Introduction to Materials Science and Engineering
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Lecture – 63
Grain boundary

We continue our discussion on two dimensional surface defects, and one of the important two dimensional surface defects are the grain boundary. Grain boundaries are internal boundaries inside a crystal and we have already met them while discussing in a dislocations, because we said that dislocations inside a crystal can end on a grain boundary. So, grain boundary is also one of the locations where a dislocation can end.

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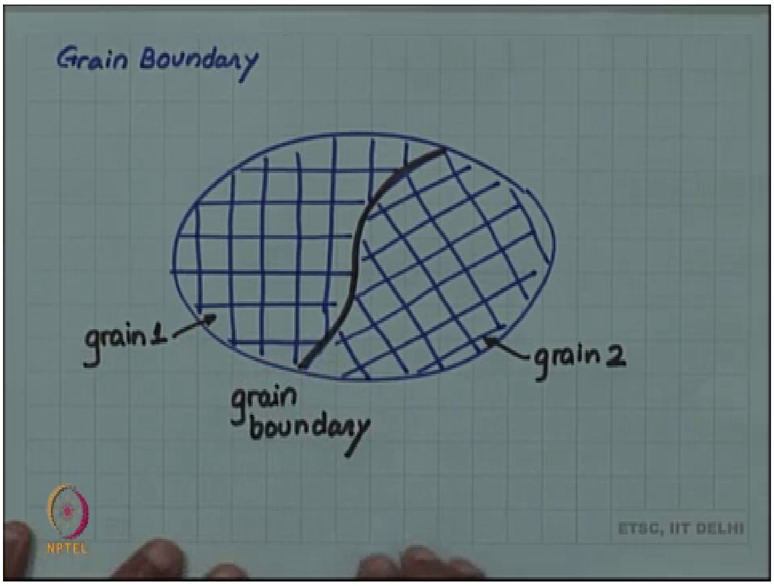

So, when discussing that we drew a picture something like this, that suppose this is a sample we are trying to indicate grain boundary. So, if the sample has the same orientation of crystal right through all, the unit cells are parallel then it will be called a single crystal, but instead if it has a boundary. So, let me draw a boundary in this and if the crystals on one side is oriented, one way this is a two dimensional sketch I am making. So, on one side the unit cell is oriented this way, but another side the unit cell orientation may be different. It is the same crystal same unit cell, but the orientation is different.

So, the crystal structure, the lattice parameter, everything is the same, but across this boundary which I have drawn the orientation changes. So, this boundary, this boundary will be called a grain boundary. This will be a grain boundary we will call this as one of the grains. So, this is grain 1, this will be another grain; grain 2 and this will be a boundary between grain 1 and grain 2.

So in fact, there are only two crystals here. So, two grains and. So, it will really be called a bi crystal, most samples of material which we use are actually poly crystalline.

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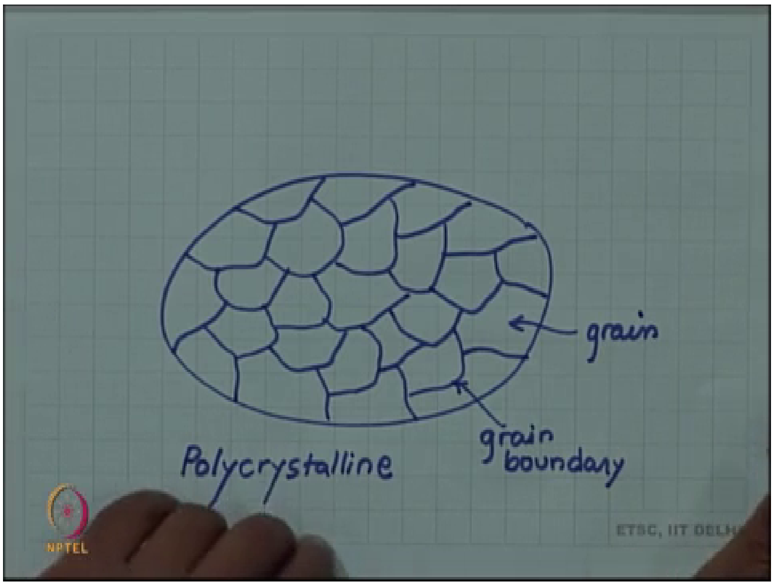

So, they will have not just a single grain boundary and two grains, but multitude of grains and each pair of grains separated by a boundary. So, I am trying to draw a cartoon sketch of a polycrystalline material.

So, this crystal that now has many grains, and each of these lines which I have drawn is a grain boundary. So, such sample will be called polycrystalline and each of these internal boundaries are the grain boundary, and each of the individual regions are the grains. So, this is typical of most material, and why we have this we will study a later in most of the cases.

