MITOCW | Student Video: Crystallography, a Visualisation Tool for CS, BCC and FCC Bravais Lattice Structures.

ALEXIS GERVAIX: Hello everyone, and welcome to this little video presenting you my project on Mathematica. My name is Alex. And I'm currently studying material science in EPFL in Switzerland. And we had this personal challenge to do something you wanted with Mathematica.

So I took an interest into crystallography, because this is a quite essential field of material science. Well, actually, it was on the request of my girlfriend, who has quite trouble to see things in 3D that I did this. And my idea was to create a tool that could be used by anyone that doesn't especially know about Mathematica, and that, without coding anything, he could create a couple of structures, have a look at the-- have an interactive part with it, and choose the atom, et cetera, and visualize more easily these structures.

So let's have a look first at a bit of theory, and first with the Bravais lattice. So Bravais lattice is one of the fundamentals of crystallography. It defines the different structure in which the atom can organize themselves.

So there is 14 of them, where we will vary the axes, the primitive cells, which are A, B, and C, the different angle. And these are the different axes. And these axes can change their length, all the angle, as you can see here.

And there is also a place where you will have more atoms in the middle, or in the same-- in the faces. So in my program, I will focus on the simple cubic, the face-centered cubic, and the body-centered cubic, which are some of the most, I wouldn't say basic, but some of the ones you will encounter more often in solids. There is also [INAUDIBLE] compact that is quite often represented, but it was quite difficult implement. So it could be nice to do it in the future, but for now, it's not there.

And I also had a look at interstitial sites. So interstitial sites are atoms that would come to put themselves in some void area of your lattice. So here is the FCC lattice with an atom on each summit and one in the middle of the faces.

And we have in pink an octahedral sets. So it's an octahedron of void place. And in the center, you have then the possibility to put an atom. So this is interesting when you are looking for alloys in metallurgy, for example, because it gives a lot of possibilities to put new atoms in your metal.

And so there are two categories, as I mentioned, the octahedron and the tetrahedron. And for each of the three structures that I have been picking, there is a different number of octahedron. For example, for cubic simple, there is only one, so in the middle. But for BCC, as we can see here, there is a lot of tetrahedraces, which are here on the faces.

So yeah, well, this is a 2D graph. And it's not always easy to really see how things are done. And I remember having a really hard time to find where the tetrahedron sites were for the BBC. So this is why I really wanted also to put in my 3D graph the interstitials. And I hope it will be useful for you as well if you use my program.

So yeah, so about crystallography in general, this is a field that gives you a lot of information about the properties of matter, because when you understand how the atoms organize themselves, you can start to understand things like metal transition. And a more advanced thing, you can start to look at the growth of monocrystals. For example, if you're working in semiconductors and you're trying to do nanowires, then you need to understand how the-- what are the different plane, how the atoms organize in plane, themselves.

And when you're working on aircraft engineering, you have the turbine that you need to do in a monocrystal of nickel. This is very important. So yeah, there is a lot of application that you can have from this subject. And I thought it was an interesting one to observe.

So let's have a look at the program. So this is some reminder about how it works. And this is the interactive part. So my program consists of two cells that you simply have to click on them and press Shift, Enter.

The first parts are the function that will define the position of the atoms. And the second part is the interactive tool, which we call Manipulate Mathematica, and gives a lot of possibilities. So you will see, this is a huge cell with a lot of code. I know that Mr. Carter doesn't like it at all. But I had to keep it like that to have my Manipulate.

And let's simply run it. So it takes a bit of time. And here we have it. So this is the panel-- maybe we should put that away-- where you have, on the left, the controls, on the right, a display with a panel of the periodic table, the 3D graphic, and a little graph that helps you to visualize more easily the parameters of the lattice. That helps you when you try to calculate the densities of these particular structures.

So as you see, we can move it. There is different type of atom here. I on purpose put NaCl,

which is salt. And now let's have a look at all the possibilities we have with this program. Because the thing is that I want you, when you have a-- you know already a structure, and you want to know what it looks like, to be able to create it.

Well, first, let's look at the different options. So we have these three structures, the BCC, the cubic simple, and the FCC. You can change the atom size. Here you can display-- you can choose if there is the [INAUDIBLE], and here, the choice of element, because I wanted that you can choose what type of atom you put in your cell. This is why there is this panel.

So I divided my graph into four parts. Basically, atom one and atom two are the atoms on the edges. And in the center are a different division that helps you to create more complex cells.

So let's have a try. I would like a body-centered cubic. And I would like an alloy which is iron and aluminum. That structures itself into a BCC. So I will put an atom two there, aluminum. And here you will see it changing.

So this is normal, because I asked the software to only update this part when I click on the panel [INAUDIBLE]. It can be improved, this part, but it was to have stability during the initialization of the Manipulate. And here I have a way to initialize my body-centered cubic with the iron atom on the edges and my aluminum atom at the center. You can, of course, change the atom size. You can click on the same atom, and this way, get a little bit bigger.

OK, so there is also FCC that you can do. There is one alloy that works with this, which is, if I remember well-- I wrote it somewhere-- aluminum and nickel. So let's circle the aluminum and this nickel here. And that should be [INAUDIBLE]-- yeah.

And here is the FCC. And here you can turn and have a look. You see that there is nothing in the middle. And for me, it helps me a lot to visualize it like that. There is also the adapted density calculation graph, where you see that this diagonal in the middle will-- no, in the face here, will help you calculate the density. And you know that this line is a square too of the lattice parameter.

Now let's have a look about the interstitial that I took some time to put-- add on my graph. And I would like to show you a little example that I had-- that I forwarded, which is this slide about the magnesium lead, intermetallic Mg2-Pb. And they said that this should look like this. And they are giving us that, so the anion, the magnesium are on the FCC site in blue. And the lead is on the octahedral site. So let's try to put it in my program.

So first, I will say, yes, I would like to have octahedron interstitial. I will stay in FCC. I would put the same atom here, magnesium, and here. And it's a bit long to update. My computer is having a hard time.

All right, so we see that it doesn't look like at all on what's [INAUDIBLE] on here. This is a bit-- all right. OK, and here is where I see that this guy did a mistake here by putting octahedron in this place, because this place is tetrahedron, the other type of interstitial. So we will remove the octahedral, put the tetrahedral [INAUDIBLE].

And here we go. [INAUDIBLE]. OK-- no, no, OK, I should do things properly. Interstitial tetrahedral and [INAUDIBLE]-- now it's better. And it looks like what we have here.

And I find it better to look like that, because now that we can change a little bit the size, it is clear now that there is nothing in the middle, which, it's not that clear when you look at this thing. So yeah, I found that it was one nice application of this little program, to visualize it more easily.

So here is for now. I hope you enjoyed this little presentation, and that it will help you by using this program to see better in 3D your crystalline structure, and that will help you to have a better idea of what you're doing with your crystallography courses. So thank you for watching.