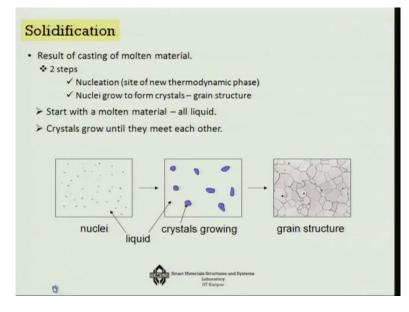
Nature and Properties of Materials Professor Bishak Bhattacharya Department of Mechanical Engineering Indian Institute of Technology Kanpur Lecture 10 The Role of Crystal Structure 3

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Crystal D	efects		
✓ Introduction			
✓ Point defects			
✓ Line defects			
✓ Plane defects			
✓ Volume defect	ts		

Today in the role of crystals, we will focus on actually the defects in crystal. So even though crystals have a very regular structure, but in nature hardly such regular structures will be followed. So hence the defects that we will we will come across in a crystal structure at various length scales, etcetera, we will focus on that today. So thus we will first give an introduction of the crystal defects. We will then talk about point defects, line defects, plane defects and finally the volume defects.

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So the 1st point is that, when the crystal is forming if you let us discuss that we have earlier also discussed about it. So let us look back at this that from liquid stage, we are gradually through a gradual process of cooling we are getting the crystal structure, right. If we want to make the cooling process to be very fast, then what we are going to get a glassy amorphous structure. So hence a very controlled uniform gradual cooling is must in terms of developing a crystal structure.

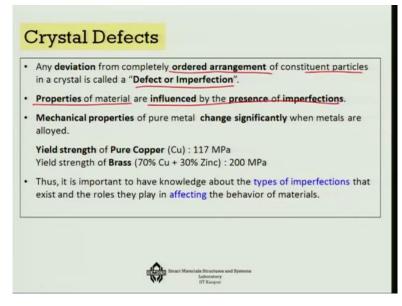
Now when you are from this molten state you are actually taking a material to the solid phase. The 1st thing that would happen is that there will be a sight of new thermodynamic phase, which we will call as the nucleation. So the nucleation as has been shown here, various nuclei will start and this nucleus will grow to form the crystals. And these crystals will start to grow up to a point when they will meet each other, then we are going to get actually the grain structure okay.

So basically, grains are crystals but they are crystals grown up to such an extent that these each crystal structure is getting in touch with another crystal structure that is when we will say that now from the basic crystal structures the grains have been formed in the system. So this is how the solidification process occurs. Now in this solidification process, not everything goes perfect so there will be lot of scopes of things getting disturbed.

And many of these disturbances will result on what we say then the crystal defects. So any deviation that we will observe in an ordered arrangement of constituent particles in a crystal, we call them to be defect of imperfections. Now why it is important because the properties of

the material are actually influenced by the presence of this imperfection that is why it is important for us.

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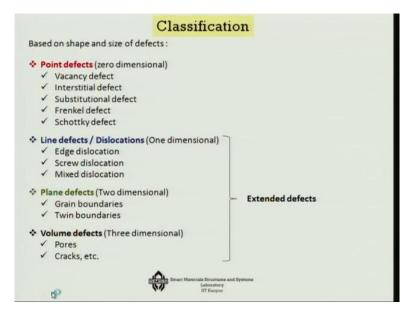


Mechanical properties for example are pure metals that changes significantly when metals are actually alloyed. Now alloys are actually intentional creation of disturbances or defects in the crystal structure to improve the material properties or mechanical properties of a metal. People have understood it initially intuitable you can say when you have talked about from the Copper age to Bronze Age okay.

People have understood that something happens when copper gets mixed with other impurities. Similarly, when we have talked about from Iron Age to steel age okay if you remember those various types of steels the early steels in southern part of India for example okay so people have realized that carbon as an impurity plays role in the crystal structure of iron to actually improve the properties of iron drastically.

So the copper for example, when you take your copper its Yield strength is 117 megapascal, but you mix this copper in a ratio of 70% copper with 30% Zinc, you get actually brass and you see the brass modulus of elasticity Yield Strength is 200 megapascal, so thus it is important for us to know about how many types of imperfections are possible in any regular ordered crystal structure, what are the roles of each one of them in terms of the material properties of the system.

