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Lecture - 17 Defects in Crystalline Materials – 3 (Line Defects, Types of Dislocations and their Characteristics)

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In the last class, we have started our discussion on line defects or dislocations, wherein we have discussed that the stress required to plastically deform a real crystal is much less than the stress calculated for a perfect crystal. The reason for that reduction in stress required for imparting plastic deformation is due to some sort of defects called line defects or also known as dislocations.

We have also discussed that the concept of dislocations was invented by Orowan, Taylor and Polanyi in 1934. Although they did not observe them experimentally, theoretically they have hypothesized that defects such as line defect should be existing in order to confirm with the reduction in stress for plastic deformation for real crystals.

However, the first experimental observation of dislocation was made in 1947. In this class we will look at more details about the nature of the dislocations and then the details therein.



Here we have a bubble raft experiment as is done by the Cambridge material science course. I have borrowed it from the Cambridge material science course available freely on web at this particular link, wherein you can actually have lot of information about the dislocations.

The way to create such a bubble raft has also been explained in that web resource. I encourage all of you to go to this web resource and see how this bubble raft has been created. So, if you look at this particular bubble raft, you can see certain point defects. For instance, you can see a defect here, a defect there, and a defect here. All of them are point defects.

This is an interstitial defect and here you can see a substitutional defect and so on. These are the different kinds of point defects. If you see here in this line where the line is shown, there is continuous line of atoms and here also a line of atoms; but here you have only a half plane of atoms. Imagine this line represents a plane in the out-of-plane direction and we have atoms in there.

Such a defect which has only an extra half plane and other half plane is missing below it is what we call dislocation and this is something that one can create using a bubble raft experiment as shown here. Similarly, such line defects and point defects can also be observed in sweet corn. If you look at sweet corn, you will see the white colored one and yellow colored corn seeds. The difference in color sort of represents your point defects, but also you can nicely observe certain kinds of line defects such as dislocations.

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Let us now look at the slip caused due to shear stress by the two mechanisms that we were discussing: by glide of plane of atoms as compared to the dislocation. We will see how this deformation takes place. Here in this animation, we will see the meaning of slip by a glide of a plane of atoms. What is happening here is that, all the bonds, atomic bonds are broken at once and then recreated.

You can see that here this atom bond, all these bonds are broken and then again recreated with the neighboring atoms. So, this atom was a neighbor to this atom before the slip has happened; now this became a neighbor to this atom. So, that is basically plastic deformation, because the neighbors are changing i.e., there is a breakage of bonds.

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If you look at slip by dislocation motion, you can see that here you have an extra half plane and here the plane of atoms is not available.

If you are applying shear stress as shown here, the slip can be seen as the motion of this line defect moving from left end to right end. That is a difference between slip by a glide of plane of atoms, all the planes of atoms are breaking their bonds simultaneously and then reestablishing, as compared to the dislocation where one bond is broken and then reestablished and so on.

That is the difference between dislocation motion and slip. In a real material, because of the presence of such defects, you can have plastic formation by dislocation motion, because it requires much less energy compared to the glide of atoms.



The stress required for slip, the theoretical shear strength when we have calculated is given by this expression $\tau_{\text{max}} = \frac{Gb}{2\pi a}$, where *b* is interatomic spacing in the plane that is called Burgers vector and *a* is interplanar spacing. We have already seen this derivation in the previous class. The shear stress required for slip by dislocation motion is this expression and was derived by Peierl and Nabarro.

That is why it is called Peierls-Nabarro stress

$$\tau_{\rm p} = G \, \exp\left[-\frac{2\pi a}{(1-\nu)b}\right]$$
$$\tau_{\rm p} = 3G \, \exp\left[-\frac{2\pi w}{b}\right]$$

where b is the Burgers vector, w is the dislocation core width. What is the size of the dislocation core?

If your Burgers vector is equal to the dislocation core width for this simple situation, τ_p can have a maximum value of $\frac{G}{180}$. This is the shear stress required for causing slip by dislocation motion; whereas this is the shear stress required for causing slip by glide of plane of atoms. You can see that this value is much smaller than the theoretical shear strength that is predicted.

The shear strength required for causing slip by dislocation motion, given by the Peierls-Nabarro stress, is a better approximation to the real value of shear stress required as compared to the theoretical shear strength.