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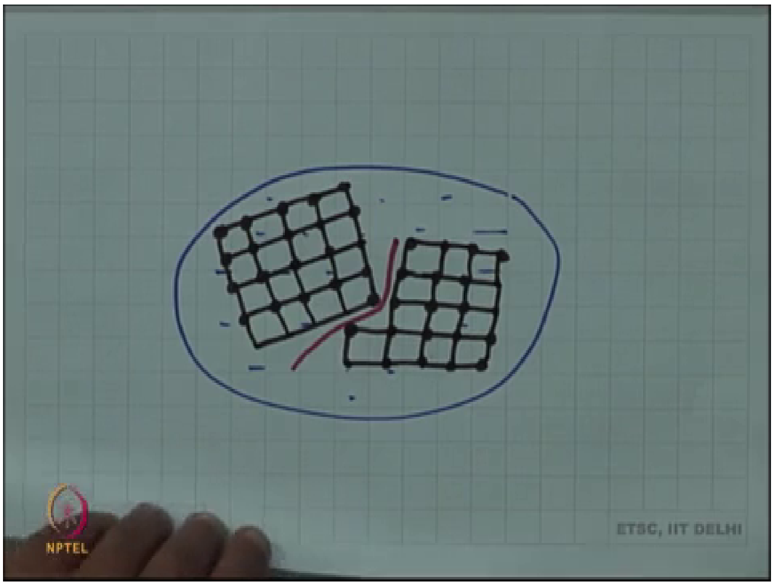

The material solidifies from a liquid and if it is solidifying from a liquid. So, suppose we were doing a casting and we had a liquid phase.

Then crystal starts forming, and in different region all the same crystal will nucleate. Nucleation will not happen in two in one, only in one region, but in more than one region and in different region, the nuclei may orient themselves differently, because this is a random process, a solid nucleus is forming inside a liquid.

So, there may be no correlation with the orientation of one nucleus with respect to the other nucleus, and then as more and more unit cells join up. So, this crystal will grow in time by adding more unit cells. This crystal will also grow by adding more unit cells and as you can see in this growth process gradually, sooner or later they will meet each other. So, in those regions where they meet, they will stop growing and that is what we will define the grain boundary, because the orientation will change in those regions.

So, in this example where two, only two nuclei were growing you can see that a grain boundary now is developing in this, this region. So, this is the reason why most materials are polycrystalline, unless and until we take a special care to make a single crystal, most materials will be polycrystalline.

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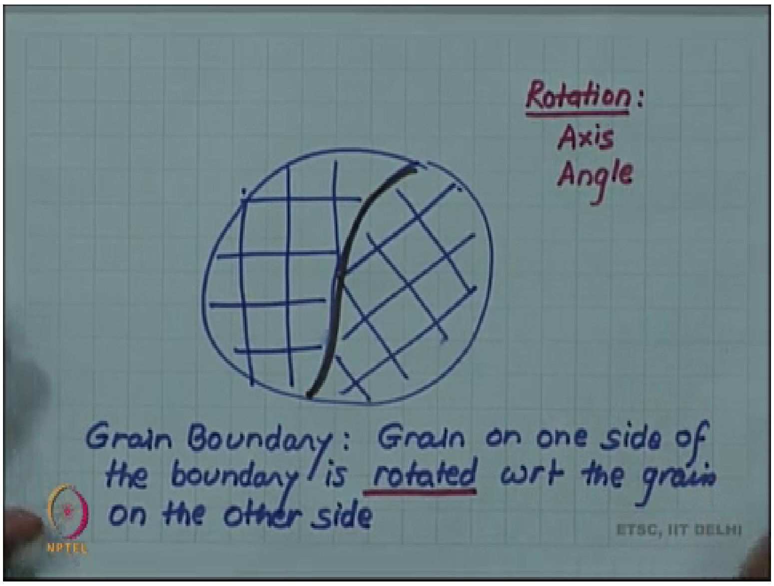

Now, since the orientation is different, as we said that across a grain boundary the orientations are different. This again is the grain boundary and orientation changes.

So, this orientation change can be represented as a rotation. So, grain boundaries or rotation boundaries grain on one side of the boundary is rotated with respect to the grain on the other side of the boundary. So, there is a rotation and a rotation can be represented by an axis, rotation axis and a rotation angle based on the magnitude of the rotation angle.

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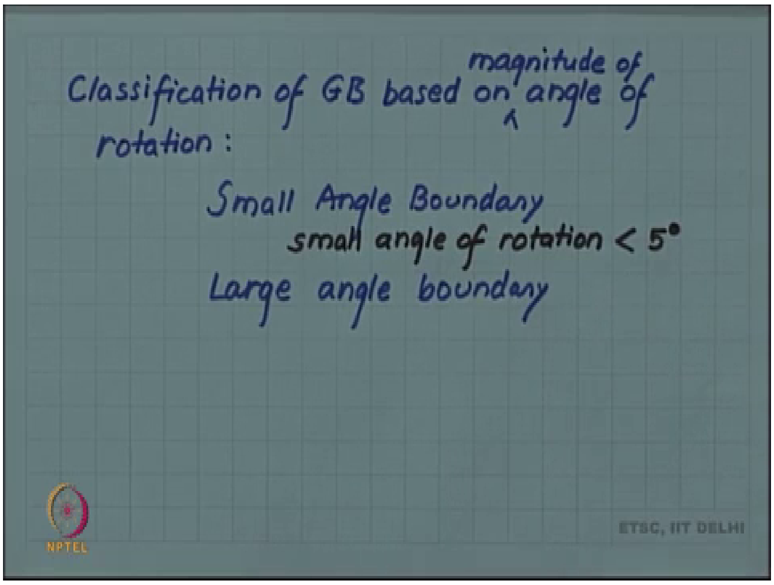

There is a classification, classification of grain boundary. I am writing G B for grain boundary classification of grain boundary based on angle of rotation, based on magnitude of the angle of rotation. We can have a small angle boundary or a large angle boundary.

