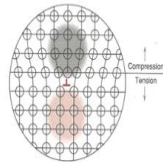**Basic Construction Materials**
Prof. Radhakrishna G. Pillai
Department of Civil Engineering
Indian Institute of Technology - Madras

Module - 3
Lecture - 13
Nature of Materials - Part 3

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Hi, we are in this module on Nature of Materials. This is the second lecture in which we will be looking at lattice structure and defects.

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So, as you can see on screen, the electron configuration, bonding etc. were covered in the previous lecture. And today we are going to talk about lattice structure and some of the defects in the materials.

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These are some of the books, which I used such as Mamlouk and Zaniewski, Callister, Illston and Domone's book. All these books and a lot of information from the internet have been used for making this module.

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Classification of materials can be done based on the chemical bonds. For example, as you see here, the 3 major type of bonds; metallic bond, covalent and ionic bond and also covalent bonds alone. Metallic bonds are present in of course, metals and typical metals which we use in construction; steel, iron, aluminum, copper, etc.

Covalent and ionic bonds, they are mainly present in most of the inorganic or nonmetallic solids like ceramics and concrete is one very good example of ceramic material along with bricks, glass, aggregates, all this. In these, you can see crystalline structure more mostly.

And then, there are other type of materials which are mainly organic solids. Examples are asphalt, plastic, wood, etc., where we see random molecular structure. Again, one more thing I want to tell, even though we said crystalline structure, it is not that they are very well crystallized in nature, but more or less; in general, we can say they are crystalline in nature.

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Now, let us look at the metallic material, which is the focus on today's lecture. Then, we will go into nonmetallic materials later in the future lectures. So, in the metallic material, first let us see the process of solidification. How do we make metals? We get the raw materials for making the metal and then we melt them. We increase the temperature of the materials so high that they melt. And then, we allow that material to cool down. In this cooling process, the solidification happens in the way we want. So, that is what is the engineering. Metallurgical engineering plays a big role in that.

One important thing to note is, most of the metallic bonds are nondirectional in nature. Why it is happening is, because when the crystal growth happens or when the molten material is cooled down or when the temperature comes down, what happens is, crystals starts forming. And depending on the rate at which it is cooled, the way in which the crystals grow also matter or the size of the crystals or the grains that are formed. We will talk more detail about

that later on. The size of the grains and the imperfections and many things inside the metal in the 3D space are heavily dependent on the rate of cooling and the temperature which we adopt, etc., mainly rate of cooling.

Here is an example of a titanium crystal bar. You can see a lot of crystals on this. These are all individually grown crystals. You can see that the nature is different in the centre of this thing and as you go away from the centre, like over here, it is slightly different. In next slide, I will show you more detail on that.

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Here you can see how the cooling rate matters. The top picture on this slide is the cross section of an ingot or we can call it a rod. On the bottom picture, you are seeing the side face or the cross section or the longitudinal face. So, if I am talking like this, something like this. So, this bottom portion, this much is shown here and this is shown here or any cross section for that matter is shown on the top image. And the bottom part is shown in the bottom image. This image is collected from the literature, so it says nickel-copper alloy. But it is not necessarily that one, I am just using this as an example.

Now, effect of cooling rate and effect of impurities in case of alloys: so, what this does is, because of this temperature changes happening, there is a possibility of segregation between the elements present in the molten material. And also that will induce some change in the grain size and shape. Here is an example. You can see the top picture, the cross section. When we look at this portion here, we can see that, near the surface it is actually very fine grained. Then, you have some region towards the centre, where you have elongated grains.

And then towards the centre, you have again equiaxed grains, where the axis in both directions are more or less similar in size. In brief, small equiaxed grains along the border, columnar grains in between and then towards the centre you have large equiaxed grains. Here you can see very fine grain.

Small equiaxed grain means very fine grain or the size of the grain is very small. Large equiaxed grain means the size is larger, but more or less similar size in all the directions. That is what equiaxed means. Although these two images are from two different literature, I thought it is good to show them together as you can see the same kind of what is happening.
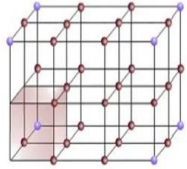
So the side view, how it would look. Here, the important thing is, at the bottom also you have similar because, if the material is a rod, it is cooling from all the surfaces. Not only the circular surface, but also from the bottom surface it is cooling. And that's why you see this kind of distribution of the grains.

So the point is, near surface of the metal might have a different grain structure and as you go a little bit inward, you might have another grain structure and as you go little bit further, you might have a third type of grain structure. Therefore, this distance from the surface might influence the rate of cooling at a particular point inside the material and that will influence the type of grains which are formed or the size of grains which are formed in a metal structure.
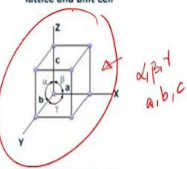
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Now, let us look at the space lattice. So, what is it? It is the imaginary network of lines. You can see a lot of lines in this drawing on the screen and also you see the intersections of those lines. What we assume is that, at every intersection of these line, there is an atom present. So, space lattice is the imaginary network of lines with atoms at intersections representing the arrangement of atoms.

As you can see in this sketch, you have lot of these imaginary vertical and horizontal lines and then you have all the intersection points. You have a circle or sphere which is drawn. This circle or sphere indicates the atoms present. Now by definition, atoms, molecules or ions arranged in a repetitive 3D pattern in long range order (meaning larger distance covered) forms a crystal structure.

You might have also heard the word amorphous materials, where the crystals are not very well defined for a larger volume. Even though they are arranged, they are arranged in short range order. That's what is an amorphous materials.

