Basics of Materials Engineering
Prof. Ratna Kumar Annabattula
Department of Mechanical Engineering
Indian Institute of Technology, Madras

Lecture – 12
Defects in Crystalline Materials – 1
(Point Defects)

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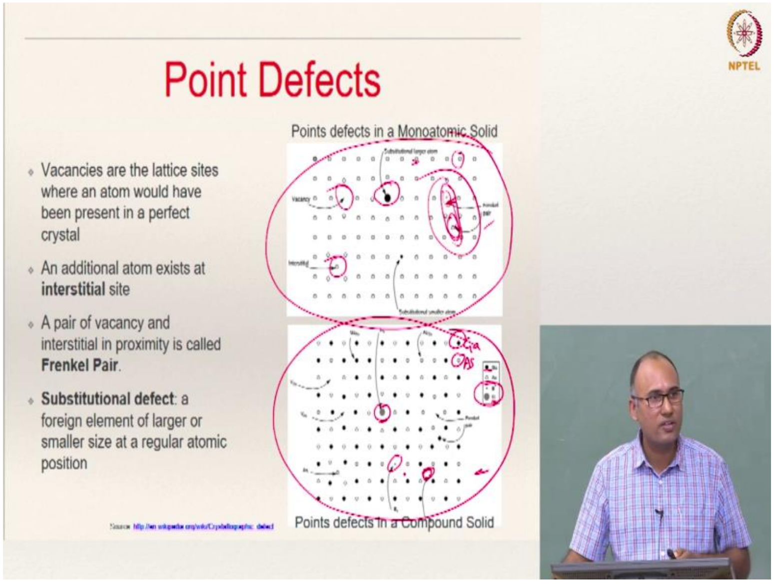

Let us now look at point defects. If you see this crystal lattice, these are the atoms or lattice sites, where there are atoms and you see that in this position, there is no atom, where it should have been, right? Such a defect is called a vacancy and here, you see that there should be an atom of this type, but some other foreign atom which is larger than this one is actually substituting for the position of the parent atom. And hence, it is called a substitutional point defect.

It is actually substituting for the position and here, if you see, this is actually not a lattice site, but this atom comes and sits in the interstitial positions available amongst the lattice sites and hence, such a defect is called interstitial point defect. Now, if you carefully look here, you have a vacancy, and very close to that vacancy you have an interstitial. Such a pair is called Frenkel pair. It is a particular kind of a defect.

So that means, you are having a vacancy; but very close to that vacancy, there is an interstitial. Probably, the atom which should have been sitting here, actually did not go there, and it is hanging around there. So, if this atom goes there, it would have become a perfect crystal and such a pair of point defects is called a Frenkel pair. What we see here is a gallium-arsenide system. The black dots are gallium and this is arsenic, and then, in that you have impurities of boron and indium. Because the size of indium is larger than all other atoms, usually it forms a substitutional point defect.

The interstitial sites will not be having enough space for indium to occupy the interstitial sites, and they are usually occupied by the impurity atoms which are smaller in size compared to the parent atoms. Boron, for instance if you see here, sometimes can actually substitute, but there is a higher probability for this boron to go and sit near the interstitials because there is free space available. It does not have to knock off the existing parent atom. When you are looking at point defects, you have different kinds of point defects depending upon the size of the atoms.

