**An Introduction to Materials: Nature and Properties (Part 1: Structure of Materials) Prof. Ashish Garg Department of Material Science and Engineering Indian Institute of Technology, Kanpur**

> **Lecture - 40 2-D Defects**

So, we will begin with lecture 40 which is the last lecture of this course in which we will primarily discuss about 2-D defects which is the remaining topic of this course.

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So, what we does, what we did in the last lecture was, so we introduced a new different, we introduced defects in the last few lectures, two lectures and we first talked about the point defects which are equilibrium defects which means they are thermodynamically stable as a function of temperature. So, except at zero Kelvin, you will always have point defects in a material and point defects are basically you can say vacancies interstitials substitutional atoms and so on.

So, these are primarily three point defects that you see in the materials and the concentration of these point defects varies as a function of temperature. So, basically this is the defect formation energy and higher the defect formation energy, lower is the defect concentration going to be which is a function of bond energy typically.

So, if bond energy materials with higher bond, energy will have lower defect, point defect concentration as compared to materials with lower bond energy and you can see that it has exponential dependence on temperature minus 1 over T.

So, as a result when temperature increases and the vacancy concentration also increases exponentially and then, second defect that we considered was lower line defects or 1 d defects and here we looked at edge dislocation and screw dislocation. So, essentially an edge dislocation was an extra plane of atoms which has been put in otherwise perfect lattice. This extra plane of atoms is useful in the sense that it allows the materials to deform. It also creates only stress fields. There is a tensile and compressive stress field and in the two particle lattice and dislocations, this dislocation can be characterized by its own burgers vector if you look at the edge dislocation if I go to edge dislocation.

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So, if you look at the top view of edge dislocation, this is the plane in which you have a dislocation line. This is the dislocation line. So, vector is t, ok. This is top view, and the burgers vector is along this direction. So, this is b vector, alright and when you apply stress, I will show that stress relation with a stress in the next slide. If you look at the side view, the side view is something like that. So, if this is the crystal ok, so here you have an extra row of atoms and these are the other rows of atoms. So, I am just making them solid lines. So, this is the perpendicular. So, perpendicular to the plane is this t vector. So, this is side view front view. So, t is normal to the plane of the paper.

So, this will be going into the plane and the burgers vector would be this and as you apply stress, shear stress, this will slowly move out on this side and giving rise to a step. So, obviously, you had a step on this side and this will create when it moves out completely, it creates a step on the other side leaving a relaxed crystal. The magnitude of that step will be equal to burgers vector. So, in this case, as you apply stress in this direction tau and that t moves, the dislocation line also moves in the same direction as off stress and burgers vector, but dislocation line is perpendicular to the stress as well as the burgers vector, ok.

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So, this was edge dislocation and then, we looked at screw dislocation which was basically you had this was one part of the crystal and the second part of the crystal was slightly sheared with respect to, so sort of sheared in this fashion. So, this is a sort of shearing that takes place, sort of this I can mark this as red. So, red one is top part of the crystal and blue one is the bottom part of the crystal and top part has sheared. If this were the bottom part with respect to quantity called as by an amount by this vector and this is the dislocation line in this case t whereas, the other part of the crystal is like this. This is the remaining part of the crystal, ok. So, the one half of the crystal is sheared.

So, when you apply stress in this case, the stress is applied in this direction. This is stress. So, stress t vector and v vector, all of them are parallel. So, when you apply stress and this dislocation line will move in this direction, eventually giving you a step which is like, so this is the top part and the bottom part will be like this or this is the top part and that is the bottom part. So, this is a step that you create. One step here, another step there, after the application of stress. So, in this case, in the screw dislocation case, your b was parallel to t and b was also parallel to tau and t moves perpendicular to the stress direction, right whereas, in the previous case b was perpendicular to t, b was parallel to stress, t was perpendicular to stress, t moves in the direction of stress, ok. So, these are the take home messages. I will just show you sort of dislocation in which you can see this.

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So, here you can see this is the motion of edge dislocation. So, you had an extra row of, you start with an extra row of atom on the left. So, this is an extra row of an atom. So, this is the extra row of atom you had and you apply stress, it moves to right. So, now it is here. After some time it is here and then, it completely moves out of the crystal, and this is how nice dislocation moves in this case and the screw dislocation on the other hand moves in a different manner.

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So, when you apply stress, so there is blue. So, these blue ones are the stress arrows. So, this is the dislocation line. The one in the orange, it moves in this direction whereas, stress is in this axis. So, as you keep applying the stress and the line moves or the crystal giving rise to steps which are here, this is one step, this is second step. Somehow the color is not coming very well, but this is how it moves in the screw dislocation, ok.