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Here we can see how a caterpillar moves. You can see that the caterpillar basically does not move by slipping, but it will actually lift the area that is between two legs and then push that; it will create a hump and then slip that hump and effectively it moves, it makes a motion in the direction of its requirement. The dislocation motion can be seen as analogous to the motion of a caterpillar.



The dislocations as we have already discussed are line defects; so you have a plane of atoms here, which are an extra half plane. If this is not there, it would have been a perfect crystal; but because of this extra half plane, then this becomes a crystal with a line defect.

When you are applying shear stress this way, the extra half plane is moving to the right eventually slipping. So, this will cause unit slip and the amount of slip caused is actually equal to the interatomic distance. That is represented by a special vector called Burgers vector, we will look at it in couple of minutes.

Here, this particular defect is called an edge dislocation and you can observe that if you see in the out-of-plane direction. You have seen this symbol, which is shown like this. So, this basically represents that you have an extra half plane of atoms. This is your extra half plane; so that means the extra half plane is existing above this plane, and below that there is no extra half plane. This is the representation of an edge dislocation. If your extra half plane is actually available at the bottom rather than at the top, then you would describe the edge dislocation as like that.

This line represents the presence of extra half plane or the line defect. This type of defect is what you call edge dislocation.

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As we have been discussing, the dislocation motion can be analogous to the caterpillar motion. So, here this is analogous to your extra half plane. This extra half plane when it moves, causes slip. The amount of slip that is caused is equal to the amount of distance that the caterpillar would have moved by moving this hump towards this edge.

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In the bubble raft, you can see that these are what we call closed packed directions; that means the interatomic spacing in those directions is minimal. If you take this direction, the interatomic spacing is actually larger than this case. These are all our closed packed

directions and it is important to realize these closed pack directions, because later in tomorrow's class, we will see why these closed packed directions are important.

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If you take this bubble raft, when you are applying a state of compression, we will see that the dislocations are moving under the action of compression. You can observe the dislocation motion happening in the bubble raft, which is a two-dimensional system. In order to visualize the movie, I encourage you to go through this link wherein these movies are available and you can see how the dislocation motion is happening under the action of compression and as well as under the action of shear stress.

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Dislocations are basically classified into two classes: one is called edge dislocation and screw dislocation. If you see this, this is what we are calling extra half plane of atoms throughout the system and this line is what you call dislocation line. The end of the extra half plane is a line.

If you connect all the atoms at the end of the extra half plane with a line in the out-of-plane direction here, that will represent our dislocation line. If you are applying shear stress in this direction, then the slip takes place in this direction and then eventually you will have slip of that kind.

In the case of an edge dislocation, the dislocation line moves in the direction of the applied shear stress. If you are applying shear stress in this direction, the dislocation line also moves in the same direction. The second figure, this figure represents another kind of dislocation called screw dislocation.

Here, that is our dislocation line; we are not able to see that, it is hidden there. When you are applying shear stress, this dislocation line moves here, eventually causing same kind of deformation. The dislocation line is moving in this way, whereas shear stress is applied in that direction.

This is going perpendicular to the applied shear stress. So, the dislocation line moves in a direction perpendicular to the applied shear stress and such a dislocation is called screw dislocation. However, although the dislocation line motion is different, the net plastic

deformation in both the cases is the same; that means the amount of slip caused is same and in the same direction.

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This is another example of edge dislocation and screw dislocation; these are called the Volterra dislocations, because Volterra has given this idea.

If you take a sheet of paper and roll it until the edges touch each other; then that is sort of representation of a perfect crystal. Normally, if this end meets here, it would have been a perfect crystal. But if you are slipping by this amount, then this is what we call the representation of an edge dislocation.

When you are starting here and by the time you come here, you are in the same plane, but you are off by certain amount, equal to this width. That is what we call an edge dislocation. Instead of slipping in this direction, if you move this plane a little bit upwards, then you can see that this is our screw dislocation. This is similar to the parking lots that are there in the shopping complexes.

In a parking lot, if you make one round starting at the ground, you go to the next floor; that is what you are basically doing. You are actually going around this axis and then by the time you reach here, you are going to the next round.

This is behaving like a screw; when you are rotating a nut on a screw thread, when we make one rotation, the nut would have moved upwards equal to the pitch of the screw

thread. Similarly, this motion creates such a deformation and hence it is called a screw dislocation.