Now, atomic arrangement also depends on the atomic size and the valency. We will talk about this unit cell here. You have this representation of the space lattice on the top right diagram and each cubical region or each unit cell (not necessarily cubic) can be explained in terms of their dimension of each of the edges and also the angle between those edges. Angles can be represented by alpha, beta and gamma and the dimensions by a, b and c as you see in this sketch here. This is essentially the building block for any metal, which we talk.

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How many types of space lattices are there or identified? There are about 14 types of space lattices. You might have studied this earlier also. You can see that all of them are shown here. These pictures are taken from the internet, so that it is easy for you to visualise the things. You have triclinic, monoclinic, orthorhombic, rhombohedral, tetragonal, hexagonal and cubic or isotropic and within this, you have other subcategories. Like in the case of orthorhombic, you have simple, base centered, face centered, body centered.

So, there are total 14 space lattice arrangements that are possible. In case of most of the metals, all these are not observed. What we mainly see are face centered cubic, body centered cubic and hexagonal close packing. These are the 3 lattice structures which we see in case of metals.

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Those 2 cubic and 1 hexagonal space lattices are found in most metals. So, let us have a little bit closer look at those lattice structures. Let's look at the face centered cubic. As you can see over here, for this cube, there are 6 faces, that is, one face, second face, third face and similarly, the other 3 faces, which you are not seeing here. From the second diagram, you can see this one and the second face and then this is the third face. If I write here also, this is 1 and then this is 2 and then let us say this is 3. So, this is 1, 2, 3. And the other sides which you are not able to see, this can be 4 and then this is 5 and then this is sixth one here. So, there are say 6 faces for the cube and at the centre of each face, there is 1 atom.

In the case of body centered cubic, you can see, this is the 1 atom which is present at the centre of the cube. I am going to call it 0. It also has atoms in the corners. That is, we call it

as 1, 2, 3, 4, 5, 6, 7 and then of course, there is a eighth one there, which you do not see in the first image. So, this is how they are. One thing to note here is that only this number 0 atom is completely occupied within the body centered cubic structure, whereas all others are in the corners. You can see that this 1, 2, 3, 4, 5, 6, 7 and 8 are all not fully occupied by the same cube.

In case of HCP, again you have similar type, but it is not in the shape of a cube. Here the section is like a hexagon in nature.

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There are 2 parameters which are very important when we talk about this lattice structure. One is coordination number and the other one is atomic packing efficiency. We will talk about the atomic packing efficiency in next slide. In this slide, let us focus on coordination number.

Coordination number is also known as ligancy. Whereas, ligands are atoms that are bonded to the central atom. So that is how the coordination number is counted.

What is coordination number? It is the number of nearest neighbours for a central atom. Now, for case of FCC, this coordination number is 12. How do we calculate that or how do we get that number?

As you can see here, this portion here is the FCC structure and this is continuing to the next unit cell. So, if this is one of the unit cell and this is the central atom which I am considering,

that central atom has these 4; 1, 2, 3, 4 and these 4, that is 4 here and then this, this, this and this; that is another 4. And then, sum of all these 4+4+4 is equal to 12. So, it has 12 nearest neighbours. That is what is the coordination number for FCC, which is 12. This is how we get that.

Now, for BCC, you can say similar way. By considering this as a centre atom, I have these 4 and then I have these 4. That is 4 + 4 = 8. That is the coordination number for BCC structure. If you take HCP structure, the coordination number is going to be 12. If you consider this as a central atom, it has 6 atoms here and it will also have another 6 atoms on the other side. Thus, that will again form 12. So this is how the coordination number is calculated.

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If you look at the atomic packing factor for lattice structure, it is dependent on the equivalent number of atoms associated with each unit cell and atomic radius. As you can see here, for FCC it is 0.74, for HCP also it is 0.74 and for BCC it is 0.68. So, if you look in the previous slide for FCC and HCP, these numbers are also similar. Now, if you see the picture on the bottom left, you can see that all the atoms are not completely occupied by 1 unit cell, some of them are also shared by the adjacent unit cell.

So, on 6 faces, half of the atoms are shared and on 8 corners, one eighth of that particular atom on every corner is shared by unit cell. Now, what you do is, you calculate the total volume of the unit cell and the volume of the atom or the share of the atom within that unit cell. When you divide the volume of atoms in the unit cell with the total volume of the unit

cell after knowing the type of atom and the radius of each atom (You know what is this distance here and you know what is this distance also), you will get atomic packing factor.

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Theoretical density of FCC lattice

Calculate the radius of the aluminum atom, given that aluminum has an FCC crystal structure, a density of 2.70 Mg/m^3, and an atomic mass of 26.98 g/mole. Note that the APF for the FCC lattice structure is 0.74.

Solution

$$\rho = \frac{nA}{V_c N_A}$$

ρ = density of the material
n = number of equivalent atoms in the unit cell
A = atomic mass of the element (grams/mole)
V_c = volume of the unit cell
N_A = Avogadro's number (6.023×10^{23} atoms/mole)

For an FCC lattice structure, $n = 4$, so

$$V_c = \frac{4 \times 26.98}{2.70 \times 10^6 \times 6.023 \times 10^{23}} = 6.636 \times 10^{-29} \, m^3$$

$$APF = 0.74 = \frac{4 \times \left(\frac{4}{3}\right)\pi r^3}{6.636 \times 10^{-29}}$$

$$r^3 = 0.293 \times 10^{-29}$$

$$r = 0.143 \times 10^{-9} \, m = 0.143 \, nm$$

Mamlouk and Zaniewski

NPTEL MOOC Course on Basic Construction Materials - Module by Dr. Radhakrishna G. Pillai, BTCM Division, Civil Engineering, IIT Madras, Chennai, India

This atomic packing factor is actually related to the density, etc. So, when you look at this, you can pause for a minute and then go through these calculations and then understand it better. If you have any doubts, we can definitely talk about this in the review session.