Basics of Materials Engineering
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Lecture - 15
Defects in Crystalline Materials - 2 (Effect of Point Defects)

In the last class, we have looked at how do we go about calculating the theoretical shear strength of a given material.

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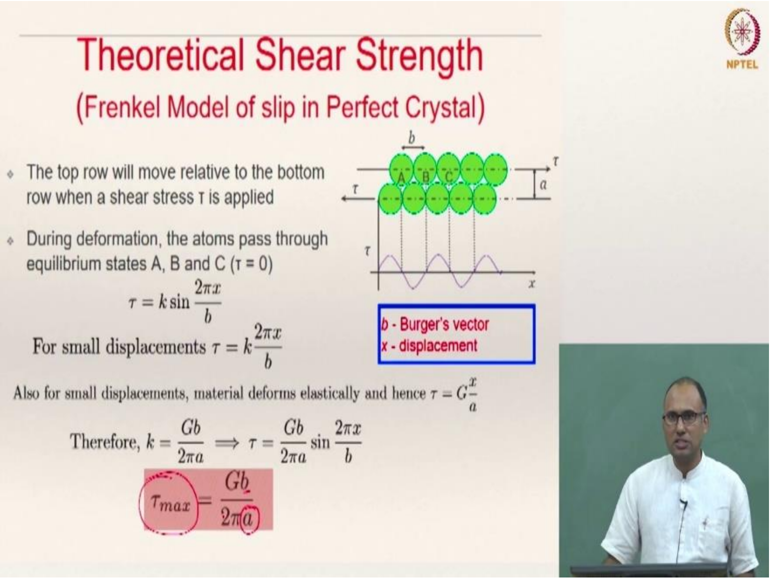

We have seen that the maximum shear stress required to cause slip of one atom plane over another plane of atoms, is given by

$$\tau_{\max} = \frac{Gb}{2\pi a}$$

where a is your interplanar distance.

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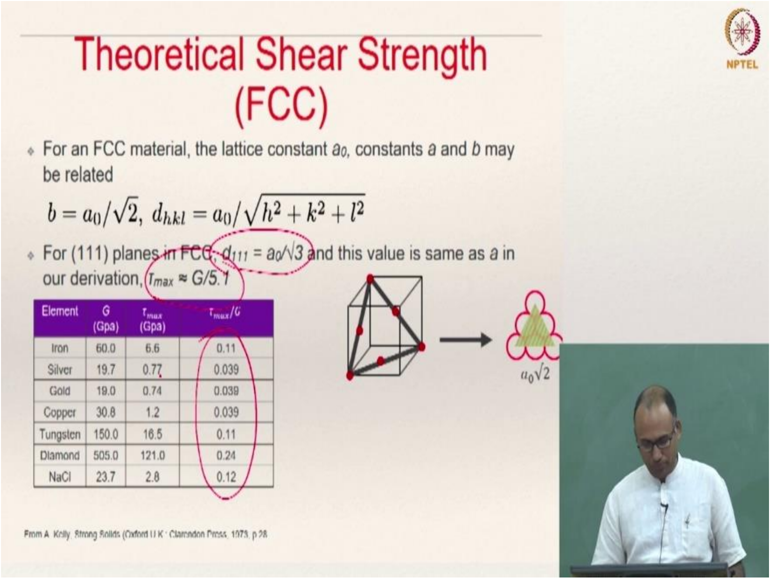

Using this simplified formula, we can actually calculate for any given material, $\tau_{\max}$ as a function of shear modulus. If it is an FCC material, and if you are talking about slipping over (111) plane -- so, for (111) planes, you know the interatomic spacing can be calculated to be $\frac{a_0}{\sqrt{3}}$, where a_0 is your lattice parameter for the FCC crystal. Then, we can find out the $\tau_{\max} = \frac{G}{5.1}$. One-fifth of the shear modulus.

The shear modulus and the shear strength of the material are of approximately same order of magnitude. But the real materials do not have such high values. If you calculate the theoretical values for the materials in these idealistic situations, they are at most one order of magnitude different, but otherwise they are all almost same order of magnitude.

