

STUDENT:

Today we're going to look at Hooke's Law in Cubic Solids. Hooke's law describes behavior of springs. What we're going to do is we're going to model the solid as a collection of springs connecting a whole bunch of atoms in a cubic lattice. Now, disclaimer-- I'm probably going to do this all wrong. But what's science if we don't make a few mistakes, right? Let's get started.

The potential that describes fairly well the behavior of the interaction between two atoms is the Lennard-Jones potential. It describes the van der Waals interaction, and it looks something like this. It's a potential with a term which goes $1/r^{12}$, and one term which goes $1/r^6$. And as you can see, as the atoms get very close, they repel greatly, and then they have a sweet spot here, which is the distance they prefer to be at.

As they get farther away, they start to repel more again. The atom like to sit right there in that little potential well. It's written up in Mathematica. You can see the equation here, what each term means. And when I come here as I take in the derivative. What that does is give me the force on the particle when it's in this potential. So as we see, the force is high and positive when it's closer to the other atom, then the equilibrium distance and the force is negative when it's farther-- so it gets pulled towards that sweet spot that I mentioned earlier. And here are the two plus together.

So with Hooke's Law, we're modeling the atomic bonds as springs. And the way that's going to work is, we have Hooke's Law which is that the force is proportional to the spring constant times the displacement. So the further you pull it, the greater the force in its linear relationship. And the problem is, though, our Lennard-Jones potential is not-- it's not a normal potential array. It's this weird wobbly shape. But for Hooke's Law to work, you have to have something that behaves like a spring, which has a parabolic potential well, which is how you get that linear force relationship when you take the derivative.

So what I've done is I've used Mathematica and its wonderful math tools to take the Taylor expansion about that equilibrium point. And you can see here, this is the second order Taylor expansion, so it's a parabola. And if you look at this little manipulate here, I have set it up so you can adjust the potential while depth can choose the equilibrium distance, And you can look at the different order Taylor expansion, so that's the first order-- it's a line. The second order is a parabola-- that's what we're going to be using.

The other ones are just better and better approximations of the action potential. Mathematica supposedly can do negative powers, but I'm not seeing that here, so could be the actual perfect model would be obviously one over r to the 12th, there's r to the negative 12th. So I differentiated that second order potential like that. And you can see here the force response for our generalized for an approximated spring bond. And so you can look at our force response here.

Notice like before, the force is positive when the atoms are close together, and negative when they're farther apart-- so it gets pulled out of that sweet spot. And I've plotted it here with the potential, so you can see how exactly it interacts with that potential. Here is the approximate potential with the actual Lennard-Jones potential. So you can see that it's not a very good approximation, but very small displacements on the order of about 0.1 times that minimum distance will probably be OK.

I simplified it here to get the-- and then I take the derivative again, just so I can get that slope-- and that'll be useful later. So here, we're modeling our cubic lattice. Say we have something like alpha polonium, which has a simple cubic structure-- the only metal that has a simple cubic structure with a single atom motif. So we have our stress over here, and our strain, and there's this fourth ranked tensor that connects our second ranked tensors with stress and strain. But, because of the wonders of mathematics and matrices, we can actually break that down into two first ranked tensors and a second ranked tensor.

Which is pretty great, because it means we don't want to do some really early math. And so we can find that infinitesimal strain tensor, if we're looking at a tiny, tiny piece of a solid, will look something like this. It's this-- ϵ_{IJ} is equal to $1/2$ of the displacements in each direction of the infinitesimal piece. And so from that, we can build that out to the second rate strain tensor, which is this tensor here.

And it looks like this, where u is the position, so we have all these displacements. As you can see along the principal axes, they're just partial to the displacements and the directions along the other axes, they're a little more complicated, because you have things moving in two directions at once. But the coolest part is that only six of these entries are unique-- because this is the same as that. That's the same as that, and that is the same as that. So what we can do is we can just break it down to these six unique things.

And then here is our second ranked tensor, like I said before, of our elasticity. But, because

we're using Hooke's Law, these are springs and this is a simple cubic lattice. So each atom is only attached to six of its neighbors, so it's not going to have any weird stresses. This is where I'm probably wrong, but at this point, we are going to do this. So here are our diagonal elasticity values. And if we do anything before and simplify that spring potential, and grab the slope of that line, we get our spring constant.

So if this were a spring, that's what the spring constant would be. And we just plug that in here to our matrix, and we get-- oh look, it's Hooke's Law. So if everything is wonderful and linear, which it's probably not, but if it were, we have the Hooke's Law, and we can use that to determine from the strain, the stress-- or vice versa. As you can see, it would look something like this-- so in the original position of the spring's the black, and then when you drag the atom over here, you get this red, deformed spring. This one here's squished, these are stretched. And yeah, that's about it.