Basics of Materials Engineering
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Lecture – 22
Defects in Crystalline Materials – 6 (Twinning, Interfacial Defects and Volume Defects)

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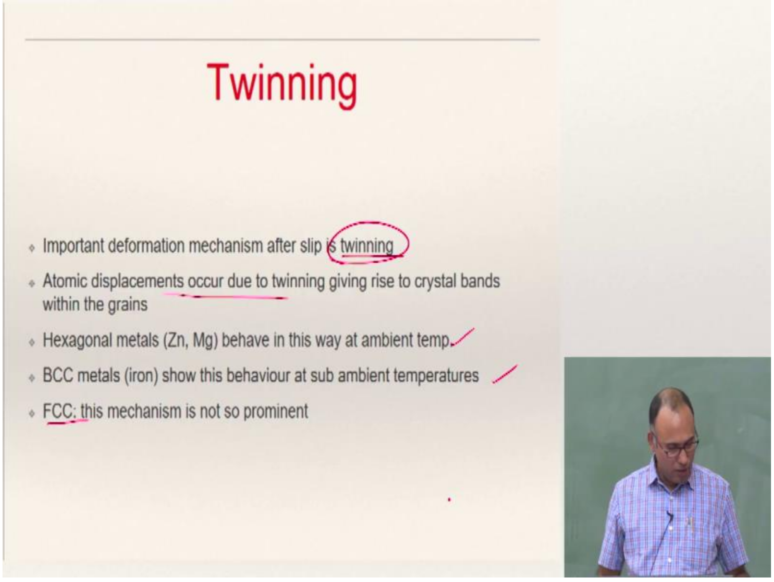

Twinning

- Important deformation mechanism after slip is twinning
- Atomic displacements occur due to twinning giving rise to crystal bands within the grains
- Hexagonal metals (Zn, Mg) behave in this way at ambient temp.
- BCC metals (iron) show this behaviour at sub ambient temperatures
- FCC: this mechanism is not so prominent

After the slip, another important mechanism is twinning. What do we mean by twinning? It is not really the kind of dislocation motion that we have discussed so for, as in the case of slip. It is primarily due to atomic displacements which are not necessarily the integer multiples of the Burgers vector.

We will see in a moment how this twinning deformation takes place. This is typically the mechanism that is observed in HCP materials and BCC materials, but not so much in FCC. FCC materials primarily deform due to slip; whereas, in HCP and BCC you can observe some twinning happening. It is not that FCC materials will never show twinning, they may also show twinning, but it is not so prominent as in the case of HCP and BCC materials.

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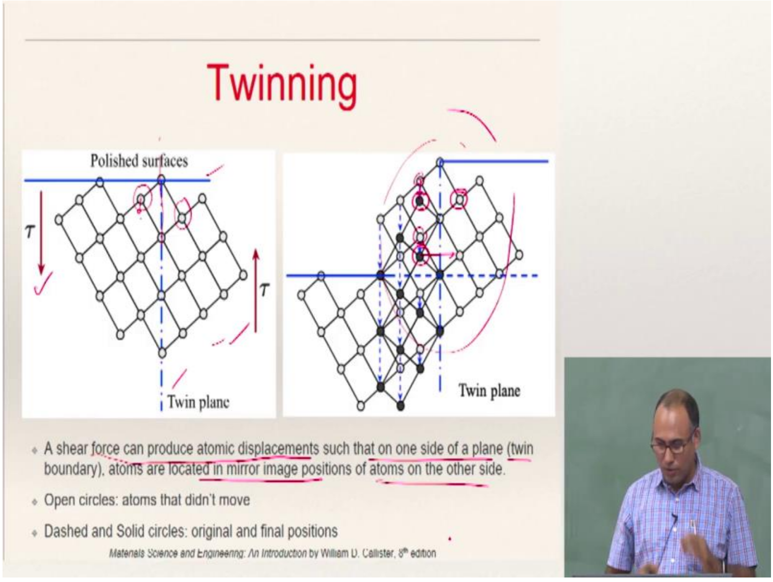

Twinning

- A shear force can produce atomic displacements such that on one side of a plane (twin boundary), atoms are located in mirror image positions of atoms on the other side.
- Open circles: atoms that didn't move
- Dashed and Solid circles: original and final positions

Materials Science and Engineering: An Introduction by William D. Callister, 8th edition

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Let us say this is your crystal lattice and you have this polished surface, and let us say this is your twin plane. Like in the case of slip plane -- we have discussed what is a slip plane, right? Similarly, let us consider this is a twin plane and now you have applied a shear stress.