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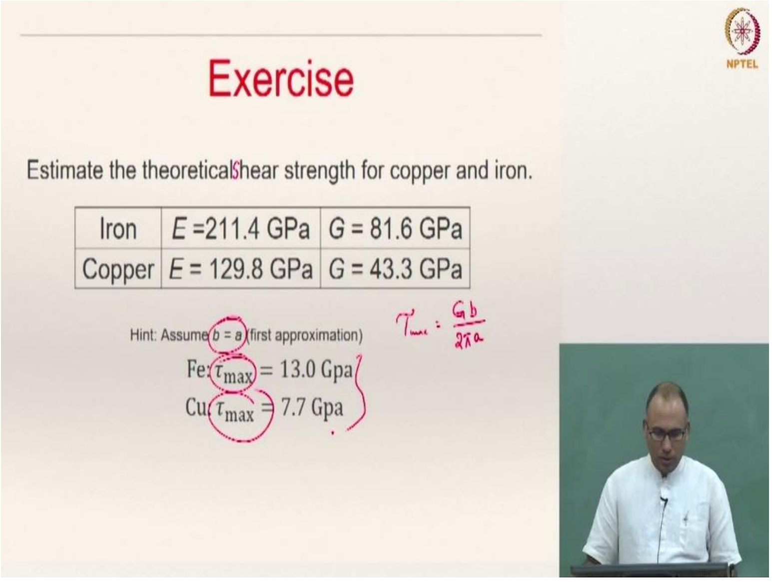

You can actually estimate the theoretical shear strength of copper and iron given their elastic modulus and shear modulus. We have just now calculated

$$\tau_{\max} = \frac{Gb}{2\pi a}$$

We can make a reasonable approximation saying that the interatomic spacing and interplanar spacing are almost similar. They are not going to be exactly same, but you can make a firsthand approximation.

If you make such a firsthand approximation, then you can calculate your $\tau_{\max}$ for iron and copper to be in the order of gigapascals. But the real material shear strength is known to be in the order of megapascals.

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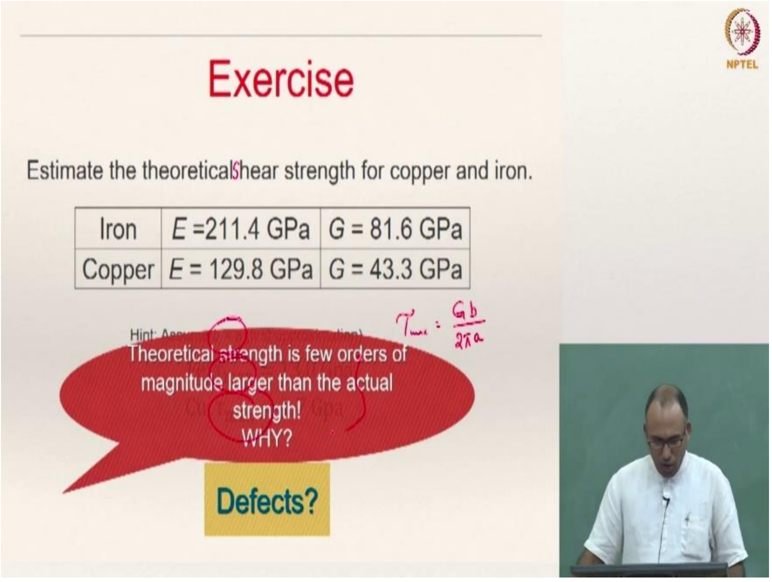

That is the discrepancy why the theoretical shear strength for ideal crystal are calculated to be much higher while the real materials do not have such high strengths.

The origin for these things may be in the defects. That is the reason why we probably need to study defects and then try to understand how these defects lead to lower strength to these materials.