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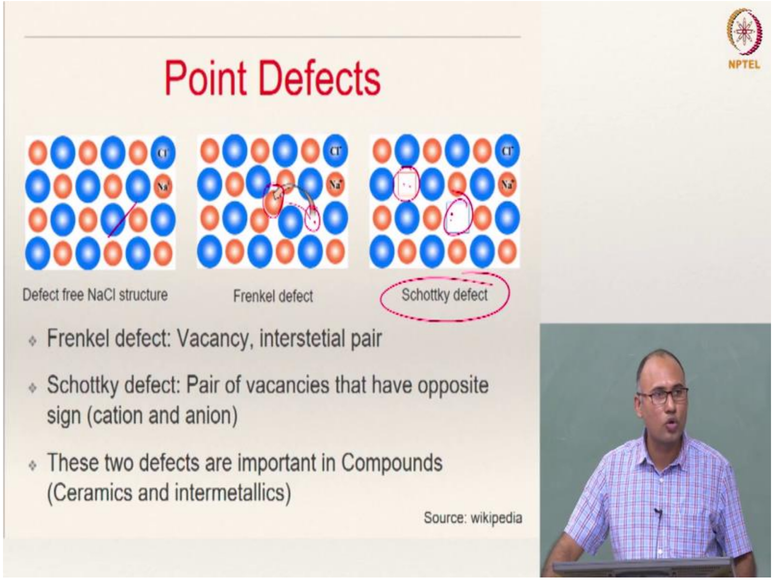

For instance, this is NaCl structure which is defect free, and here you have a Frenkel defect. Frenkel defect means an interstitial and a vacancy side by side. If you have a vacancy here and you do not have an interstitial here, but far away, then those two cannot be called as Frenkel pair because they should be close to each other. And there is another kind of defect which is called Schottky defect.

What is a Schottky defect? Schottky defect is a pair of vacancies that have opposite signs. You have both elements, sodium and chlorine; one is positively charged and one is negatively charged, and you need to have vacancies of these two ions together.

Here, what should have been there? Sodium should have been there; here, chlorine should have been there; both of them are missing. So, you have a pair of vacancies which are of opposite sign; one is an anion and another is a cation, which are not present in the crystal lattice and such a pair is called Schottky pair or Schottky defect. So, these two kinds of defects are usually found in ceramic compounds and intermetallics. So, it is very important to understand these two kinds of defects and their role in the mechanical behavior of the ceramics.

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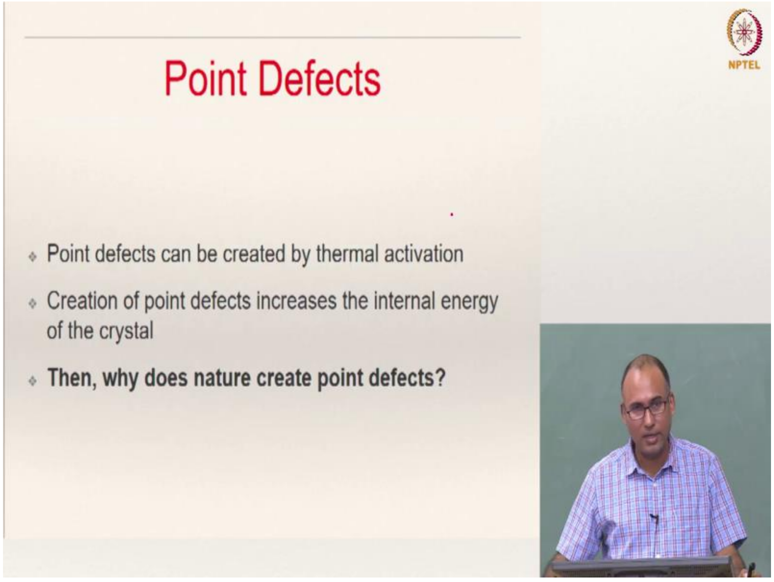

How can you create point defects? Is it possible to create point defects? Yes, they can actually be created by thermal activation; that means, if you increase the temperature of a material, then what will you do? By increasing the temperature, you are providing energy to your atom. If you provide sufficient energy, the atoms can actually jump out of their equilibrium position and move around. When you create a point defect, what happens? The internal energy of the system or the crystal increases. If the creation of point defects increases the internal energy of the crystal, why does nature create point defects in the first place?

What does nature try to do? For every system we will try to minimize the energy. But by creation of a point defect, you are going to increase the internal energy of the system, because you are actually creating the local distortion and that will increase the internal energy of the system. If that is the case, ideally nature should not be actually creating point defects. But you have point defects in the materials. What is the reason for that? Alright, that is the question that we are trying to address now.