Then what happens is the atoms on one side of the twin plane move with respect to the atoms on the other side of the slip plane in such a way that they become mirror images about the twin plane. For instance, this atom should move in such a way that this becomes mirror image of this atom and so on.

Let us see how that happens. The dark circles now show the deformed configuration of the same system. I have increased number of atoms but that does not matter. Now, you see that this atom is here and that is the mirror image of that atom about this slip plane. Similarly, this atom has moved here and this became mirror image of that atom and so on.

As a result, what is the amount of atomic displacement? It is actually less than the interatomic spacing in the direction. Whereas, in the case of slip, the amount of slip is always integer multiples of the Burgers vector. Burgers vector is the direction of the slip.

The amount of slip caused by dislocation motion is always expressed as integer multiples of Burgers vector. Whereas, in this case for twinning you should not have that much of a deformation. The deformation is constrained by the requirement that about that twin plane, you should have a mirror image of atoms on one side with the atoms on the other side. If you have a plastic deformation of that kind then such a deformation is called twinning deformation.

Like in the case of slip, you can also have plastic deformation by glide of a plane of atoms compared to motion of dislocations. Individual atoms break the bond and re-establish the bond. There is a difference between the amount of energy that one needs to spend in order to create slip by glide of a plane of atoms compared to slip by dislocation motion. The amount of energy required to cause slip by dislocation motion is much smaller than the amount of energy required to cause slip by glide of a plane of atoms; that means the dislocations are helping you to do slip.

Similarly, here what we have shown is how the twinning deformation takes place in a perfect lattice. Same as in the case of slip, the dislocations here can help twinning. The amount of theoretical strength required for causing twinning deformation is usually much larger compared to when the dislocations come and help this twinning deformation.

Then, the slip will not be equal to integer multiples of Burgers vector, but some non-integer multiples of Burgers vector, as we can see here. A shear force can produce atom displacements such that one side of a plane of atoms that is called twin boundary, are located in a mirror image positions of the atoms, on the other side.

It does not mean that only atoms on one side of the plane should move. Both of them may be moving, but effectively they should move in such a way that after the deformation you should be able to find the mirror image positions across the twin plane; that is what we mean by twin deformation. Typically, it is much more difficult energetically compared to slip.

If slip turns out to be difficult and if you do not have enough favourable slip planes for dislocation motion to happen through slip, all the energy that you are putting in maybe in such a way that it actually can trigger twin. In some materials, you can actually initiate plastic deformation by twinning rather than by slipping; that is typically the case in BCC and HCP materials.

But then, the amount of plastic deformation or the plastic strain caused by twinning is usually much smaller than the slip.

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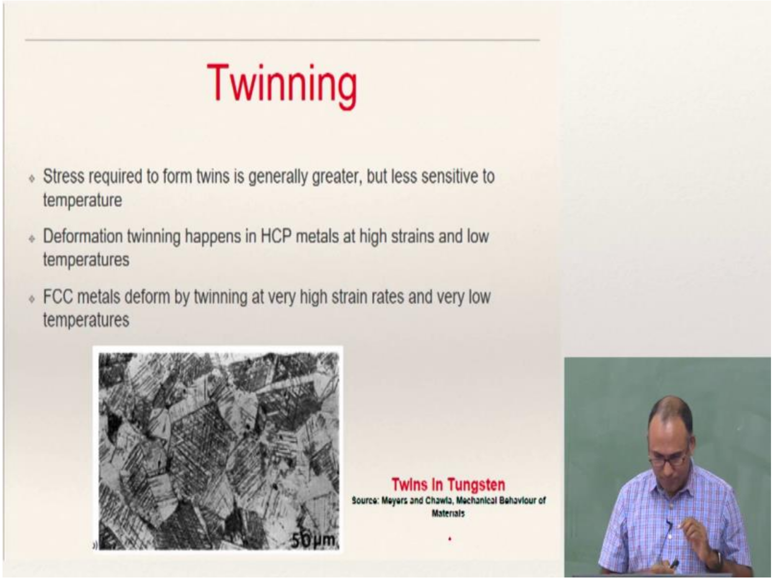