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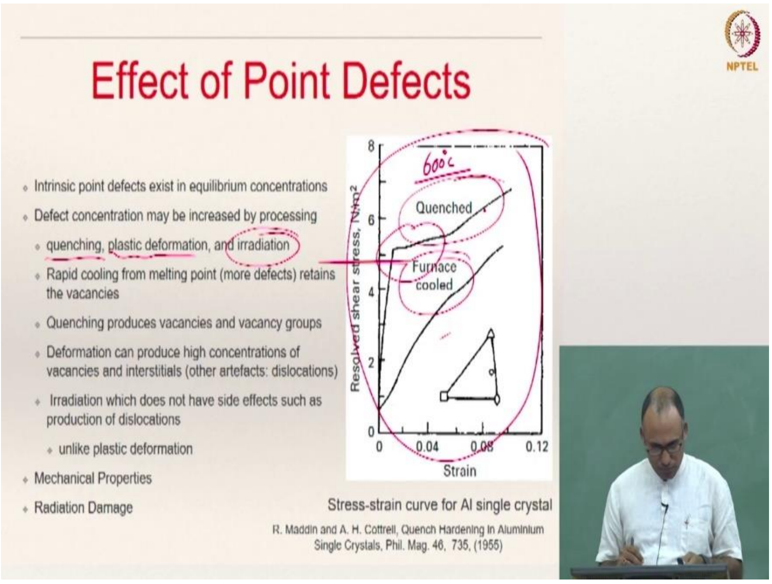

So far, we are have looked at point defects. Let us now look at the different effects of these point defects. We have already discussed in the last class and have derived an expression for equilibrium concentration of vacancies. During that process, we have realized that even at room temperature, without actually doing any additional thermal excitation, every material will have some number of vacancies or point defects -- this is equilibrium concentration of vacancy.

The intrinsic point defects always exist in equilibrium concentrations in every real material. The concentration of these point defects can be increased by different kinds of processing. You can increase the point defects by thermal activation or by doing some mechanical work as well. You can increase the concentration by quenching. Quenching means sudden cooling of the material from high temperature.

By plastically deforming the material, you can increase the number of defects in the material. Another way that the point defects in particular can be induced in a material is through irradiation. However, the nature of point defects that are generated due to irradiation is something that needs to be looked at. We will discuss about the effect of irradiation on materials in a moment.

Here if you see this graph, this actually shows the stress-strain curve for aluminum single crystal. And there are two lines; one of them is a quench sample, another one is the furnace cooled sample. Both these samples are cooled from 600° C. They are initially at 600° C. One of them is quenched; that means, suddenly cooled may be by putting in open air or in water. So, the rate of cooling is very high.

The other one is furnace cooled; that means, you keep the sample in the furnace and gradually reduce the temperature of the furnace and hence it is a much slower rate of cooling. You bring them to room temperature in both these cooling methods, and then do the testing on these sample. What you would see is both of them behave differently. The quenched sample shows much higher strength compared to furnace cooled sample.

Because of quenching you are imparting point defects to the material, or you are introducing defects in the materials and these defects act as barrier for plastic deformation. The number of defects that you produce depend on the rate of cooling and that is because, in quenching the rate of cooling is much higher and hence you will produce more defects and then you have more obstacles for plastic deformation.

If you quench a material, you are going to increase the strength of the material. The yield strength of the material is much higher here in this case comparatively. But then it also comes with a problem. You are reducing the ductility; that means, the material becomes brittle. You might increase the strength, but the at the same time you are reducing the ductility, or you are increasing the brittleness of the material which may not be a desirable property all the time.

You might also want to increase the strength, but at the same time you do not really want to sacrifice your ductility; you do not want to impart brittleness in ductile material. You need to understand how the defects that are generated through different processing routes contribute to the mechanical behavior of the materials.

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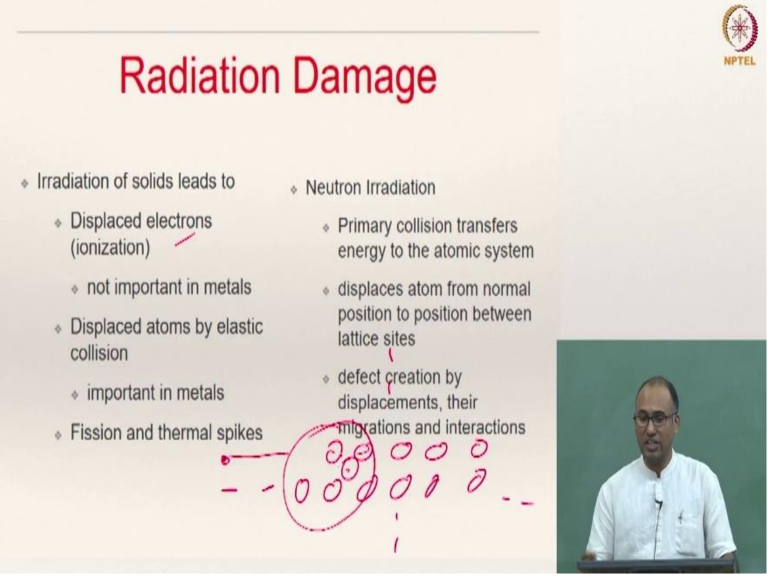