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This is a perfect crystal in 2D and here we are showing in 3D. The 2 D picture is good enough to explain the Burgers vector of edge dislocation; whereas 3 D picture is required for explaining the Burgers vector of screw dislocation. We know that, when you have an edge dislocation and you are applying shear stress, you will have slip. The direction of the slip and its magnitude is described by a quantity called Burgers vector.

Let us say you are at position M. Let us say you are at this point and now if it is a perfect crystal, if you make a loop -- so, this is our starting point and I am going one, two, three steps vertically and four steps horizontally; then I go in the opposite direction three steps and again the opposite direction of the horizontal displacement four steps. Then, the starting position and ending position are the same. That happens when you have a perfect crystal or in the loop where there are no defects.

Now, let us take this situation wherein you have an extra half plane here, this is an extra half plane. I am starting at M and moving one unit, two, three units vertically and one, two, three, four units horizontally. Since I came down three units, I go up three units like that. How many units have I moved horizontally? One two, three, four, four; four units horizontally to the left.

Now, I move to the right one, two, three, four. So, I stopped at Q. That is my starting point and that is my finish point. If I draw a vector from start to finish, that is what is called Burgers vector.

The Burgers vector represents the direction in which slip is taking place and the magnitude; this will be the magnitude that you would have by causing the dislocation motion. If your direction of the slip is like that, then the Burgers vector is also in the same direction of your slip. This is your dislocation and the dislocation line is in the out-of-plane direction, i.e., perpendicular.

When you are applying slip like this, the dislocation line is also moving. Suppose if you are applying slip, the dislocation line is moving in this direction and the Burgers vector is also moving in the same direction. That is what we said when we have defined edge dislocation; the dislocation line and the Burgers vector move in the same direction as the applied shear stress.

Let us now look at the Burgers vector in the case of screw dislocation. Not here, but at a later stage I will show you a detailed view of looking at screw dislocation.

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The Burgers vector describes the magnitude and direction of the lattice distortion associated with the dislocation.

The nature of the dislocation is identified by the relative orientation of the dislocation line and Burgers vector. In an edge dislocation, the Burgers vector and the dislocation line are perpendicular to each other, as we have seen here.

In metals, the Burgers vector will point in close packed direction with magnitude equal to the interatomic spacing; because the close packed direction is the direction in which your slip takes place. The dislocation density is a quantity that describes the total length of dislocations in a material per unit volume of the material.

If you take a unit volume of material, what is the total length of all the dislocations? For instance, if you take a carefully solidified material, the value of dislocation density will be something like 1000 mm of length of dislocations per mm³ of the sample. So, $10^3/\text{mm}^2$ is the dislocation density.

Some people also describe the dislocation density as number of dislocations per unit area. But the better definition for dislocation density is the length of the dislocations per unit volume of the material. If you have heavily deformed metals, then the dislocation density is going to be very high. You can see almost 10^{10} mm/mm³.

It is almost six orders of magnitude higher than that of a carefully solidified; that means during deformation, the dislocations multiply increasing the density of dislocation significantly.

The concept of Burgers vector was invented by the two professors at Delft University, Jan Martinus Burger and Wilhelm Burger. These two people are responsible for the definition of the Burgers vector.

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This is a typical TEM image, transmission electron microscopy image of dislocations in titanium alloy looked at magnification of 51450 and you can see these lines are dislocations.

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How do we go about looking at a screw dislocation? This is a dislocation line and the Burgers vector is parallel to the dislocation line, as opposed to being perpendicular in the case of edge dislocation. In the top view of this figure, you can see AB is the dislocation line, and all the open circles represent the atoms in the top layer and the dark circles represent the atoms in the bottom layer. The upper front region of the crystal is shifted by one atomic distance to the right relative to the bottom portion, as seen here. Usually, an edge dislocation is represented by symbol like that; a screw dislocation is represented by a symbol like that.

How do we go about defining the Burgers vector? We have shown this here, right? Let us say we start there and we are going one two, three, four units down here and one, two, three, four, five, six units to the left and one, two, three, four, five, six units up. And so, again we have to go back; to the right, we have to make six units. Since we already made four units here and remaining two units, because you have gone six units here, -- so, I have to go by two units and then you will end there; that is our end point. So, you have not come back to its original position. When we are making this loop, we should ensure that you are actually going around the defect; if you are not going around the defect, you would find that it is a perfect crystal.

