

Basics of Materials Engineering
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Lecture - 09
Crystal Structure - 7 (Single Crystal and Polycrystalline Materials)

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The slide is titled "Crystalline and Non-crystalline Materials" in red text. It features a list of properties of single crystals, each preceded by a diamond symbol (◊). The items are: "Single Crystals", "Semiconductors (single crystal silicon etc) for microelectronics", "High strength materials with low thermal creep, e.g. turbine blades*", "Single crystal copper has better conductivity than polycrystalline copper", and "Single crystal Sapphire for lasers". The words "High strength" and "turbine blades*" are circled in red. The slide also includes the IIT Madras logo on the top left and the NPTEL logo on the top right. A small inset video shows a man in a red shirt speaking at a podium.

- ◊ Single Crystals
- ◊ Semiconductors (single crystal silicon etc) for microelectronics
- ◊ High strength materials with low thermal creep, e.g. turbine blades*
- ◊ Single crystal copper has better conductivity than polycrystalline copper
- ◊ Single crystal Sapphire for lasers

So far, we have talked about a unit cell which is stacked in three directions, and we have not talked about any issues with the orientation mismatches. So, these things are called single crystals. Until now what we have talked about is a single crystal; that means, the crystallographic orientation is unique.

The single crystal materials are extremely important materials for several technological applications. For instance, you use single crystal silicon for semiconductor applications, and turbine blades for instance, are required to withstand very high temperatures. Have you heard of a steam turbine and a gas turbine in your advanced thermodynamics courses or application of thermodynamics courses? So, there, these components are subjected to very high temperatures. You ideally want to operate them at high temperatures in order to increase the thermal efficiency.

When they are working at high temperatures, they are subjected to a phenomenon called thermal creep, and you want to have materials which have high strength at high temperatures. So, if you want to have something like that, you want to make the

materials with single crystals, so that you the material will provide very high thermal creep resistance.

So, that is why the turbine blades are usually made of single crystal materials. If you have a single crystal copper, it is known to show better electrical conductivity compared to a polycrystalline copper. The lasers that we use in pointers are sapphire lasers which are single crystal materials. So, there are several technological applications for the single crystal materials.

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The slide is titled "Crystalline and Noncrystalline Materials" and features the NPTEL logo in the top right corner. On the left, there is a list of bullet points: "Polycrystalline Materials", "Most crystalline solids are collection of many small crystals or grains", and "Grain Boundary". To the right of the text are three diagrams: a top diagram showing several small crystals with different orientations (marked with 'X' and '+'), a middle diagram showing a 3D lattice structure with a grain boundary, and a bottom diagram showing a 2D network of grain boundaries with some regions numbered 1 and 2. In the bottom right corner of the slide, there is a small video inset showing a man in a red shirt speaking.

But there are several other applications where we use polycrystalline materials. What is a polycrystalline material? Most of the crystalline solids that we use in our engineering applications are polycrystalline in nature. For instance, if you are growing a crystalline solid from liquid state, when we are solidifying your liquid metal, there will be several nucleation sites. So, first there should be a nucleation and then the material gets solidified.

For instance, in this picture you can see that there are different nucleation sites and each one of them having their own orientation, isn't it? When all of them meet together, you have incompatibility at the position. This is crystal 1, 2, 3, 4, 5, 6. When 1 and 2 meet there is an incompatibility in terms of orientation. This is one grain and this is another grain; this is what we call a grain boundary.

This crystal has one orientation, this crystal has another orientation, and this is what we call a polycrystalline material, because the polycrystalline material will have several grains and each one of these grains have their own orientation. Had it been a single crystal, it has one single orientation everywhere, there is no grain boundary, there is no incompatibility between each of these grains. So, when they come together, you will not see any incompatibility, and you will see that it is a single grain.

Most of our materials are polycrystalline and hence, we need to understand what happens when you have a polycrystalline material to the deformation mechanism that is something that we will discuss in the next module and it is important to know that it is extremely difficult to actually make a single crystal material. Why is it very difficult? If you were to make a single crystal material, what is that you need to do? Suppose you are coming from liquid state to solid state, what is that we need to do?