Twinning

- Stress required to form twins is generally greater, but less sensitive to temperature
- Deformation twinning happens in HCP metals at high strains and low temperatures
- FCC metals deform by twinning at very high strain rates and very low temperatures

Twins in Tungsten

Source: Meyers and Chawla, Mechanical Behaviour of Materials

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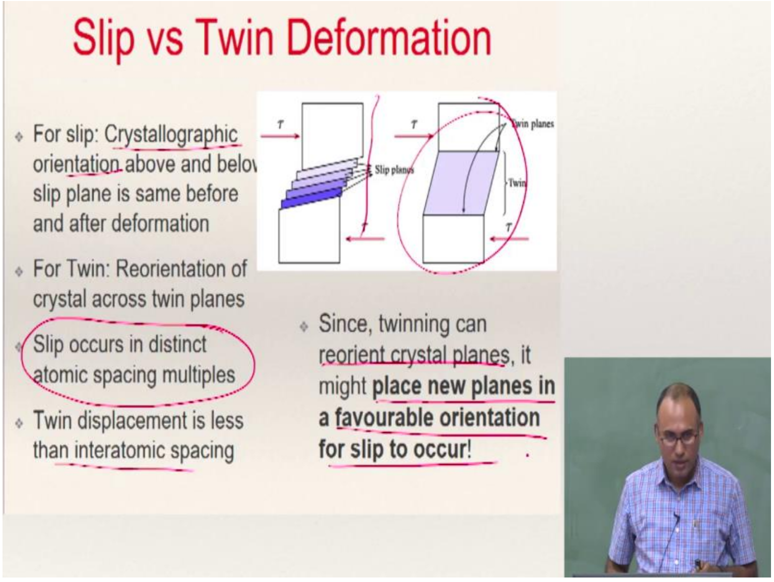

Slip vs Twin Deformation

- For slip: Crystallographic orientation above and below slip plane is same before and after deformation
- For Twin: Reorientation of crystal across twin planes
- Slip occurs in distinct atomic spacing multiples
- Twin displacement is less than interatomic spacing
- Since, twinning can reorient crystal planes, it might **place new planes in a favourable orientation for slip to occur!**

Why is that? What happens when you have a twin deformation? If you see the primary difference between the slip and twin deformation, and this is how slip happens and this is how the twin happens. For slip, the crystallographic orientation above and below the slip plane remains same during the deformation.

But for twin what happens is, because the atom motion is in such a way that there is a mirror image of one atom on one side of the plane to the other side, there is actually a rotation of the lattice around the twin boundary. As a result, if you have initiated twin deformation, it is possible that by rotation of the grain, you may be actually bringing new slip systems into action which were not available otherwise. Just by twin deformation, you are actually changing the orientation of the crystal planes. Your direction of the loading is the same, but because of the twin, the crystal orientations are changing -- reorienting, as a result the new slip planes and new slip directions are coming into action

And that is how you will cause slip followed by twin, and that is typically what happens in many of these BCC and HCP materials. Initially you will cause twinning and then the twinning deformation reorients the plane in such a way that you will activate new slip systems. What do you mean by activate new slip systems?

Your direction of the loading has not changed. Activating new slip systems means that the ϕ and λ values are changing without actually changing the direction of the orientation in your Schmid factor. How are ϕ and λ changing? Only when the crystals reorient themselves. The twinning is causing this reorientation and hence bringing new slips systems into action, and that is how you can cause the slip.

As we have discussed, the slip occurs in distinct atomic spacing multiples; whereas, twin displacement is less than interatomic spacing. The most important effect of twinning in a material is actually to reorient crystal planes such that it places new planes in a favorable orientation for slip to occur the way that we have discussed just now.