For instance, if you make such a loop in this region, you will see that you are coming back to its original configuration; that means this loop is not including the defect, here this green loop is actually including the defect, and hence your start position and end positions are different.

As we have discussed in the previous case of edge dislocation, if you draw a vector from start to finish, that is the Burgers vector, which represents the amount of slip and the direction of the slip. You can see that the Burgers vector here is parallel to the dislocation line.

However, if the Burgers vector direction is also parallel to the slip direction here.



The open circles are plane above and the solid circles are plane below for the screw dislocations. The Burgers vector is parallel to the dislocation line in screw type; whereas in edge type that is perpendicular to the dislocation line.

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Here we have another system, wherein you have mixed dislocations; here you have a screw type and here you have an edge type dislocation. Several real materials not necessarily have only pure edge type or pure screw type, they may have mixed dislocations. Here, this is our dislocation line. So, here it has screw nature, here it has pure edge nature; in between it has a partial screw nature and partial edge nature.

That means, with respect to the dislocation line here in this region, the Burgers vector will be parallel to the dislocation line; in this region the Burgers will vector will be perpendicular to the dislocation line. The dislocation line is like that and then the Burgers vector is like that, so that is perpendicular. But in between, the Burgers vector will not be either parallel or perpendicular; it will be at certain angle to the dislocation line.

Note that in this figure, the dislocation is changing its nature being screw here to the edge here; but the Burgers vector will not change its sense. In all the cases, the Burgers vectors direction is the same, it is only the dislocation line that is changing its direction; that means the nature of the dislocation is changing, eventually the Burgers vector direction is remaining the same. That is an important concept to understand.

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Let us now look at the characteristics of dislocations. The plastic deformation in metals usually leads to an increase in internal energy and dissipation as heat. When you are applying external stress, there is some amount of plastic deformation. A lot of amount of energy is dissipated as heat and some amount of energy is stored as strain energy and this strain energy is usually associated with the dislocations. In this figure here, if this extra half plane was not present, this would have been a perfect crystal. But because of this inclusion of this extra half plane; what happens? The atoms in this region which are close to the extra half plane are sort of squeezed together; whereas the atoms below the extra half plane are pulled apart. Let us say this above this plane, you have an extra half plane of atoms; there the atoms are squished together and as a result the atoms just above the dislocation line or adjacent to the dislocation line are in a state of compression.

The atoms below are in a state of tension, for the case of an edge dislocation. The atoms elsewhere which are not immediately above or below might be in a state of shear. The tensile compressive and shear lattice strains are possible for edge dislocation; whereas for screw dislocation only you will have shear lattice strains. So, the lattice distortions take place as strain fields are emanating from dislocation line because of the presence of this extra half plane.

The region which is having this extra half plane will experience state of compression in an edge dislocation and the one below experiences a state of tension.

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If you are applying shear stress, the slip takes place in this plane, right? This is something called positive edge dislocation and let us say this is what you call negative edge dislocation. If you have same sign of dislocations in the identical slip plane, when they are coming close to each other, they try to repel each other, because the atom planes are squeezed together and this will also have a squeezing together kind of a stress strain field.

As a result, you see that when these two of same sign are coming together, they repel each other; either positive edge dislocation or negative edge dislocation.

However, when two dislocations of opposite sign and in the same slip plane are coming together, they attract each other in order to annihilate; they annihilate and become a perfect crystal. Because you have an extra half plane here and an extra half plane here, these two become a perfect crystal. The dislocations can either repel each other, attract each other, by attracting they annihilate; so that means, the dislocations actually can interact.

During plastic deformation, the dislocation density increases drastically. The strain fields associated with these dislocations and the associated forces causes something called strengthening mechanisms, that leads to a special property called strengthening for the crystal lattice.

We will discuss about these strengthening mechanisms. When you have a dislocation of opposite signs coming together due to plastic deformation, they start repelling each other. If the dislocation of the same sign is not there, this dislocation would have moved this way.

Because of the fact that there is another dislocation which is of opposite sign, further deformation of these two dislocations cannot happen. That means, the dislocation motion is sort of impeded and that will require additional higher strain to overcome the resistance caused offered by these repelling force fields of the same sign dislocations. That is what is seen as an increased strength of the crystal lattice.

So, we can discuss about these different kinds of strengthening mechanisms from the characteristics of dislocations in the next class.

Thank you very much.