MARCELO GONZÁLEZ: This video is about crystals and structures presented by me, Marcelo Alejandro González. Well, first of all, I would like to say, don't focus on the code. And second of all, one of the basic things-- most basic concepts-- that we need to see for crystalline structures is first, what is a crystal structure and second, what is a unit cell?

Well, a crystal structure is just the way in which atoms, ions, and molecules are spatially arranged in 3D. And a unit cell is its smallest repetitive volume, which means that it has to contain the complete lattice pattern. As you can see here, we have a crystalline structure, of course, but what do you think that is the unit cell of this crystal structure?

This is the unit cell. The unit cell is just a simple cubic crystal, where the lattice constants and the interfacial angles are the same, which means that the unit cell is actually represented by a cube. This is just one of the seven different crystal systems that actually exist. However since we've already started talking about the simple crystal structure, let's not concentrate on different crystal systems and let's go deeper into this types of structure.

A simple lattice is indeed just a cube, as you can see here. It's a cube that has atoms in all of its corners, so it has eight atoms. These eight atoms have 1/8 of themselves inside the unit cell. and at the end, it makes the unit cell have one complete atom.

Well, another important concept in crystalline structures is the coordination number. The coordination number is just the number of nearest neighbors each atom has which are the closest to them. In this simple cubic structure, the coordination number is six. It's hard to see it in just one unit, so what we're going to do is create another visualization with eight unit cells put together with different colors, so it is a lot easier to see which ones are the nearest neighbors. Here, you will be able to see it.

Now here, you see how the red atom has six nearest neighbors, which are the yellow atoms. Actually even though this is the simplest crystal structure, there is only one type of atom that can arrange in this structure, and that is alpha polonium. I am sure none of you guys has ever used polonium before. One of the reasons why is because it's radioactive. But the main reason why only alpha polonium goes into this crystal structure is because of the packing factor. This type of crystal structure has a very low packing factor, and that's why not a lot of atoms would crystallize into this type of structure.

But actually, what is the atomic packing factor? Well, the atomic packing factor, as we can see here in this formula, is just the volume of atoms in a unit cell if we assume they are hard spheres and the volume of the entire unit cell.

So to calculate the atomic packing factor, I just created a function to use it, which means the number of atoms and the radius of this atoms if we actually think about the mass spheres. Thinking of the atoms as spheres is actually the easiest way to calculate the atomic packing factor because the formula to calculate the volume of the sphere is pretty easy. It's just 4/3 of pi times radius cubed.

Now, what we need to find is what is the radius of these spheres? In this case, the easy way to do it is having two atoms in two corners. If you have two atoms in two corners, you can see that from the center of each of the atoms, you have one length of the lattice.

Here, the lattice is just a cube, so its volume would be the length of the lattice to the power of three. And since we have two atoms in one length, the radius of each of these atoms is just going to be half of the length of the lattice. Therefore using the function to calculate the atomic packing factor, knowing that there is only one atom and that the radius is half the length of the lattice, you get an APF of just 0.52.

Well, we've already gone through the basics of a simple cubic structure, but let's go a little bit more complicated now. We're now going to the body-centered cubic lattice. Well in a body-centered cubic lattice, imagine you're an atom. You want to be like alpha polonium, so you want to have your space. You know, you want to not have a very large packing factor. You're trying to get together with seven other atoms in a unit cell, and then just an atom comes in between all of you.

This is what happens. This is as you can see here in the visualization. And just an atom is in between the unit cell. We can see it a little better with a lot more separation. So there is an atom in between all of you. So as compared with before, there is not only one atom per unit cell, but now there's two-- the one that's right in the middle, which is complete, and still the 1/8 of the whole eight atoms there are in the corners.

Now, we knew that the coordination number for the simple cubic cell was six. And now, for the body-centered cubic, it's eight, which means that it has a lot more atoms closer to him. That would, in principle, say that the atomic packing factor would be higher, but that we will see

later.

We talked about the coordination number being eight. And here, we can see by putting eight unit cells together, we can see the eight nearest neighbors for the red atom here in the middle. It's actually pretty hard to see it with bonding, so now we can see it a lot better. So it has eight layers neighbors-- this red atom in the middle. And these eight nearest neighbors are the yellow ones that can be seen here.

Well now, we can start talking about the atomic packing factor of a BCC structure. It is actually not as trivial as the simple cubic structure because since you have an atom in the middle of the unit cell, the corners of the same unit select don't actually touch. So it's not as simple as just saying that it's half the length of a lattice. Now, we actually need three atoms, as you can see here in the visualization, that are going through the inner diagonal of the cube.

If you remember from your old math classes, the length of the inner diagonal of a cube is actually just square root of three times longer than the length of a lattice. And as you see here, we have four radii going through this inner diagonal of the cube, so actually the radius of all of these spheres is square root of 3 times the length of a lattice divided by 4. Why? Because we have four radii through this whole diagonal.

So now using the function we used before to calculate the atomic packing factor, we know that there is two atoms. I've already explained how to calculate the radius. So then using this function, we get an APF of just 0.68, which is considerably higher than 0.52 for the simple cubic lattice. Some of the examples for these body-centered cubic structure are chromium, tungsten, iron, tantalum, and also molybdenum.

Lastly, we can talk about a face-centered cubic lattice. In a face-centered cubic lattice, you can see that the unit cell is a lot more densely packed than the other ones. Why? Because here, we have eight atoms which are in the corners. That means one complete atom in the unit cell. But now, we have six atoms in all of the faces of a cube, which are six. And half of these atoms are inside the unit cell, which means that we have six atoms per six faces-- half of them as an inside 6/2. It means three more atoms, so the total number of atoms in this unit cell is four. That will mean that the atomic packing factor will actually be higher than all the other two we've seen, but that we'll actually talk about later.

Now if we want to see the coordination number here, it is actually pretty hard to do it with eight unit cells together, as you can see here. So what I'm going to do is put two of these unit cells

one on top of the other, so you can see the coordination number, which is actually 12. That is also goes together with the atomic packing factor. As you can see it here, even with the bonding-- I changed the colors now-- the atom in yellow has 12 nearest neighbors, which are the atoms in red. That's the coordination number.

Now finally, for the atomic packing factor of an FCC structure, it's actually also not so trivial. Now instead of using the diagonal of a cube, we're going to use the diagonal of a square. Not so hard to remember from your math classes, since you know that the diagonal of the square is just square root of 2 times larger than the length of this same square. So using the same principle, the radius of these spheres-- since we know that we have four radii here-- would be square root of 2 times the length of the lattice over 4.

And of course, we know that now there are four atoms per unit cell. And this APF gives us 0.74, which is the highest one you can get from atoms, as I said before, that have the same radii. Then you can try to concentrate on mixtures of atoms, not of pure atoms and elements, as I have mentioned here. That's a little bit more complicated. Some of the examples for this FCC structure is aluminum, copper, nickel, silver, or gold-- fairly well-known metals.

That's all for this lecture, guys. Thank you very much for watching the video. I would like to acknowledge Bianca Eifert and Christian Heiliger because they're the authors of the package Crystallica, which made this Mathematica notebook possible. Thank you. Goodbye.