**JURGIS RUZA:** In this demonstration, I'm going to show you how to construct 2D Brillouin zones and hopefully achieve a better understanding of them and what they are.

So a Brillouin zone is an important concept in material science and solid state physics alike because it is used to describe the behavior of an electron in a perfect crystal system. So what is a Brillouin zone? A Brillouin zone is a particular choice of the unit cell of the reciprocal lattice. It is defined as the Wigner-Seitz cell of the reciprocal lattice.

It is constructed as the set of points enclosed by the Bragg planes-- the planes perpendicular to a connection line from the origin to each lattice point passing through the midpoint. Alternatively, it is defined as the set of points closer to the origin than to any other reciprocal lattice point. The whole reciprocal space may be covered without overlap with copies of such Brillouin zone.

OK. So that was a rather convoluted definition. Let's do it again. Let's brush up and be sure that we understand this definition. We're going to define the reciprocal space and the Bragg planes as well. But to define both of these, we'll also do a quick revision of what is the erect lattice so that we can go from there to the reciprocal lattice.

The microscopic perfect crystal is formed by adding identical building blocks. So to say unit cells consisting of atoms and groups of atoms. A unit cell is the smallest component of a crystal that, once tacked together with pure translational repetition, reproduces the whole crystal, which essentially means that you can take the same thing over and over and over again and get the whole system done.

So the groups of atoms, these unit cells that form the microscopic crystal by infinite repetition, is called the basis. OK. That seems quite clear. And the basis is formed in such a way that it forms the lattice, more commonly known as the Bravais lattice. Every point of a Bravais lattice is equivalent to every other point, which means that the arrangement atoms in a crystal is the same when viewed from different lattice points.

OK. That also seems quite understandable, and you should probably know that by now. So any fundamental lattice must be definable by three primitive translational vectors-- a1, a2, and a3. The combination of these vectors is usually to find the crystal translational vector r, such that r is equal to a1 n1 plus a2 n2 plus a3 n3, where n are just arbitrary integers to show the size of our lattice.

The crystal lattice is repeated an infinite amount of times to create the perfect crystal structure, and each of those lattice are translationally symmetric. Another way to look at it is that one cannot tell their position in the crystal structure because every lattice looks the same. OK. So that seems to make sense. So now, let's go through reciprocal space.

So every lattice has a reciprocal lattice associated to it. In crystallography terms, the reciprocal lattice is the fraction prior of a crystal, or in quantum mechanics it's describe as k space, with k being for k wave vectors. In 3D lattice, the vectors would be b1, b2, and b3. And they can be denoted as-- we'll look at just b1. b1 is equal to two parts of the cross-products of the vectors a2 and a3 from our direct lattice divided by the triple cross scalar product of a1, a2, and a3, in which case this cross-product of a2 and a3 is the area of our vector of our two vectors, and the triple scalar product is the volume of our system.

By simplifying it, we can just get 2 pi over the height of our unit cell, or we can put it this way. The larger our direct lattice, the smaller in comparison our reciprocal lattice becomes. Another observation that could actually be made by the reciprocal lattice is that the reciprocal lattice of the reciprocal lattice is the direct lattice.

But OK, for simplicity's sake, let's look at a transformation from 2D lattice to a reciprocal lattice. So we have a visualization here where we can change the length of our x vector in direct space and the length of our y vector in direct space. And we can change whether or not we're seeing this as a direct lattice or whether we're seeing this pattern as a reciprocal lattice. So as we can see, by increasing the length of our direct vector, we change the sizes of our reciprocal lattice vectors, and the other way around.

So now we had a definition of the reciprocal space and direct space. Let's go back to our definition. So the first Brillouin zone can be defined as a set of points in reciprocal space that can be reached from a specific point of origin without crossing any Bragg planes.

So what are Bragg planes? A Bragg plane, or in this case, a Bragg line, is a Bragg line which perpendicularly bisects a reciprocal lattice vector-- a vector which connects two lattice points. And the closest Bragg planes are essentially crossing the Brillouin zone.

Now, we can show the Bragg planes with the closest neighbors, with this being our original lattice point. And these are the four closest neighbors in a simple, I'd say cubic, but it's actually just the square lattice because it's in 2D. And if we add the second largest vectors, for the second closest neighbors you can see these ones. And essentially, it conveys the same information. When we go to a higher order of closest neighbors, we can see that the system gets a lot more complex.

So now we've seen what are Bragg planes, we can go towards Brillouin zones. So this is the first Brillouin zone. It is what it seems it is. As you can imagine, the Bragg planes just go here. And the Brillouin zone shows us the area in reciprocal space that is closer to our lattice point than any other lattice point, which are essentially the Bragg planes as well.

As we can see, our reciprocal lattice origin point is in here. The square is closer to this point than to any other point. And after these lines, it gets the other way around. So we can move on forward to a higher order of Brillouin zones.

And this is the Brillouin zone for the second closest neighbor. As you can see, it is rather similar. It's just takes the second closest neighbors and essentially draws another square. But it's a bit tilted to the edge.

So now let's look at the third one. For the third Brillouin zone, it gets a bit more complex because if we scroll a bit backwards, we can see that the Bragg planes for the third closest neighbors are these ones. So we might think that this whole thing would be the third Brillouin zone, but it's actually not, because with every next system it gets a bit more complex. And it's actually taking account both the third Bragg planes and the first ones.

So now let's do another thing. Let's turn on that we can see all the Bragg planes and turn up another notch. So here we can see that the fourth Brillouin zone gets a lot more complex. And we can see all of the Bragg planes for the closest neighbors. And these lines get quite difficult to understand by drawing themselves, but we can help ourselves out with this visualization.

So yeah, we can see that they start to interact with each other, and thus make a more difficult structure. And if we go to the fifth one and show that we can see all the Brillouin zones-- so here we can see that it becomes quite a nice drawing. If we were to keep adding them-- I mean, let's just do it. Let's add until the ninth one.

So here we can see a high order Brillouin zone. It actually looks kind of nice, which is also interesting because it's also an art form drawing high order Brillouin zones. The higher you go, the more complex and more discrete the system gets. And it essentially looks nicer.

So after looking at this, we can get a short definition of how to construct 2D Brillouin zones. So n-th Brillouin zone can be defined as the area, or volume if we look in 3D, in reciprocal space that can be reached from the origin by crossing exactly n minus 1 Bragg planes.

So we can look also at a Brillouin zone for a system where the atoms are not perfectly in a perfect square lattice but are offset a bit, making, so to say, a triangular lattice. And as we can see here, the first Brillouin zone is a hexagon. And the second one already gets a bit more difficult by forming a star shape. And the third one is, again, so to say, a hexagon. And it goes on like that.

And then, so what information does the Brillouin zone hold and what does it give us? In short, vectors in the Brillouin zone or on its boundary characterize states in the system with lattice periodicity. For example, phonon or electron states. But for that, a whole other video.

This code for this demonstration was taken and edited from mathematical demonstrations made by Jaroslaw Klos.