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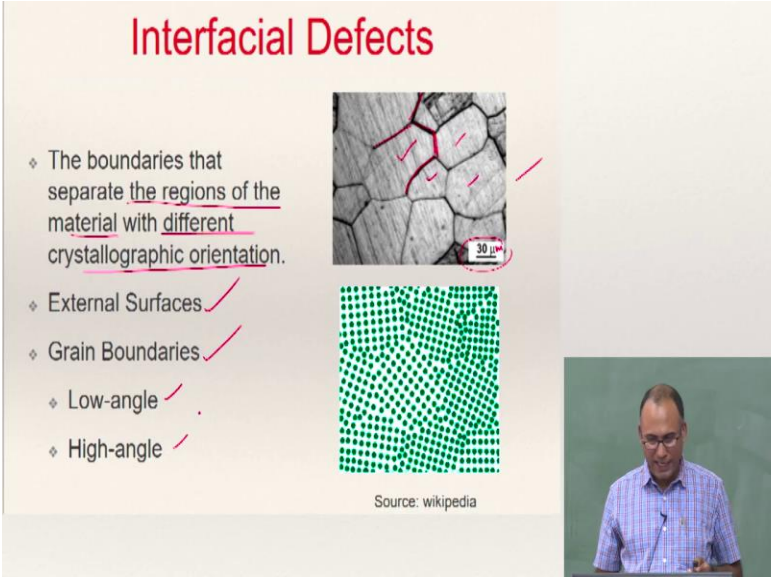

Interfacial Defects

- The boundaries that separate the regions of the material with different crystallographic orientation.
- External Surfaces
- Grain Boundaries
  - Low-angle
  - High-angle

Source: wikipedia

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That is about one-dimensional defects or line defects.

The next kind of defects are interfacial defects. There are different kinds of interfacial defects, what are these interfacial defects? They are basically the boundaries that separate the regions of materials with different crystallographic orientation. You have a material; in one place, you have a particular crystallographic orientation in another place, you have another orientation. The boundary that separates these two orientations is what you call an interface.

Every material, even a single crystal material will have a boundary. What would that boundary be? The external surface, right? For every material you have an external surface and the order ends at the external surface. The atoms on the external surface are not surrounded by the same number of neighbours compared to its bulk. It is missing neighbours on the outer side of the external surface. As a result, the energy of the system increases; that is what your surface energy is called.

Suppose if you take a liquid, on the external surface all the water molecules are not bonded by equal number of neighbours below. As a result, the surface increases its energy, but the system should always try to minimize its surface energy. As a result, what it should do?

It should reduce the surface area and that is the reason why liquids form spherical droplets, because they are the minimum surface area. However, it will not be always spherical. It will have other shapes, because of other forces coming into picture, but eventually it will have to minimize its surface area. But what happens for solids? Is the external surface of a solid always going towards spherical shape?

It is not possible because of the rigidity of the solid. The solid has other factors coming into picture and hence it cannot. But nevertheless, because of the free surface the external surfaces have some energy -- that is what increases the energy of the system.

If you are talking about a perfect crystal, external surface is a defect. Normally the long-range order is stopping at the external surface, you can also see that as a kind of a defect and the second important defect is the grain boundary. Here you can see a micrograph. The scale here is 30 μm.

You can see that this is one grain with a particular crystallographic orientation, this is one, this is one and this is one, and this interface, is your orientation mismatch. When you look under microscope, that nicely comes out as a grain boundary.

Here you have a different kinds of grain boundaries. How do you distinguish different kinds of grain boundaries? They are typically low angle grain boundaries and high angle grain boundaries. What do you mean by low angle grain boundary?

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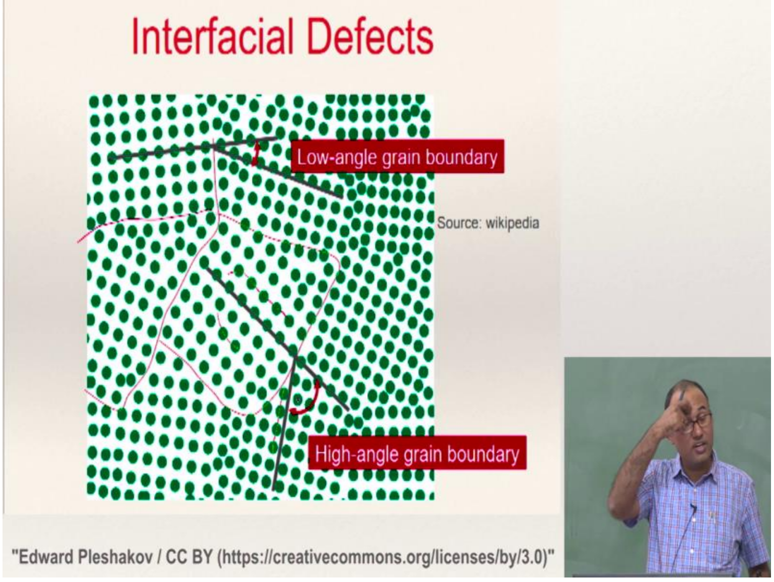

Interfacial Defects

Source: wikipedia

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Let us say this is a cartoon of a crystalline material with different grain orientations. Can you see the different orientations here? So, that is one boundary, right? There is also another boundary here. This is one grain, this is another grain and so on, and this is another boundary. Like that you can draw all the boundaries.

