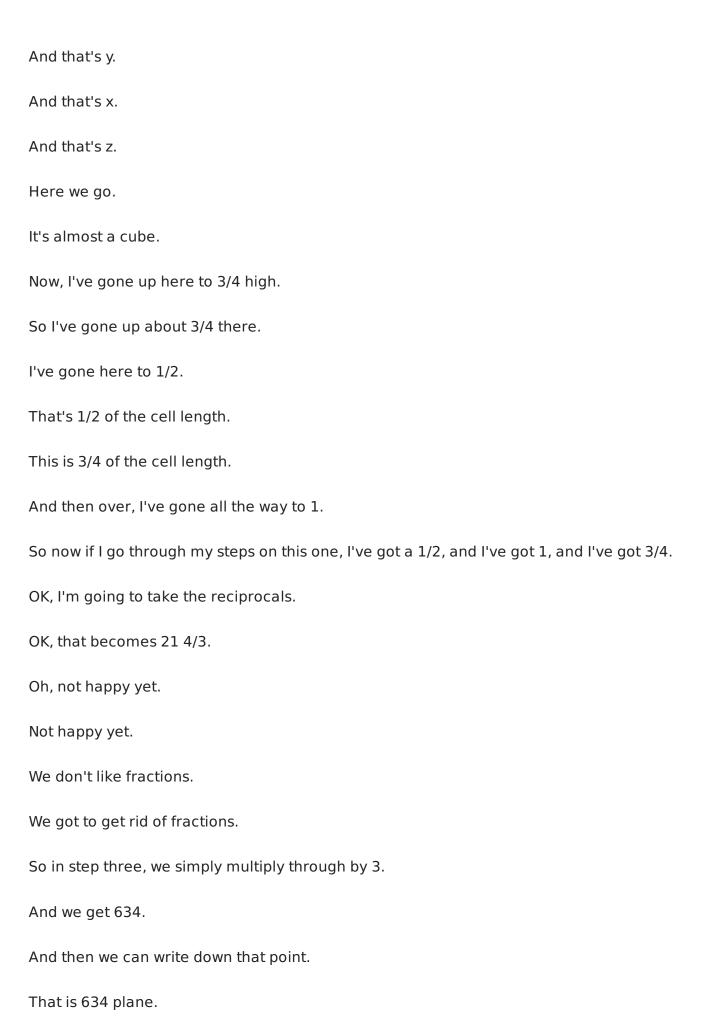
So I'm intercepting at 1.

But the thing is, oh man, crystallographers don't like infinity either.

They don't.

And so what they do is they just take 1 over.
That's a nice way to fix infinity.
And so step two, this would become 00 and 1 over 1 is 1.
Right, 1 over infinity is 0.
Now we reduce to integer values and there's no work to do there.
And then we are very careful about this.
We use parentheses.
No more brackets, parentheses.
Do not get this wrong because you might be talking about a vector by accident.
You don't want to talk about a vector by accident.
So this is the 001 plane, no commas.
Remember the dislike of commas.
It's the 001 plane in this crystal.
That is a cut.
OK, good.
And that's called a Miller plane.
Well, if I do another example, do one more, so that is this one.
I have it.
I've got a bunch of examples here.
And they can draw it, you know, better with the shading and stuff there.
But you see, that's what we just did.
We did the 001 plane that one there





And so on and so on. Now, let's go back to-- let me erase this. There's a couple of things about the planes that once we know what the plane is, we know some other things about it. So let's talk about that now. All right, if I-- first of all, a Miller plane is not just one plane. A Miller plane is not just one plane. A Miller plane is an infinite set of planes. OK so when I say a Miller plane, well, very often what you do is what we've been doing, which is you define the plane that's kind of closest, somehow, to the origin. In the unit cell, the one that cuts it. You define it that way. But actually, what Miller planes are are infinite sets of planes. And so I'm going to put-- Now, I'm not a crystallographer so I can write infinity. I'm OK with that. It's an infinite set of planes. OK.

They are equally spaced and here's the key, one should always be going through the origin.

If you want to look at it as a set of planes, you've got to put one at the origin.

That will help you think through what I mean.

OK, so if one goes through the origin, then what you see right away is how they repeat.

Because you know, it's not just that I go-- in that case, let's take that one, the 001.

Now you say, where's the next 1 in this infinite set of planes? OK, well, put that one at the origin and make another one. Then put that one at the origin again and make another one. That's how to think about this infinite set of planes. OK? So if I had one that went half way, a 200 plane or an 002 plane, as it would be if it's properly noted with Miller indices, well then you say, well, OK, I've got one half way. You know, isn't that it? No. The set of infinite planes also would have one at the origin, one half way, one at the top. Because each time you put it back and you do your next one. That's how to think about this infinite set of Miller planes. So you get this infinite set of planes that have-- I'm going to go to this picture. There it is, a 100, that just go on forever. Those are the Miller planes. And what they have is a spacing between them. And this is really important. So this is the next thing I want to tell you.

It's an infinite number of them.

All right, so I've got-- so a Miller plane isn't just one, it's infinite.

And what that means is that when I give you-- when I give you this, right, or that, or any Miller plane, I know what the spacing is between them.

That is enough information.

Because the distance between planes is-- actually, here it's very easy to see.

The distance between these planes is a.

But the difference between the 200 planes is a over 2.

And in fact, for a cubic cell, there's a formula that you can use for any two planes.

The distance between, well, let's see.

I'll write the notation first.

The distance and the plane there is equal to a.

And the distance of a 200 plane between planes is equal to a over 2.