Let us now look at radiation damage. What do we mean by radiation damage? The radiation can be through different means. You can have neutron irradiation, ion irradiation; so, different particles going and hitting the material.

Irradiation of solids in general can lead to different things; they can ionize the material; that means, they can knock out electrons from the shells around the nucleus, and hence, ionize the material, which is not typically the mechanism that you observe in metals particularly; or you can actually displace the atoms from their lattice sites.

When you subject crystallographic lattice sites to irradiation, you can displace the atoms from their lattice positions. This is one of the important damage mechanisms when a metal is subjected to radiation. Let us look at neutron irradiation which is typically the major problem that is observed in nuclear reactors.

You have high energy neutrons that go and hit the structural material. The shell of a nuclear reactor is made of some special steel. These high energy neutrons go and hit the surrounding casing material. Because of that, they can displace atoms from their crystallographic lattice positions. What happens when you have a very high energy neutron coming and hitting an atom and the atom displaces? You are having a vacancy. You are actually creating point defect.

Imagine you have a nicely ordered crystal like that. Crystal means you have this order till long range and let us say you have a high energy neutron coming and hitting. If the energy is sufficiently large, this atom will be knocked off. It may be moving to some other position in the crystal lattice because of the high energy that you have imparted. So, you have created a vacancy and what happened locally? Locally the order got disturbed.

If you try to look for the crystalline order, then your local order is disturbed. Locally it is not crystalline anymore. But if you have so many such high energy neutrons, they can be bombarding everywhere in your material, and in the long run, they can actually make your material non-crystalline, you can actually get your material amorphous.

You create so many point defects. So, the primary collision; that means, the first neutron comes and hits an atom, the energy will be transferred to the atomic system and usually you will displace the atom from its normal position to somewhere in between the lattice site. It can go anywhere. Because it has high energy, it can actually stretch the bonds and actually sit in the interstitials although the space is not enough. But now, it has energy; it can push aside and thus you create point defect in the case of radiation.

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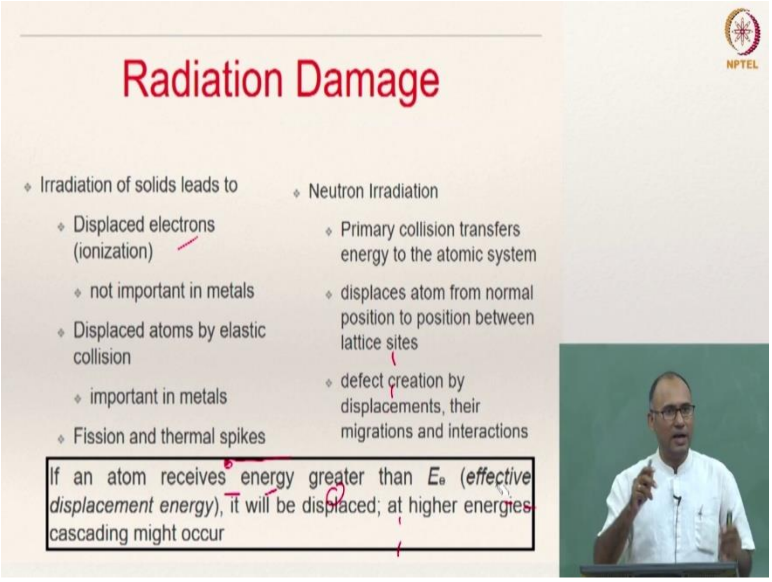

If an atom receives energy which is greater than effective displacement energy; what do you mean by this effective displacement energy? Energy, that is required to displace an atom from its equilibrium lattice position.