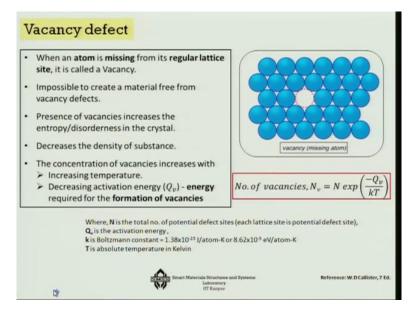
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Now to do that we have to clearly classify the types of defects, so the major types that we can say is that the Point defects which are actually 0 dimensional, we will put more emphasis on that in this lecture. Also there are other defects like Line defects, which is like Dislocations that is 1 dimensional in nature, Plane defects which are like 2 dimensional in which grain boundaries will come, twin boundaries will come and find the Volume defects which are 3 dimensional in which pores, cracks, etcetera will come.

Now in the point defects itself, there are about 5 to 6 categories of it for example, the Vacancy defect, Interstitial defects, Substitution of defects, Frenkel defects and Schottky defect, so we will talk about all these types of defects in today's lecture, so let us 1st start with the Point defects. Now this is associated with the atomic sites happening inside a crystal structure and it may not be very regular in nature, it may be just irregular in the sense that in a regular lattice, it may not be periodic in nature.

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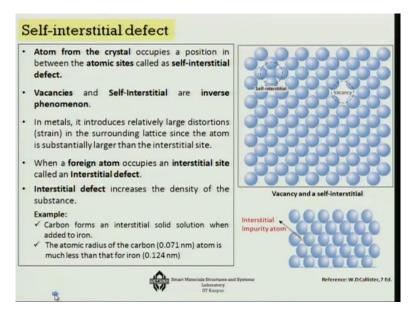


At different points you may suddenly see that one atom is missing from the regular lattice site. If this happens, then this is called the vacancy. So and this is something that is very real in the system it is impossible to create a material which will be free from the vacancy defect. Now the here is an example that you have a regular structure, suddenly one atom is missing here okay, so there is a vacancy here.

So presence of this vacancy, naturally what happens it increases the disorderness or the entropy in the crystal that is one thing. What are the other things that is happenings, it actually decreases the density of the substance because there is nothing that there are (())(07:18) type of a thing there in the atomic structure, so it is going to decrease the density. The concentration of vacancy increases, when there is an increase in temperature okay.

So at higher temperature it is found that vacancies are more why, because atoms are more mobile basically and in fact something more happens at that high temperature that decreases in activation energy okay. So in fact, the number of vacancies you can actually compare it is in erroneous law that the number of vacancy is actually varying with the activation energy and temperature okay. So as the activation energy is reducing, as the temperature is grieving, you are you are actually going to get more number of vacancies in the system.

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Now there is another form that can happen when the vacancy is there and suddenly an impurity because you will never see a very pure materials, suddenly an impurity goes and say okay there is a vacancy, let me push myself inside it, so that is called interstitial defect. Now if the atoms from same group goes and pushes it, then it is actually self interstitial defect. Sometime atoms of different kinds or impurities okay foreign atom can occupy then it is not self interstitial, but it is just in interstitial defect.

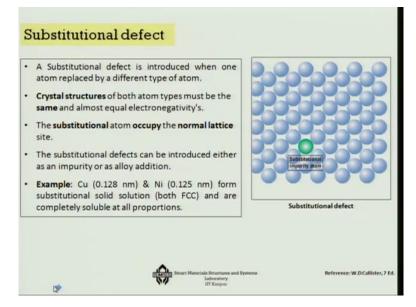
In fact, if you can see that a vacancy and the self interstitial defect may be actually kind of an inverse way of 2 phenomena because supposed where there is a vacancy, there is supposed to be an atom there. But due to the increase of temperature, due to the decrease of the activation energy, this atom has jumped out of its location and then pushed him in one such place.

That way it is stressing the region here and it is creating a kind of a pore here. So that is what is happening that vacancy is happening at one place and this sometimes self interstitial phenomena is happening at another place and both of them may become actually coupled with each other. There are some examples like carbon forms and interstitial solid solution when it is added to iron.

