POOJA REDDY: Hi. I'm Pooja. And I will be talking to you about how you can visualize the energy of defects, specifically focusing on screw dislocations.

So crystals have an underlying lattice structure. But in reality, they're rarely perfect. They usually have mistakes in them which we call defects. A point defect can be a vacancy where an atom is missing from the lattice. And it can also be an interstitial, where there's an extra atom in the lattice.

Another type of defect are dislocations, which are linear defects. Here is an example of an edge dislocation. The red arrow here shows a line direction in the defect, which is at the edge of this extra plane here that's in the lattice.

Another type of dislocation is a screw dislocation. The blue arrow here shows a line direction of this defect. Here, items on one side are higher than the other. Here, it's lower. And you see this almost spiral shape that forms kind of like a screw. From these pictures you can really see how defects distort the 3D lattice.

So why do we care about defects? Turns out that they really do affect material properties. Some properties depend heavily on defects. And those include conductivity, especially in semiconductors, hardness and ductility in metals like brass, and diffusion coefficients of materials.

So lattices exists because they are low-energy configurations. It would make sense then that errors in the lattice, like defects, should increase the energy of the lattice. So how can you think of the energy of atoms in a lattice, or just in general?

One way we can calculate the energy of atoms is using Lennard-Jones potential. Lennard-Jones potential approximates the interaction between a pair of neutral atoms. In this graph here, the x-axis is the distance between atoms, and the y-axis is a measure of potential energy. And you can really see in this function how there is a energy well or minima.

So what happens is when atoms are too far away from each other, there's an attractive force, and they come together to reduce energy. And when they're too close, there's a repulsion force, which is used to reduce energy. And at the energy minimum the atoms are actually this specific distance away from each other. What you actually find is that the bond length

corresponds to this distance found at the minimum of potential energy.

But how about in the lattice where there are a lot of atoms? Energy still does want to be minimized. So these atoms try to minimize energies by sitting in multiple energy wells with their neighbors.

Also, it's good to remember that an atom will be interacting with this one and this one and this one, and just all the atoms around it. Although the effects will probably become smaller as the distance between atoms increases.

So an interesting question to then ask is how would defects affect the energy of particles in a lattice when a lattice is a low-energy configuration? In this notebook I will aim to visualize the energy of defects. I will mainly focus on first, vacancies in a 2D lattice, and then move on to screw dislocations in a 3D lattice.

So here is a 2D lattice with a vacancy. What I've done is I've used Lennard-Jones potential to calculate the energy of each atom. I then use this energy to color the atoms. And blue is low energy, and red is high energy.

What you find is interior is mostly blue, while the surface has these yellow and red energies which are higher. One way to think about this is that these atoms have fewer neighbors, so they sit in fewer energy wells. This higher energy we find on the surface is actually known as surface energy. Also, notice how the energies immediately around the vacancy are also higher.

For fun, here's a cool simulation of multiple vacancies moving around a lattice. You can see here how the energies around vacancies change when vacancies are next to each other or near the surface.

Now that we've had a taste of how you can color atoms to indicate energies, let's move on to the good stuff-- screw dislocations. First, here's a cubic lattice. Like with the 2D lattice, there's a surface energy. This higher surface energy can make it difficult to see how the screw dislocation changes energies of atoms in the lattice. So what I'm going to do is only visualize the inner atoms excluding the surface ones.

To really see how screw dislocation works, here is an inner layer of the lattice. The Burgers vector represents a magnitude and direction of the lattice distortion resulting from a dislocation. As I increase the magnitude of the Burgers vector, you can really see this kind of

spiral staircase shape happening around the dislocation.

Now I'm going to extend this layer to show all the inner atoms in my cubic lattice. As I increase the magnitude of the Burgers vector here, you can see how the atoms right around the dislocation become more red or higher energy. So the energy around the dislocation is higher, very similar to what we saw with the vacancies.

Now what I'm going to do is chop this in half and only look at half the atoms. And as I increase the magnitude of the Burgers vector, it becomes really clear that the energy becomes higher just around the dislocation, where here is a dislocation, here's a very high energy red, and here's the lower energy.

The only thing is it's kind of hard to see how the inner atoms energies change. So what I've done below is I've created a simulation where the higher the energy, the more opaque the atom.

So we start with a pretty translucent lattice because everything's lower energy. So as I increase the magnitude of the Burgers factor here, you start to see that atoms around the center become more opaque. And you can really see where the locations of high energy are.

Here is kind of this column of high energy right in the center. These parts have higher energy as well because they're more exposed. They have fewer neighbors.

So now that we've looked at cubic lattice, let's look at a hexagonal close packed lattice, or HCP. So here I visualize an inner portion of the HCP lattice. Again, I'm not looking at surface atoms. And all atoms here are pretty dark blue, so they're lower energy.

As I introduce my Burgers vector, the energy does clearly increase right around the center. And what you'll also notice is that atoms are becoming less blue, which means that the energy of all the atoms is kind of increasing.

And something cool happens if I keep increasing the magnitude of the Burgers vector. What I find is that I have this area of yellow, kind of higher energy. And an area of much higher energy right outside of that. And then the energy starts to decrease again.

So let me go down here where I have colored my particles also based on opacity. And you can really see this super high energy opaque red lines near the center where my dislocation is.

And this is a pretty cool result of simulating screw dislocations. I expect energies to be higher right around the dislocation, which I saw pretty clearly with the cubic lattice. But in HCP, in addition to energies being higher, energies become a lot higher a little ways away. So this is a neat example of how simulations can really teach you something more about a system that you didn't know before.

In the above simulations, I varied the magnitude of Burgers vector. But we also know that defects can propagate through lattices. In my simulation before, I actually had the vacancies moving around. So now I'm curious to see how my screw dislocation can propagate through a lattice.

What I've done below is I've fixed my Burgers vector to a magnitude of 1, and have propagated the terminus of the screw dislocation. Here is a cubic lattice. And as I move the terms of the Burgers vector through, you see this layer of high and low energy moving through the whole system until it passes all the way through. And now you have the geometry that you can tell is of a screw dislocation.

Now if I only look at half the atoms, and I start moving my Burgers vector terminus through, you can really see how the blue or low energies are where the atoms are being squished together, and the red is where they're being spread apart. And also above where the terminus has passed through you have this geometry of a screw dislocation, and below you still have the cubic geometry of the cubic lattice.

In hexagonal closed pack I still do see a really similar thing of this layer of lower and higher energy passing all the way through the lattice. At the end, you just have this geometry that we remember before of a screw dislocation. The interesting thing is you can still see that the energy is higher around the line of the screw dislocation, just like how we saw before.

So here are some takeaways. First, I went over a couple of basic types of dislocations. Then I talked about how lattices are low-energy configurations. I also showed how you can use Lennard-Jones potential to calculate energies of atoms. I then visualized energies of defects using Lennard-Jones potential and focused in on screwed dislocations.

I first varied the magnitude of the Burgers vector. And this was to show you how energy was higher on the position of the dislocations. I then showed you how a lattice changes as you move the terminus of the Burgers vector through it.

I hope you've enjoyed learning about the energies of defects.