GLORIA CHYR: Hi there. My name's Gloria Chyr. And for the next few minutes, I'll be talking about how to find the perfect diamond and why that might actually be impossible.

Let's start with what a perfect diamond looks like. A quick Google image search for the perfect diamond yields this as the first result. And it does look pretty perfect. But just because it looks perfect doesn't mean that it actually is. To determine if a diamond is really perfect, we have to look at its structure.

A diamond consists of carbon atoms arranged in what we call a crystal structure. More specifically, diamond form a cubic crystal structure made up of tetrahedraly arranged atoms as shown in this 2D depiction. An important thing to note is that diamonds are not a stable form of carbon. They're what we call metastable, which means that they're energetically unfavorable, but there is a high activation energy for it to decompose so it stays how it is for a very long time.

Besides the fact that diamonds aren't forever what really makes finding the perfect one impossible is that it probably doesn't even exist. What real diamonds look like is something like this. It's the same structure as the last slide, but there's a carbon atom missing. This is called a vacancy, which is a type of defect that can exist in crystals like diamond. Defects are imperfections and crystals, and vacancies are not the only kinds.

All crystals in the real world have a number of defects ranging from vacancies, to grain boundaries, to edge dislocations. There's quite a number of them. But for the purpose of this video, I'll be referencing vacancies in diamonds. Keep in mind that anything I say about them also applies to other kinds of defects in other kinds of crystals.

OK, so now that we know why crystals aren't perfect, we want to know why this happens to begin with. The reason that these defects form is because a crystal will always be tending to equilibrium, also known as the state of lowest Gibbs Free Energy. The formation of defects in a crystal may seem counter-intuitive because it costs energy, which is not favorable. But the formation of defects also increases the amount of entropy in the system which is favorable.

The entropy gain can sometimes outweigh the energy cost of forming a defect. So a perfect crystal can actually decrease its Gibbs Free Energy by forming defects. This can be seen in the following equation where delta G equals delta H minus T delta S. So formation of defects becomes a battle of enthalpy versus entropy. If the enthalpy cost of forming a defect is greater than the entropy increase of the system, then the defect does not form. If the entropy increase of the system is greater than the cost of forming a defect, then the defect does form.

The change in Gibbs Energy of forming vacancies depends on several factors, including a number of vacancies already present in the size of the crystal. So the energy cost and entropy contribution of vacancy formation actually changes with each defect formed. What we see is that there's actually happy spot for the equilibrium amount of vacancies.

This here is a visualization of how the number of vacancies affect a Gibbs Free Energy of a crystal at various temperatures. On the left is a plot of Gibbs Free Energy where the x-axis represents a number of vacancies documented in a crystal, and the y-axis represents the Gibbs Energy of the system. On the right is a visualization of what the lattice looks like at equilibrium.

In this demo, the crystal is a square lattice made up of 400 atom sites. I am using a 2D square lattice instead of a three dimensional diamond lattice for ease of viewing and understanding this topic. These concepts apply the same way to diamond crystals, which are much more complicated. As you can see already, there is a vacancy present in this lattice.

It may be a bit difficult to see on the left, but this is because at equilibrium the Gibbs Free Energy plot is actually not linear, but curved. This becomes more apparent as we increase the temperature. Higher temperatures provide greater entropy increase of defect formation. So we see vacancies are more likely to form.

Here we can see that the lowest Gibbs Free Energy doesn't occur at 0, but actually in around 50 vacancies per 400 sites. This seems pretty high. But if you think about it, this is at 5,000 Kelvin. So the atoms in the diamond crystal are actually moving around quite a bit. So it makes sense that you won't find all of the atoms in the right places. If you would like to see how this visualization was made, the code is accompanied with this video.

In summary, what we found is that the perfect crystals don't exist because the equilibrium state of lowest Gibbs Free Energy occurs with some number of defects. Since diamonds are crystals, it turns out that finding a perfect one is impossible. But that doesn't mean we can't find a diamond that looks perfect.

Thanks for listening. And I hope this quick lesson has made understanding why defects form a little clearer. The notebook that accompanies this video is a written version of this video. And with that, I would like to thank Professor Carter and Professor Keenan and the help of 31.6 TA's Emma, Burhan, and Philippe.