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So, this is sort of the summary of two dislocations. In edge dislocation b is perpendicular to t, in a screw dislocation b is parallel to t. The relationship between line vector and burgers vector is in edge dislocation. It is perpendicular in the screw dislocation. So, b and t are per perpendicular to each other in edge dislocation whereas, b and t are parallel. In screw dislocation, the slip direction, the direction along which dislocation line moves is parallel to burgers vector. In case of edge dislocation is parallel to burgers vector again in screw dislocation. So, movement is parallel to burgers vector. In both the cases, the direction of dislocation line movement with related to burgers vector is parallel to burgers vector in edge dislocation and it is perpendicular in the screw dislocation.

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Finally, I just wanted to show you the type of burgers vectors in cubic crystals that you see. So, the translation or burgers vector is always from between two lattice sites. So, it is from one site to another site identical lattice sites, ok.

So, for monatomic face centered cubic crystal, it is half 110 axis and direction and monatomic BCC, it would be half 111 monoatomic simple cubic. It will be 11100 for sodium chloride, it would be half 110 because its FCC lattice; however, for a cesium chloride structure, it is 100 because there is a cesium atom sitting at simple cubic position and chlorine atom sitting at simple cubic positions. As a result the vector is of simple cubic, although structure looks like BCC. It is not some BCC diamond cubic. Again the FCC structure for this will also be half 110. So, it has to go according to crystal system, not just the position of atoms.

So, it has to move from one identical atom to another identical atom and they have to be one lattice point or the lattice point, ok. So, complete lattice translation basically, this is where we finish the edge dislocation part. We will now take up the surface defect part of the remaining. So, now we will introduce what we call as is surface defects or 2-D defects.

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Now, basically these are many kind of interfaces or surfaces in the materials. So, for example, you can have grain boundaries. So, first defect could be your if I list them out your grain boundaries, then you can have stacking faults, then you can have twin boundaries and you can also have grain boundaries can be both low angle and a small angle depending upon the angle of measurementation and basically the free surfaces,.

So, there are many more other examples of and basically any kind of interfaces,. Interface, it could be homo. Into homo, it could be interface between the two same materials, it could be interface between two different materials and so on and so forth. So, let us just go about this one by one.

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So, grain boundary basically means suppose you have as I explained in the last lecture, suppose you have this volume of material. So, let us say we have, so what could happen is that in this part of the crystal, you can have atomic arrangement like this, and the other part of the crystal, your atomic arrangement could be. So, basically they are not closed pack items, they are stacked in a fashion which is slightly different from the previous one or it could be same orientation, it could be close packed layer oriented differently.

So, this is another kind of orientation. You can have orientation like this and you can have another orientation somewhere here so on and so forth. So, you can see that if you take a particular vector let us say this is the closed pack direction, in this case this closed pack direction in this case lies in this direction in this region. It lies in this direction, in this region, it lies in this direction. In this case, it may lie in this direction. So, as a result these have they create boundaries between them which are the regions of misorientation where they do not, orientations do not match.

So, these are the regions of you can say crystallographic mis orientation and this is what. So, the region in which the orientation is all same is called as a grain and this is called as a grain boundary. Now, depending upon the angle of misalignment, these could be called as high angle or low angle grain boundary. So, grain boundary can be furthered categorized as low angle or high angle.

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So, if I show you now images of these two samples, so this is what it would look like if you look at this image. So, here this is one region in which all the atoms are arranged in one manner and this is another region in which atoms are arranged in other manner and this is one region in which atoms are in particular manner. So, this is the direction of let us say closed pack direction within this plane and this is the direction within this grain and if I calculate the angle between the two, I get the angle of misorientation. So, you can see that between the grain on the left and the right and the misorientation angle is smaller. So, this is the angle let us say theta and between these two. So, if this is grain 1 grain 2 and this is grain 3. So, between grain theta 1, 3 is smaller than theta 1. If I take the same direction in grain 2 and grain 1 and then, calculate the angle, this angle is larger, ok.

So, this grain boundary will be called as high angle grain boundary. This would be called as low angle. I will come to the magnitude in a short while and if you look at the grain structure of materials in optical microscope to look at, to visualize this, you need to normally subject the material to an acidic treatment, which is called as ethant, use of ethant. So, basically this ethant is nothing, but a mixture of few assets dilute acids which preferentially removes the atoms come back grain boundary area because grain boundaries are lose part of the material. It has higher energy. So, it gets etched preferentially as compared to the grain. So, when you subject it to optical microscopy, the light gets scattered more at the grain boundary. So, there is more reflection from the

grains than at the grain boundary. As a result, grain boundaries appear darker in comparison to the grain. So, the region which are dark are the grain boundaries whereas, regions which are bright are the grains and the grains may also have different color because different color represents different orient, may represent different phases as well as different orientation of grains. So, depending upon the crystallographic orientation of the plane, the reflectivity of the plane itself may be different, ok.