In this grain, this is the orientation and in the neighbouring grain this is the orientation, isn't it? If that is the orientation of that grain and this is the orientation of this grain, the angle between those two is called misorientation. If the angle is large then it is called high angle grain boundary. For instance, if you take these two grains that is one of orientation, this is another orientation here comparatively, this is a low angle grain boundary.

This is in a polycrystalline material, because it is not a single orientation. If it is a single crystal material, you will not have these boundaries, because there is no misorientation. If it is a polycrystalline material, then you will see different kinds of grain boundaries; low angle grain boundary, high angle grain boundaries and so on.

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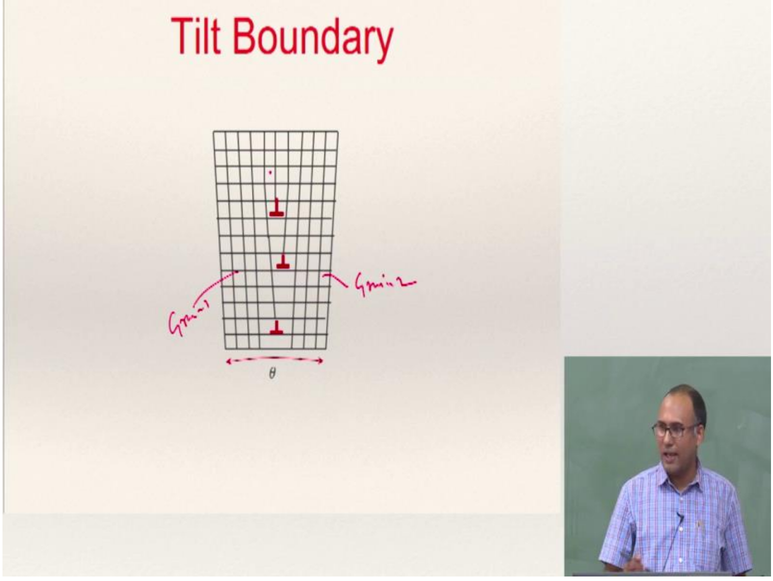
Tilt Boundary

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There is another thing called tilt boundary. This is your grain 1 and this is your grain 2 and this is your misorientation. It can also be caused by these dislocation structures. If you have dislocations of this kind then eventually you will have a tilt boundary as we have shown.

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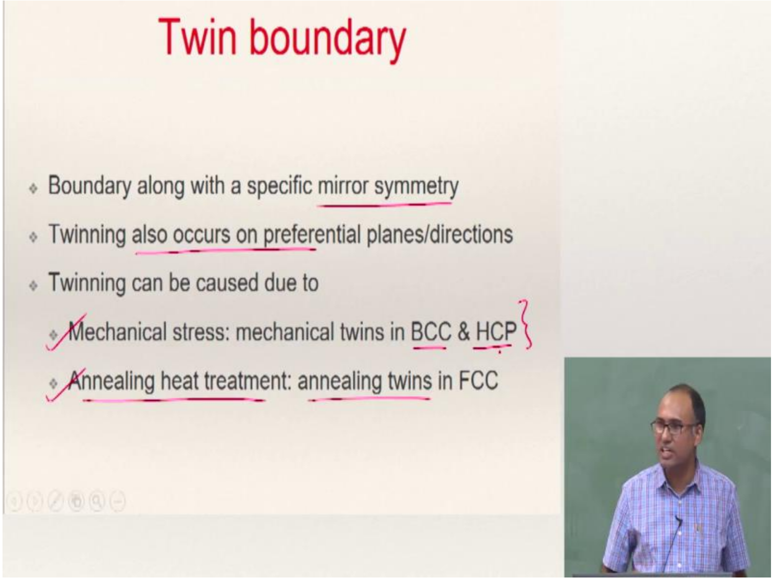
Twin boundary

- Boundary along with a specific mirror symmetry
- Twinning also occurs on preferential planes/directions
- Twinning can be caused due to
  - Mechanical stress: mechanical twins in BCC & HCP
  - Annealing heat treatment: annealing twins in FCC

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The twin boundary about which you are having the misorientation is also a defect; the twin plane that we have seen. The twin boundary is a special boundary along which you will have a specific mirror symmetry. But the long-range order is actually going to be disturbed along the twin boundary as they are constrained to move in a specific fashion. As we have discussed slip, twinning also occurs on preferential planes and preferential directions.