If the energy supplied to the atom is larger than the energy required to displace the atom, then the atom will displace. Otherwise, whatever energy is imparted to the atom will be transferred to neighboring atoms. The atom will be oscillating about its mean position and if you are giving a higher energy, then its oscillation amplitude will increase and the energy will be transferred because it is elastic.

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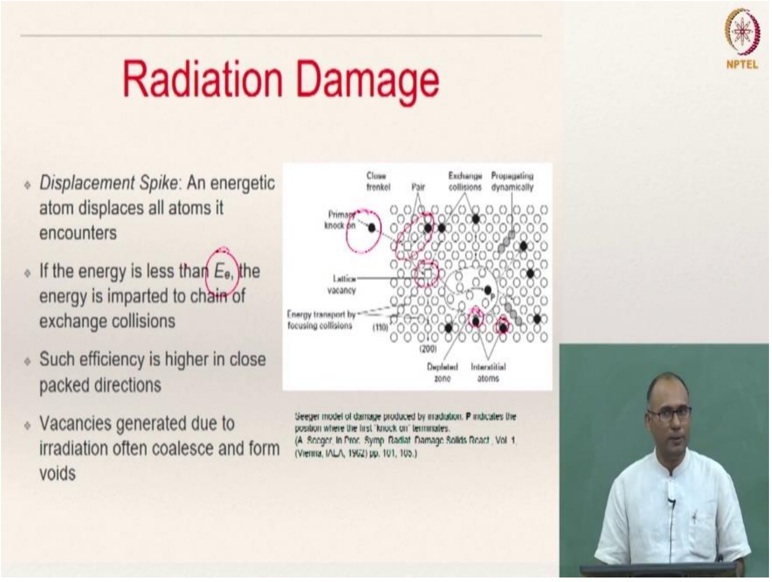

This is a typical picture of radiation damage; a cartoon that shows the various processes that one can discuss in the case of radiation damage. For instance, if you have a high energy atom, if you had energy from a very high energy neutron for instance this primary knock on atom, it will go and hit the atom positions in the lattice and then gradually they displace the atoms from their actual positions and create different kinds of point defects. For instance, here you have a vacancy and here you have vacancy-interstitial pair, and so on. And here, exchange collisions and then here you have a large sort of void alright and here you have created interstitial atoms and so on.

You have got some energy to this atom and when this atom is moving and whatever comes in its way, it actually pushes away and then gives away energy to the surrounding atom and this process is what is called displacement spike. When this energy that is imparted to the atom is sufficiently large and if it is larger than displacement energy E_e, then you will create point defects.

These point defects i.e., either vacancies or interstitials, now act as obstacles to plastic deformation. What do we mean by plastic deformation? We will see in a moment. If we create more and more point defects, all these point defects are going to stop the plastic deformation. And as a result, what happens?

The material offers more and more resistance for further deformation and hence you have higher yield strength. You will not be able to impart plastic deformation at a position where you would normally impart when the defects are not present in the material.

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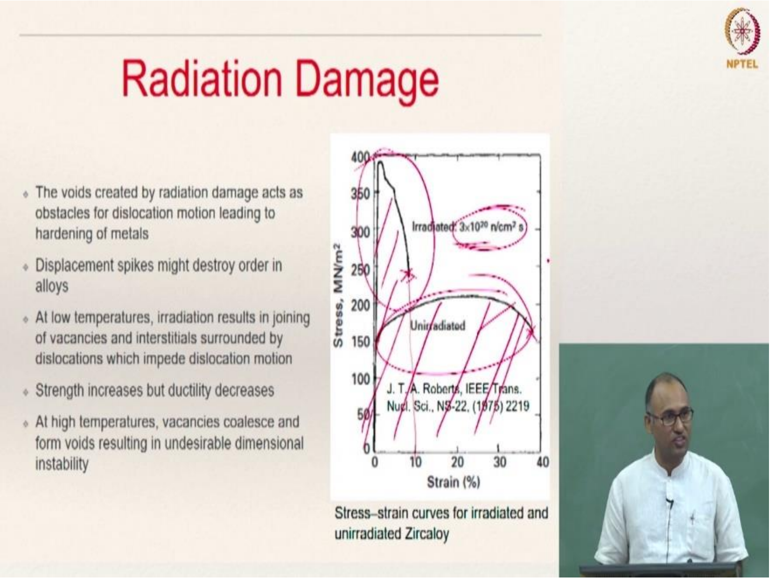

This is the stress-strain graph for zirconium alloy Zircaloy. This is an irradiated sample and this is an unirradiated sample. So, this is the dosage and you can clearly see that the material has become extremely brittle. After this much of irradiation, the material has become extremely brittle.