So, in a normal optical microscope, you see this black and white contrast, the white ones are typically grains and black ones are the black boundaries are called as a grain boundary. So, these are grains and these ones are the grain boundaries,.

One uses an ethant to preferentially<br>remove atoms form the g.b.<br>hune hight is neglected from a<br>graing than grain boundaries<br>(J/m<sup>2</sup>)

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Basically one uses an ethant to preferentially remove atoms from the grain boundary and as a result more light is reflected from grains than grain boundary and these grain boundaries are regions of reason of misorientation. Basically they are an interface. So, as a result every grain boundary is associated with a grain boundary energy, energy which is in joules per meter square gamma gb,. So, typically a higher angle grain boundary will have higher energy as compared to a lower end angle grain boundary in the materials.

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The angle of misorientation between the two is typically about, so that the way you define them is if theta misalignment is less than nearly 10 degrees, it is called as low angle grain boundary and if theta misalignment I think it is about 9 to 10 degrees. If it is greater than 9 to 10 degrees is called as a high angle grain boundary. Often in many materials, the low angle grain boundary can be viewed as is an array of dislocations. So, basically what happens is that there is an atom to atom correspondence up to certain distances and then it breaks off.

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So, if I would like to show you an image of that, so this is how a low angle grain boundary looks like. So, here b is the burgers vector, h is the height between the, distance between two dislocations. So, this is you can say the grain. So, this is number 1 grain, this is number 2 grain and they are oriented in such a fashion that there is atom to atom contact at various places. Only between the dislocations, you seem to have the atom to atom contact missing.

So, it is like an array of dislocation. This is like a vertical array of dislocations, ok. So, they may have some strain at the interface, but atomic density at the interface is higher than the high angle grain boundary. So, this defines the net energy of the low angle high and low angle grain boundaries. So, these are two energies, these are two grain boundaries that we talked about. Now, the second thing is called as Stacking Fault.

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Now, a Stacking Fault is something which typically is observed in close pack crystals. You can say it is typically a structure such as nickel, copper and basically it is a disturbance in atomic stacking. So, we saw that in FCC structure for example, you have abc kind of packing. So, you have a plane, you have B plane, you have C layer so on so forth, right. ABC and they are all same atoms. Now, suppose if I introduce a stacking fault, it may appear something like this. So, you have ABC, you can have after C, it can be just. So, CAB then again A, then again say, so here if I just mark it you have ABCAC, then again it could be ABA AB before it becomes ABC again. So, you have this region of the crystal which has different stacking as compared to the previous one. So, here you have ABC, but you end up having a stacking which is ABAB kind of stacking in some region of the crystal. So, this is the stacking fault. Obviously, it is again different stacking sequence as opposed to the normal stacking sequence in the materials. The good thing about stacking fault is that since it is in it happens in close pack crystals, there is no change in the number of nearest neighbors. So, whether it is AB AB stacking, whether it is ABC AB ABC stacking, the number of neighbors for each atoms remain 12. There is no change in that however what it changes is there is a shift.

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So, if you look at for example, this layer, so alright ok. So, that is how you form that. So, now let us say I have two kinds of voids here right A and B. So, now let us say the second layer of atoms, it goes here one, on here second, on here third, on here now somewhere. So, these kind of voids, they are used for basically I am not filling these voids. So, these are for the next layer. So, let us say this is the layer A, this is the layer B or it could be BC or whatever, right. Now, suppose the next layer somewhere in the crystal, so I can see that voids are empty, not covered. These are not covered. Similarly, you will have these are not covered. Now, somewhere in the crystal let us say I start having an atom sitting here.

So, I can see it right now, the orientation is two atoms up, one atom down and so on and so forth in this case and the site which I may want to fill is this, this, ok. Now, you can see what happens between the two of these layers, there is a region of disturbance, right. They have to accommodate in such a manner, so that they maintain the backing of the layer, but at the same time they have the two orientation have to fit with each other which means this is let us say AB, this is AC. So, B and C, layer B and C stacking have to accommodate themselves within the same layer. So, as a result there will be a shift in the translation within the layer.