You need to control the nucleation sites. You can only have one nucleation site and you should not have several nucleation sites, and then only from one nucleation site you should be solidifying the material so that, the crystal orientation will not be having any incompatibility with the neighboring crystal because there is no neighboring crystal.

But to do that, you have to do the solidification process with extreme care, and that will increase the production cost and hence, single crystal materials are usually very expensive compared to your polycrystalline materials. That is why your turbine blades have to be made with utmost care and then obviously, the cost is going to go up.

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Crystalline and Noncrystalline Materials

- ◆ Anisotropy
 - ◆ Physical properties of single crystals might depend on crystallographic orientation
 - ◆ For polycrystals (with no texture) this variation averages out and may behave as isotropic

Metal	[100]	[110]	[111]
Aluminum	63.7	72.6	76.3
Copper	66.7	130.3	191.1
Iron	125.0	210.5	272.7
Tungsten	384.6	384.6	384.6

(Source: Materials Science and Engineering, Callister & Rethwisch)

If you take a unit cell and you stack them in all the directions, we know that we have different crystallographic planes, and each plane has different crystallographic linear density and planar. Let us say you take a crystal and you are applying a load; you are pulling the crystal; you are doing a tensile test which you have done in -- have you completed your applied mechanics lab? So, you must have done the tensile test on a polycrystalline material.

What you have done is you have applied a load; you are pulling right? When you are pulling what are you doing? What is actually happening within the material? When you are applying an external load, what is happening to the atoms? The atomic bonds are getting stretched, right? That is what happens first, and if you are in the elastic regime, then what happens? As soon as you remove the load, it goes back; that means, atomic bond is not broken, it is only getting stretched. And that is what you mean by elasticity.

When you apply a load, you get a displacement. You can actually plot a stress-strain curve, and depending upon which direction you are applying the load -- if your loading is in [100] direction or [111] direction or [110] direction, the amount of resistance offered by the material to this deformation is going to be different.

In other words, the stiffness offered by the crystal will be different depending upon the direction of the load that you have applied and hence, the material property, for instance

the elastic modulus of the material is not going to be the same in all the directions; it changes from one direction to another direction.

For instance, if you take a single crystal aluminum and then, you apply the load in [100] direction, your elastic modulus will be 63.7 GPa. If you do the same thing in [110] and [111], again you will measure the elastic modulus to be different, and so is the case for all other materials.

For copper you will see much larger difference. In [100], it is much softer and here it is much stiffer 130.3 GPa. And [111] is the stiffest, right? So, this means the material does not have the same property in all the directions and hence, by definition it is an anisotropic material. It will not show you the same property.

Have you observed different elastic moduli depending on which direction you cut your sample in your laboratory, did you? What was the elastic modulus that you have observed for steel? All of you have done the experiment I suppose, you must have reported the elastic modulus as one of the outcomes of your experiment, did you? What was the number?

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Louder.

Student: (Refer Time: 09:45).

Student: 200.

As a mechanical engineer, if you do not know, if you do not remember the elastic modulus of steel and yield strength of the steel, it is not acceptable.

Student: 200.

It is not acceptable. 200?

Student: 10.

Newtons?

Student: (Refer Time: 10:08).

210.

Student: GPa.

Unit

Student: GPa.

GPa. 210 approximately 200 right; 210 GPa. But how come all of you got the same number or almost the same number 200, 210 something like that? Obviously, the samples would not have been cut in the same direction. You take a block and then, if you have cut the sample in this direction and I cut the sample in this direction, you will not know once I give you the sample, right? -- whether I have cut in this direction or in this direction. But all of you have all of you seem to have got the same number, you do not seem to observe any difference in elastic modules. Why is that? Where is the isotropy coming from?

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Because the material that you have tested was not a single crystal material, it is a polycrystalline material. So, when you have several of these orientations coming together and meeting at the grain boundaries, effectively all the anisotropy cancels out, and hence, you will measure the material property to be the same in all the directions.

So, for a polycrystalline material (not necessary all the time), if it does not have any texture, then the material property will be isotropic. For instance, elastic modulus, you measure it to be same in all the directions. That is why it did not matter whether the sample is being cut in the longitudinal direction or a transverse direction.