And what will happen if we look at it that the atomic radius of carbon is only 0.071 nanometre, which is much less than that of iron, for iron it is 0.124 nanometre. So that means, there are plenty of space in between the iron atoms, where this 0.071 nanometre carbon atom can go and push itself inside it. The moment this happens, it actually generates a stress on all

the neighboring iron atoms and that actually significantly changes the material properties of the system.

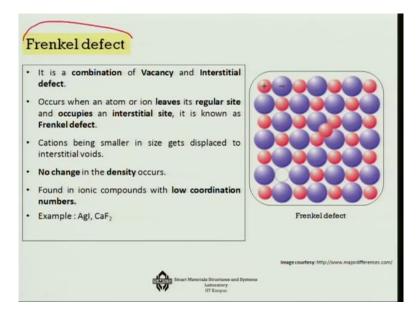
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Now sometimes there will be substitution defects also. Substitution happens when the atom that is substituting is nearly of the same size of the original atom, so they will not disturb the crystal lattice and also the atom which has come in, the foreign atom itself should have crystal structure which is very much similar like the atom in which it is going to go and sit itself. So this happens many times between copper and nickel because if you look at it, copper's atomic radius is 0.128 nanometre and nickel's atomic radius is 0.125 nanometre and both of them actually create a FCC solid solution.

So it is very easy for copper to substitute nickel okay, so that is how this Substitutional defect can get formed in the system. Now, there are 2 more varieties of this actually Point defects. These are specifically this thing arise for ionic structures okay, where I mean crystal structures which is which is mostly having ionic bonds, let us say salts or ceramics you would see this more.

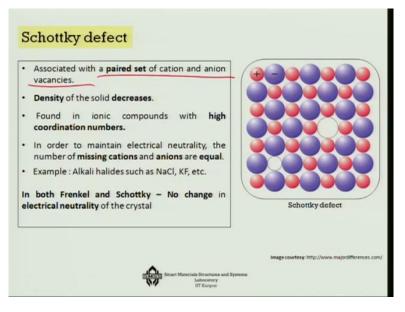
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The 1st of them is called actually the Frenkel defect. It is a combination of vacancy interstitial defect, the only thing is that this is happening when an atom or an ion leaves its regular site and occupies an interstitial site okay, so then it is known as Frenkel defect. Cations are generally smaller in size and they get displaced to interstitial voids. Now in such a case because one ion is leaving its position and it is going to another position, so generally this happens continuously and as a result no change in the density occurs.

And this is very peculiar that this is generally absorb in ionic compounds which has actually low coordination numbers okay, something like Calcium fluoride. So that is where you will see the Frenkel effect. There is another point defect that is known as Schottky defect. And here it is always, it has to be a paired set of cation and anion okay.

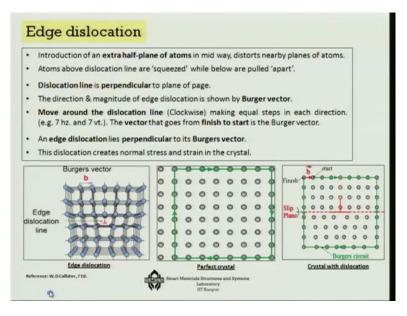
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That emphasis on pair is important because then there will be an electrical neutrality in the crystal. Now in this case, the density of the solid decreases because it has to happen pairs, so there will be lot of actually vacancies so the density of the solid decreases and it is found in ionic compounds with generally high coordination numbers. And in order to maintain the electrical neutrality as I told you earlier, the number of missing cation and anion are to be equal, so something like Sodium chloride, Potassium fluoride, et cetera.

In both Frenkel and Schottky, no change in electrical neutrality of the crystal is observed. So thus we have kind of gone through various types of point defects okay, we have talked about the vacancy defects. We have talked about what you call interstitial defects and then we have talked about in a Substitution type of defects and then Frenkel and Schottky defect. Now let us look at the linear counterpart okay, so from the point now we are going to line defect or dislocations.

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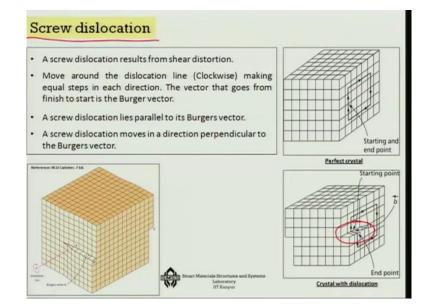


Now there are even though we call it line defects, it need not be like a straight line it can be in a curve okay, so it can be in terms of edge dislocation, it can be in terms of a screw dislocation or rotational dislocation, et cetera. Now what is this dislocation? In this case it is actually not a phenomenon with one single atom, but rather by building up the crystal structure for some reason because of various disturbances, one layer of crystal structure may not get completed.