So, as a result there is a shift vector. So, basically within a layer, you have to identify them using a shift vector if you bring it closer. So, this layer will basically get shifted by a vector in the previous layer, in the next layer and this as a result you need to identify using a shift vector to depict the shift in stacking, ok. So, you are going from ABC, then you have AB AB, ok. So, the moment you go from A to B, the B shifted with respect to C layer, right. So, there is a shift vector. So, this shift vector will go from this side to that side. This is the shift vector. So, as you go from ABC ABC ABC to let us say I can make it BC, and then, again ABC. So, I can see that, you can see A to B, B to C and then, C to 8 instead of C to A, you have C to B.

So, there is a shift in the position and the shift in the position is basically from one side to another side, ok. So, this is the shift vector. So, this is a shift vector. In the first plane, there is this is the shift position. This is the position in the first plane, this is the position in the second plane and if you take this, if you subtract the coordination of the two, you will get a shift vector, and the shift vector basically happens to be of the type of. So, basically it happens to be type I think it is 1 by 6 1 1 2.

So, essentially what happens here is the full dislocation gets broken into two parts which is called as partial dislocations. Unfortunately I cannot go into partial dislocations in this course, but basically one full dislocation which is half 110 gets broken into two dislocations of type half of 211 and if it is 110, then obviously it is going to be 1 by 6 to 1 bar 1 and this would be 1 by 6 1 2 bar 1 2 1 this sort of reaction will occur. So, basically a stacking fault would look something like this within the layer you have stacking fault somewhere in.

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So, this region is stacking, stacking fault faulted region, this is unfaulted region and between the two they have these vectors which are basically partial dislocations which correlate the two regions. Anyway this is useful plus a deformation, but I just want to tell you that something called as stacking fault in materials which is present, which is useful in deformation. So, basically it is change in the layering sequence.

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atoms across the boundary<br>  $-$  Surface  $\rightarrow$  tve energy (J/m<sup>2)</sup><br>  $-$  v annealing or defamation

Now, next thing that we have in crystals is called as twins. So, you can have for instance I can show you a image here.

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So, this is how a stacking fault may be viewed as. So, this is taken from professor Anna Subramanyam. So, you have the stacking sequence. This is the perfect region of the crystals in which you have ABC ABC kind of stacking or BCA ABC and here you have a broken region BC AB BA AB and then CA. So, this is the faulted region. This faulted region is basically the loop with partial dislocations. So, stacking fault is again a surface is a surface defect as energy of the order of 0.1 to 0.5 joules per meter square depending on the type of material.

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These are called as twins and twins basically you have two parts of the crystal. They are misoriented to each other in such a fashion, so that across one boundary which is called a twin boundary, the atoms look as if they are arranged in a mirror like position. So, you can see that this atom is a mirror image of this atom, this atom is mirror image of this atom, and this atom is mirror image of this atom. So, this is called as a twin boundary and twin boundaries are again useful in deformation. There are two kinds of twins; an annealing twins and deformation twins. These boundaries can form as a result of annealing or as a result of deformation and the crystals again it is a surface, it has a positive surface energy.

So, twin boundaries also have energies. Any kind of 2-D defect has a surface energy which is a positive surface energy whether it is grain boundary, whether it is twin boundary or whether it is stacking fault.



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So, these are certain twins you can see within the crystals. So, this is twin. For example, I think in the brass, it is in the copper sample. So, within the copper sample, you can see that this is a twin and across the twin, you have this is the sort of these are twin boundaries. So, these are the twins. So, there are twins. Basically they are not very, they can be sharp, they can be because the atomic orientation has to be mirror like. As a result these boundaries are typically quite sharp, and then, we have something called as normal surface which is basically you can say twin is a mirror like across the boundary. So, its

surface has and these can be fine formed after annealing or deformation and it has a positive energy in joules per meter square. And then finally we will just look at the surfaces.

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So, if you look at the surface of copper 1, one surface of copper, so this 1 1 1 surface of copper each atom has 6 neighbors within the plane, ok. It will have three neighbors below the plane and if there was a next layer present, it will have three neighbors out of the plane, but suppose it terminates here, this is the final surface. There is nothing above which means the bonds are broken, right. As a result there is some positive energy because creating a surface creates requires you to break the bonds. As a result, there is a cost to create a surface.

So, every surface has a surface energy, because of energy cost to create a surface as a result, you can calculate the surface energy of let us say the surface energy gamma s for a surface, it can be calculated estimated for given surfaces. Now, basically it is related to number of atoms per unit number of atoms on the surface per unit area multiplied by how many bonds each atom is making. So, basically you can say it is nb per atom multiplied by what the energy of that bond is. So, basically gamma b or we can say gb or eb energy of the bond. So, this is number of atoms per unit area, number of bonds per atom, number of bonds broken right number of broken bonds. Not all bonds number of broken bonds and this is bond energy and since each bond is sheared by two atoms, you divided a factor of two.

