TINA CHEN: In this video, we will be exploring the effect of bond energies on vacancy diffusion using a Mathematica simulation. Even the most carefully produced materials have defects. These defects often affect the physical properties of the material.

One type of defect is a vacancy in which an atom or molecule is missing from a point in the lattice. Vacancies can diffuse or move around. In this video, we will investigate diffusion of a single vacancy in a binary AB alloy.

To simplify the simulation process, this AB alloy will have a two-dimensional, square lattice. In order to simulate the movement of a vacancy, we must consider, on the atomic level, the interaction between A and B. Specifically, we will look at the bond energies.

Here, we have our AB alloy square lattice with randomly placed atoms A and B. If we have a vacancy here, then the vacancy can potentially jump to one of four places. We look at the energy required to jump to each of the four places.

If the vacancy wants to jump to this lattice point, then it has to break each of the bonds connecting the atom to other atoms. The same is true for the vacancy to jump to any of the other lattice points. It has to break the bonds connecting the atoms to other atoms.

The frequency with which the vacancy jumps to any of the four neighboring lattice points is proportional to E to the bond energy. The specific equation relating these two is the Arrhensius equation, which shows that the frequency is also proportional to V, the Debye frequency, which is a property of the material, and the temperature.

For our simulation, we will only look at how the bond energy affects vacancy diffusion. Since we only have two types of atoms in this alloy, there will only be three types of bonds-- AA, BB, and AB with corresponding bond energies, VAA, VBB, and VAB.

For our simulation, we will start with a 2D square lattice with randomly placed A and B atoms. We will see the ratio of the atoms is 1 to 1. We will also have a randomly placed vacancy. We will then simulate a single jump of the vacancy by comparing the frequencies with which a vacancy will jump to the four neighboring lattice points.

We will consider only the case that the vacancy jumps. That is, it does not stay at it's lattice point, and it can only move to one of the four neighboring lattice points. Then we can calculate

the probability with which any of the four jumps occurs.

This probability will be the jump frequency for a specific lattice point over the sum of all the jump frequencies. Note that we could have considered the possibility that the vacancy did not jump, but then the value of the Debye frequency would be needed.

And when we use the probabilities instead of the actual jump frequency, the Debye frequency cancels out, and we can consider a general binary alloy. Now that we have the probabilities P_1, P_2, P_3 and P_4 of jumping to the respective lattice points, we can simulate what the vacancy at this lattice point surrounded by these atoms will do.

First, we pick a random number from 0 to 1. The value of the random number will determine where the vacancy will go. From 0 to P_1, the vacancy will jump to the first lattice point. From P_1 to P_1 plus P_2, the vacancy will jump to the second lattice point and so on. This is the areas for which the vacancy will jump to the third and fourth lattice points.

The number picked by our random number generator will fall in one of these four areas. And the area that number falls in is the lattice point the vacancy will move to. The vacancy then jumps to the lattice point indicated by the random number.

In this way, we are using random samples to simulate the randomness of the vacancy moving, given then calculated probabilities to one of the four lattice points. To complete the simulation, we then repeat the computation of the probabilities of jumping to the neighboring atoms, the random number sampling that chooses where the vacancy moves, and actually moving the vacancy.

First, we will look at the case when atoms of the same type have lower bond energies than atoms of different types. The animation allows us to visualize how the vacancy will move within the lattice.

We can wait and see as T gets larger, something seems to occur. And that seems to be the agglomeration of the same type of atom. For instance, we can see the accumulation of red atoms in this area.

We can let the simulation run or we can see the beginning and end points after 10,000 steps. We see here that originally the lattice was pretty random. But after 10,000 steps of the vacancy, we can see accumulation of red atoms here and blue atoms here.

Next, we will look at the case when atoms of the same type have higher bond energies and atoms of different types have lower bond energies. Again, we animate and see what happens.

Now, atoms of the same type seem to be going away from each other. And instead, order seems to be appearing in this system. We see here red, blue, red, blue, red, blue, red, blue, red, blue.

Again, we can look at the initial and final products. And we can see the initial lattice was quite random and the end lattice is very ordered. It's almost completely ordered.

Finally, we will look at the case when atoms of the same type and atoms of different type have similar bond energies. We can animate, and we can wait a while, but nothing particularly special will happen.

Again, our end products can show us what will happen after 10,000 steps. And we see that there is not much significant going on. The beginning and end lattices are both rather random. So how does a lattice decide which form to approach as T gets very large?

The answer is, the strength of the bonds between A and A, between B and B, and between A and B, as we said before. That is, do atoms of the same type like or dislike each other?

Based on the answer, atoms are the same type will either conglomerate, as in the first case, into regions of A and regions of B or atoms will rearrange into an ordered form, as in the second case, to be closer to the type of atom it likes.

The affinity of an atom type for other atom types is given by the bond energy. And the type of lattice that will be formed is given by the effective interchange energy, which is given by VAA plus VBB minus 2VAB.

If epsilon is greater than 0, then atoms of one type like the other type more than they like each other, so the vacancy will allow the crystal to obtain an ordered lattice. If epsilon is less than 0, then atoms of the same type like each other more than they like atoms of the other type, and they will conglomerate by the vacancy diffusion mechanism. If epsilon equals 0, then disordered, solid solution occurs.

This is because neither the VAA, VBB, nor the VAB phases are favored. Instead, they maintain a random order. To create the simulation, me use the type of modeling called Monte Carlo simulation. The Monte Carlo method is simply a class of computational algorithms that use

repeated random sampling for simulation.

In this case, we used random sampling in addition to the probabilities to determine how likely a destination for the vacancy each lattice point is. Now take the model of the single vacancy diffusion and imagine many, many more vacancies.

We can see now why defects can cause changes in the physical characteristics and even structure, in this case, of a material. I'd like to thank professors Craig Carter, [INAUDIBLE], and Dwayne Johnson for their help and advice with the coding in this video.