In a small angle boundary, as the name suggests the angle of rotation will be small. Of course, how small is cannot be precisely defined. Roughly speaking one can think of any boundary with less than 5 degree rotation as a small angle boundary. So, those with angle higher than 5 degree will be called a large angle boundary. So, the structure of the grain boundary depends upon whether this angle of tilt is small or high. Generally small angle boundaries will have lower energy compared to the large angle boundary.

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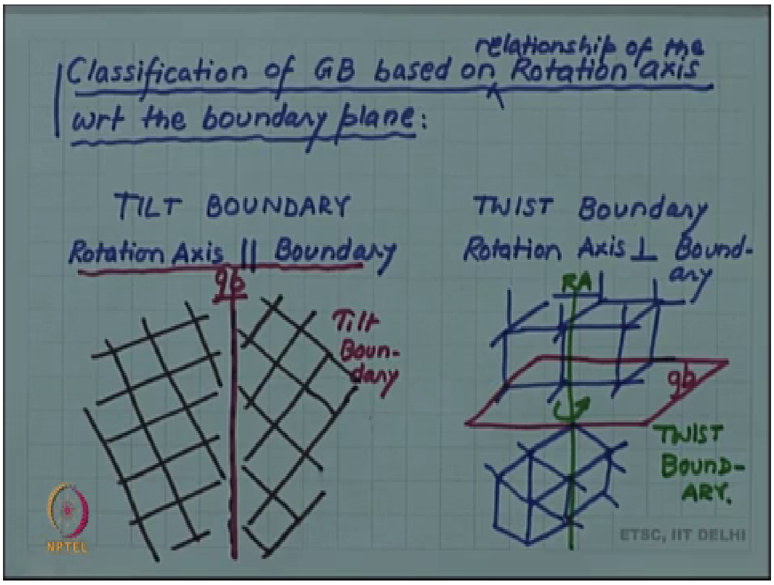

We also have a classification based on the rotation axis. In fact, the relationship of rotation axis to the boundary plane based on, let me write it based on relationship of the rotation axis with respect to the boundary plane.

In this basis of classification we have two types which we call a tilt boundary or a twist boundary, twist boundary in tilt boundary the rotation axis. Rotation axis will be parallel to the boundary plane parallel to the boundary in twist. The rotation axis will be perpendicular to the boundary plane . So, let me try to show you what we mean by this.

So, if we, let me think of boundary here, it is going to be a boundary, and I make a crystal on this side in this orientation, and then on the other side I have the crystal in a rotated orientation . So, you can see that there is a rotation of, and this is my boundary, this is the boundary plane, go grain boundary plane. So, if we think of the rotation of grain on one side with respect to the other side, you can see that the rotation is in this way; that is the rotation is in the plane of the figure which I have drawn. So; obviously, the rotation axis is normal to the plane of the figure.

So, if I want to get this orientation from this orientation, I have to rotate in this sense and. So, that would be about an axis perpendicular to the plane of the figure, and where is the grain boundary, also its separating these two grains. I have drawn a two dimensional figure, but you can extend it into the third dimension, normal to the plane of the paper. So, the grain boundary which is shown as a line on the paper is actually a two dimensional surface which is perpendicular to the plane of the paper. So, since the grain boundary is perpendicular to the plane of the paper, and the rotation axis is also perpendicular to the plane of the paper, rotation axis lies in the boundary plane. So, this boundary will be a tilt boundary. So, this will be a tilt boundary.

Now, let me try to create a twist boundary which will be little more difficult exercise, but let me try to draw it. So, let me say that this is the boundary plane and let me make a unit cell above the boundary plane in this orientation. I am drawing only one unit cell, but of course, I can extend and you can extend in your imagination and think of many unit cells in all possible directions, but the orientation is like this. And now suppose I rotate to get the orientation of the grain below this boundary plane, I rotate this orientation which I have shown here about an axis which is perpendicular to the plane which I have drawn.

So, on the lower side I draw my cube like this. Of course, again you have more grains, sorry more unit cells extending in all direction. So, now, you can see that the rotation axis here to get this orientation with this orientation, I am rotating about an axis which is vertical. So, this rotation axis, this is the rotation axis is perpendicular to the grain boundary plane. So, this grain boundary then will be classified as a twist boundary.

So, this kind of classification also is important, if one is going into the details of the grain boundary structure we will not go into lot of details, but one special case we will consider and that is a small angle tilt boundary, because a small angle tilt boundary we will find, can be nicely described as a series of parallel edge dislocation. So, it shows how one kind of defect is related to the other defect dislocations, which are line defect or can give us a grain boundary or a small angle tilt boundary, which is a two dimensional defect. This way we will consider in the next video.