But there's a general formula of any HKL.

HKL, the Miller indices.

Those are just variables.

But if those are the variables of the Miller plane, then the distance between two of them is the length of the edge of the unit cell, a, divided by the square root of the squares added together, a squared plus k squared plus I squared.

So you see, OK, if it's 100, that a.

That works.

If it's 200, that works.

And it's general.

So now, just by knowing, but because I figured out how to write a plane in HKL notation, I also know the distance between these infinite planes.

That becomes very, very important once we shine x-rays on crystals next week.

That becomes very important.

OK?

OK, so what else can we know from the Miller planes?

OK, so that's the distance between them.

Now the other thing that actually becomes fairly self-evident when you play around with this a little bit, and that was on the slide before, is that-- let's see.

The plane and direction with the same Miller indices are orthogonal.

And you can see this from this very simple picture.

There's the 001 plane.

But that's also the 001 vector, just as we defined it today.

So the 001 plane and the 001 vector are orthogonal.

So this is an example, the 001 plane is orthogonal to, oh, now gotta get this right, the 001 vector.

Oh, no commas.

Brackets, parentheses, no negatives, no fractions, no infinities.

I followed the rules.

And because of that, these indices have meaning as I'm showing you, because of that.

Now, you can play around with this but this can also be fairly straightforwardly derived, things like this.

But you don't need to know that derivation so I'm just telling it to you.

OK, so these are the kinds of things that you can do with Miller indices.

As I said in the beginning.

One of the things that you would want to know what planes you're talking about is because you want to know what the packing in that plane is.

Just like we talked about packing, right-- well, we talked about it before on Monday, the atomic packing fraction, there it is, the max packing fraction in a volume.

We also want to know, especially if a crystal is anisotropy, we want to know about packings in planes. And so, you know, if you take a very simple example like a simple cubic, there's a simple cubic lattice. And now we're all good with our notation. There's a simple cubic crystal. The basis is one atom. I don't have anything else in here. Those are the atoms. It must be polonium. And there's the 100 plane, the 110 plane, and the 111 plane, 111 plane, 110 plane, 100 plane. Now as you can see, the density of atoms in these planes is different. The density of atoms in these planes is different. And that has a real serious impact on the properties. So if we look at this-- so I'll do a couple of quick examples. If we look at this example of simple cubic, that's a very easy case. And so for a simple cubic with a lattice-- this a is called the lattice constant. I've mentioned it a few times. Lattice constant a. Then you know, if we look at the 100 plane, then the area is a squared. The area of that plane is a squared. But the question is, how many atoms are in that a squared. Well, you do the same thing that we did before.

So I'm looking at a plane here.

And I'm trying to figure out how many atoms are in this-- well, you know this is being shared in this whole big plane that goes on and on.

It's being shared by four other squares.

And so there's a fourth of each atom in there.

So there's one atom, effectively, in that plane.

Again, this is in one of the simplest cases.

But the number atoms equal to 1.

And so the density of atoms per area is equal to 1 over a squared.

That's a pretty easy case.

If I did the 110 direction, it's a little bit different because the area is now different.

So the area in this case is root 2 a squared.

You see that?

The area in that plane is different.

So the density of atoms in the plane is different.

So the density in the plane affects properties.

And I want to give you just a quick example of that and why this matters.

Because in fact, this is one of the things, all the way back to Hook and his cannonballs, and even way before that, people noticed this stuff.

I broke something, but it always seems to slice in a certain way.

Why is that?

Why would something always break in the same way every time?

With the same kind of-- what does way mean here?

It means like the angles that form. So why are those angles always kind of the same? Well, it has to do with the strength, the relative strength, of the planes inside of these crystals. And in fact, here's a beautiful piece of work on stretching a wire. All right, so here you're taking a wire that is crystalline and you're pulling it. And you can see how it breaks. You can actually see how it breaks. It's breaking along the weakest plane. It's breaking along the weakest plane. So if you want to think, then, about well, OK, how do I know how to make this stronger, for example? So it stops breaking-- you know, the weakest link is the weakest link. That was deep. So then that's the plane of the crystal that I need to think about. How are bonding together or packing in in that plane? This is real stuff. This comes about in many of the properties, not just the fracture, but in many of the properties of these materials. The property, as I said before, depends heavily on which plane you're in. And we'll see that more and more. As one last example of this, you could go a little-- So again, you go back to your periodic table. And you take-- there was copper.

Let's do nickel.

All right, you take nickel. And let's see, I know that the atomic radius of nickel is 1.52 angstroms. I've looked that up. But I also know that it's BCC. And this gives it away. This gives me what I need. The crystal symmetry, the lattice, gives me what I need. Because once I know that it's BCC, then I also know that the lattice edge goes as 4r over root 3. Remember, for an element like nickel, the packing direction is along the body diagonal. That's what gave me this relationship, back and forth. Unit cell edge, radius of the atom. So that means that in nickel, it's 3.5 angstroms. And once I know what a is, well then I can know what like the-- you know, in one of the planes I say, which plane is that? I don't know, let's look at the densities in the plane. So for the 100 plane, it's-- I'm just going to give you the answer-- 0.59 is the packing fraction. Packing density. This is the-- sorry, that's the fraction. All I did is I used the periodic table to do what I just did for the simple cubic case but now for BCC.

And think about how the atoms are packed differently within the anisotropy of the crystal.

And I can compare this plane with another plane with another plane.

we're able to do this kind of calculation.

And it's because of all the things that we've learned in the last two days, in the last two lectures that

OK, Friday, bring parents.

Bring parents.