If you take the area under this curve, this area is much less comparatively. What is this area? This is the energy. So, let us say this is fracturing here, this is fracturing here, the total energy that can be absorbed by this material before it can fracture. Here, you have much less energy and also much less strain.

Here, you can actually go up to 35 percent strain, here your strain is only 10 percent; that means, when the material breaks, you will not have enough time for response. You will not be given sufficient number of notices that it is actually going to give away, whereas, this material will give you some sort of an indication that this is going to a break. And that is the problem with irradiation.

You really do not want to have a material which gets embrittled during its service, and that is a reason why the design of pressure vessels that are used in nuclear reactor is extremely important. And once you do it carefully taking into account of the effect of irradiation and that is a reason why you need to check for the health of these material from time to time. Otherwise they can create catastrophes, because if your pressure vessel becomes brittle over time and even if you have a small crack, the crack gives through suddenly.

When it becomes a critical crack, the crack gives through suddenly in a brittle material in comparison to a ductile material. You do not want to break this pressure vessel all of a sudden, because then it creates a much more dangerous accident. That is the reason why you need to understand the effect of these defects on the mechanical behavior of the materials.

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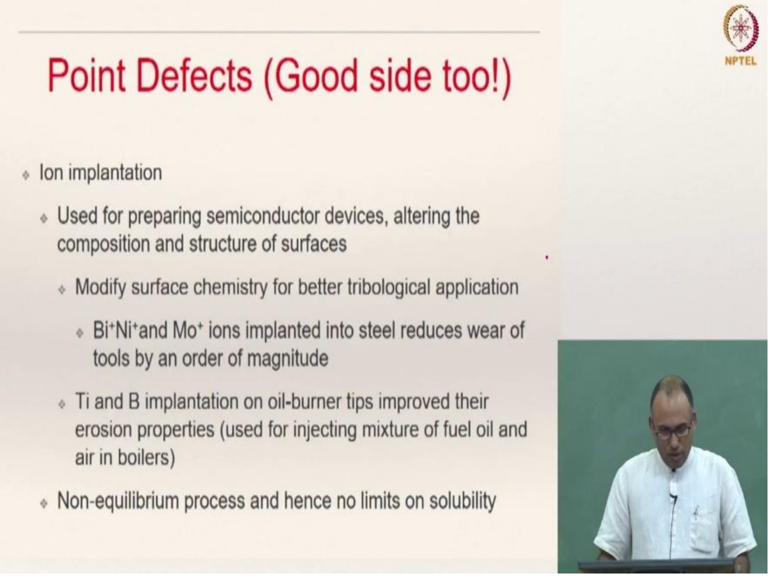

So far, we have discussed these point defects and how they affect the mechanical properties, how they are going to negatively impact the mechanical behavior of the material. But as we have discussed, the defects are not necessarily always bad for you, sometimes they can also be good.

For instance, the ion implantation; you can use them for preparing semiconductor devices and also changing the composition and structure of surfaces of the materials.

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For tribological applications; tribological application means where you have a lot of wear and tear. When two surfaces come in contact, and then they are moving fast on another, there is a possibility for the material to get worn out over the time. If you want to minimize this wear, then you can actually do some processing to the surface -- some surface treatment. People have shown that you can use bismuth, nickel, molybdenum ions and you can use them to implant on the surface of steel in order to enhance their wear resistance.

Similarly, titanium and boron implantation on oil burners improves their erosion properties because they work at high temperatures. If you want to improve their erosion properties, all you need to do is some surface treatment. So, basically here, if you do the ion implantation of titanium and boron, then that enhances the erosion properties. Like this, you can actually see several other useful sides of point defects.