And this twinning can be due to two mechanisms. One is due to mechanical stress, another way you can initiate twinning is through heat treatment; annealing heat treatment. We will see what do you mean by annealing towards the end of this course when we discuss heat treatment. When you apply a mechanical stress, you can initiate twinning in a material and that is typically the mechanism observed in BCC and HCP materials.

FCC materials at room temperature, deform by slip, they do not have to go towards the twinning mechanism due to the fact that there are so many favourable slip systems. In FCC materials, you can also initiate twinning through annealing. But otherwise, at room temperature, normally it is not a predominant mechanism. The twinning is primarily seen in BCC and HCP materials.

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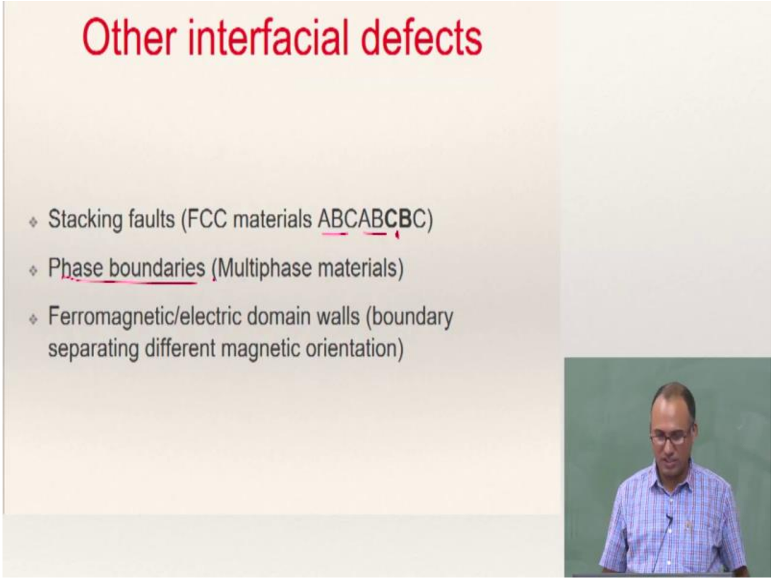

Other interfacial defects

- Stacking faults (FCC materials ABCAB**CB**C)
- Phase boundaries (Multiphase materials)
- Ferromagnetic/electric domain walls (boundary separating different magnetic orientation)

What are the other interfacial defects? Stacking faults -- we have discussed, stacking faults, right? ABCABC close packed directions and so, for instance in FCC structure, ABCABC, and here A should be there, A is missing. If only one is there then it is a narrow stacking fault, and if there are so many defects then it is a wider stacking fault. You also have phase boundaries. That means, if you have a material with multiple phases, the boundary between one phase to another phase is called phase boundary. Similarly, you have ferromagnetic and ferroelectric materials in which you will have domain walls.

What are these domain walls? For instance, if you are talking about a ferromagnetic material, the magnetic orientation vector changes from one region to another region. The boundary that separates the orientation difference is called domain wall. When you look under microscope, you can observe these domain walls in these magnetic materials.

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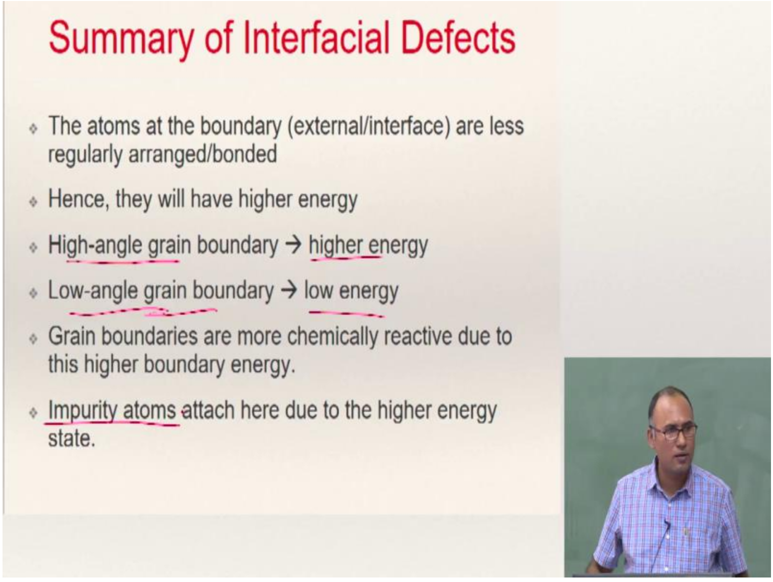