So, this is basically the bond energy of the surface energy of free surface. So, here basically this is in number per number of atoms per meter square. This is basically number, this is essentially you can say joules and per bond and this is number of bonds. So, you can see that the energy is joules per meter square or you can say it is called as Newton per meter. Since, it is a positive energy, most of the surfaces try to minimize their energy as a result surfaces are always sort of some sort of tension. So, the surface energy of the materials is always depicted in terms of surface tension, ok. So, often we call about call of it in the form of surface tension.

So, there are various materials for which you can have different surface energies, for example sodium chloride has a surface.

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Energy of gamma s of about 0.3 joules per meter square, magnesium oxide has surface energy of 1.2 joules per meter square whereas, silver has a surface energy of 1.14 joules per meter square, copper has a energy of 1.64 joules per meter square. So, these are surface energy, sort of values of most crystals, they are within the range by and large they are within the range of 1 joules per meter square, 1 joule plus minus 0.5 or so by and large. However, some crystals have lower surface energy as well which means they can have large surface area, ok. So, this is about the defects.

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So, what we have discussed so far is you have three kinds of defects; zero defects which are called as point defects, 1d defects which are called as line defects or dislocations and 2-D defects which are called as basically surfaces interfaces, right. So, among these, these are equilibrium defects zero point defects, but these two are not equilibrium defects. So, their concentration can be basically if you take a single crystal, you eliminate dislocations nearly completely, and surface energy is you can make a single crystal, you can get rid of grain boundaries for example completely.

So, surfaces can be minimized for practical reasons. They are always going to be surfaces. All we are going to be present because surfaces terminate somewhere, but theoretically speaking they are not equilibrium defects, ok. So, what we have done in this course is basically we have covered the aspects related to structure of materials we started with atomic structure.

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There we talked about the bonding in materials in and this bonding and atomic structure led to crystal structure analysis. A crystal structure theory of crystal structures were we looked at how the atoms arranged in space, what is a primitive lattice, what is the non primitive lattice, what kind of crystal systems you have, what are symmetry considerations, what kind of, what kind of structures are followed by material such as covalent, in covalent solids and then, we looked at structure of solids basically, right and in between we also looked for the completeness miller indices, right. So, here we looked at the concept of lattice, the concept of primitive and non primitive lattice, concept of motive concept of crystal system, Bravais lattices, concept of symmetry, how symmetries related to crystal structures, how does it define various crystal systems, then we looked at miller interstitials in the materials and then, we looked at structure of various solids based on the bonding criteria.

So, we looked at structure of metals which are metabolically bonded structure of covalent ceramic solids which are ceramic materials basically which are mostly covalently ionically bonded solids and then, we looked at the structure of you can say crystalline solids in this case, right and then, we looked at non crystalline solids basically glasses and polymers which are also technologically important materials and then, we looked at a structure determination using x-ray diffraction and finally, we looked at basically defects in materials because materials are not perfect. They do contain defects whether they are equilibrium defects or non equilibrium defects.

Defects are a reality of life and we need to know them because there are a lot of times they are useful. For example, point defects are useful in conduction phenomenon materials, they are also dependent, they are also useful in expansion contraction of materials for lot of ceramic materials, the conductivity is manipulated by point defect concentration. Similarly, in case of edge dislocation, screw dislocation, they are useful because they allow deformability to metals. Metals will not be able to deform. If you did not have dislocations and 2-D defects also useful because surfaces often provide means for you need to understand surfaces because most of the materials make certain bond with each other in various application.

So, in characteristics of interfaces are to be known and interfaces are important because they provide pathways for diffusion, pathways for inter facial reactions. Concept of surface is very important in phenomena such as grain growth and centering. So, any phenomena where there is a large change in the grain boundary area or surface energy occurs where surface energy plays the important role, it is important to understand the concept of surfaces.

So, I hope it has given you a brief overview of structure and structure of materials, it is not by all means it is very at the first level. If you want to get into details, everything all of these topics form a subjecting themselves. So, you can have a course in atomic structure and bonding, you can have a course in crystal structures, you can have a course in a structure of solids only and you can have a course on glasses and polymers as well as the x-ray diffraction.

So, in this course, I have tried to give you a bird eye view of structural materials. If you are interested, there are various references, various books available. You can go through to read in detail about each of these things. So, I hope you have enjoyed the course.

Thank you very much.