Summary of Interfacial Defects

- The atoms at the boundary (external/interface) are less regularly arranged/bonded
- Hence, they will have higher energy
- High-angle grain boundary → higher energy
- Low-angle grain boundary → low energy
- Grain boundaries are more chemically reactive due to this higher boundary energy.
- Impurity atoms attach here due to the higher energy state.

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These are the different kinds of two-dimensional defects. What is the summary of these interfacial defects? We know that the atoms at the boundary, whether it is an internal surface or external surface, internal boundary or external boundary, they are usually less regularly arranged or bonded and as a result, the boundary will have higher energy.

If you see the energy state near the grain boundary and the bulk, grain boundaries will have higher energy state, because the atoms are not regularly arranged. For instance, if you have an impurity in a material, it preferentially tries to go and sit near the grain boundary so as to minimize the grain boundary energy. It is already a high energy state, it will go and sit there so as to minimize the grain boundary energy. As a result, total energy of the system is minimized.

You have high angle grain boundary and low angle grain boundary, because high angle grain boundary means that the misorientation is larger. When the misorientation is larger; that means, you have a large irregularity, as a result you will have higher energy and in a low angle grain boundary, the irregularity is less and hence you will have low energy.

Because of the fact that the grain boundaries have higher energy, they are chemically more reactive compared to the bulk. If you have any chemical reaction that needs to take place, that preferentially happens near the grain boundary, because they are already in the high energy state. Because of the same reason that the grain boundaries have higher energies, the impurity atoms in a material typically try to go and sit near the grain boundaries, so that they can minimize the total energy of the system.

It is important to know why this impurity atoms go and sit near the grain boundaries and why chemical reactions take place near the grain boundary. That is going to help us understand the solidification process when we talk about phase diagrams. You guys have already got introduced to phase diagrams in manufacturing processes?

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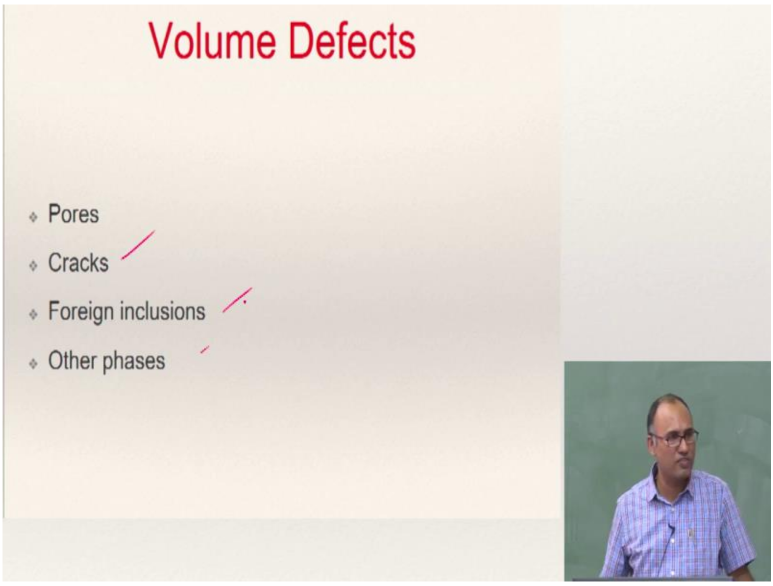

Volume Defects

- Pores
- Cracks
- Foreign inclusions
- Other phases

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That is something that we will end with in this course, ok? And then, the next level of defects are volume defects like pores. If you have porosity in a material, that is a volume defect. Cracks, foreign inclusions, other phases - these are the other kinds of defects that you can have in materials. We are not going to discuss much about them, but we can look at their effect on the plastic deformation.