And by nature it is just like nature that one extra half plane of atoms is let in between. Now this extra half plane that is there, it will actually distort all the nearby planes and then actually this dislocation is coming into picture. Now, this dislocation line in this particular case as you can see is perpendicular to the plane of the edge itself okay, so this is edge dislocation that we are talking about.

The direction and magnitude of this dislocation is given by a vector, which is known as Burger vector. So how do we get this dislocation, okay so to do that you have to move around the dislocation line in a clockwise manner making equal steps in each direction. So the vector goes from finish to start position in the Burger vector okay. And what you will see is that when you will reach the dislocation point you will see that the edge dislocation is generally perpendicular to the Burger vector.

And this dislocation creates normal stress and strain in the crystal actually and also it affects the other material properties like strength and plastic flow, et cetera. So you need not have a planar dislocation always okay, you can have a dislocation which is like a Screw dislocation okay, which is actually something like a shear that is happening in the system.



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So if there is something like a shear, once again you can move around the dislocation line clockwise as has been shown here and from finish to start with the help of Burger vector and this Burger vector what you will see is actually parallel to the dislocation in this case. In the last case that it was perpendicular to dislocation and here it is parallel to the dislocation. So a screw dislocation lies parallel to its Burger vector and it moves in a direction perpendicular to the Burgers vector, so that is when you have screw dislocations.

Now, how do we avoid dislocation? 1st of all, why do we need to avoid dislocation? Well, in most of the cases it is a defect which is something which is not negligible because it is a long scale of a defect; it is not just one single atom missing, but rather entire plane missing.

So what the way it can effect is one definitely terms of the strength of the system. And there are other things also possible that are in terms of the nature of the system at a high temperature for example; the creep behavior of the system and also it affects the damping of the system. Now one way to avoid dislocation is that dislocation is happening when crystal structures there are many crystal structures and suddenly one half planes is missing in a poly crystal structure.

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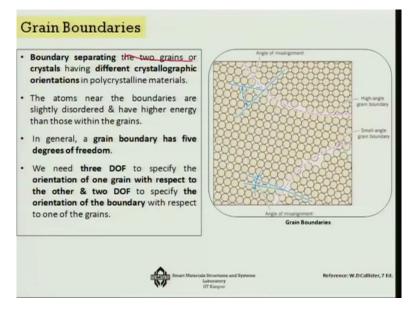


If you use a single crystal structure, generally to do that you actually control the environment to a very good degree, you can avoid the dislocation for example, turbine blade making this is done, but it is very expensive okay, so that is why it is not usually done. The other way to do is actually work hardening. Now because dislocations are happening inside the grain structure okay, so you what you can do is that through work hardening you can move all the dislocations to the grain boundaries.

So when the dislocation will become essentially a part of the grain boundary, then we can say that this strengthening plastic deformation has happened and there is a work hardening that has taken place in the system. This is done in a regular manner particularly for developing very high strength surfaces let us say, wherever there is a point contact and there is a danger of wear and abrasion the work hardening is required. And there this can this can work in much better way.

The other way to avoid dislocation is actually introduce impurity into the atom, so that it goes into that dislocations space, it fills up the space okay and thus it makes the whole system to be strong, so there are these various ways or actually dislocations that you can control. Now that is about the edge dislocation, if you expand that what you are going to get is called Surface or Planar defects.

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So the Planar defects are something that what you will see in general is in the grain boundaries itself. The boundaries that separate the 2 grains of crystals having different crystallographic orientation okay, this is where you will see this grain boundaries which is a 2 dimensional defect. Now how it is going to affect the material property because the atoms which are near to this grain boundary, suppose here we have grain boundary, right.

So the atoms which are near the grain boundary, they are slightly distorted you can say and have higher energy than those within the grains. Now, in general a grain boundary is assumed to contain 5 degrees of freedom. This 5 degrees of freedom out of that there are 3 degree of freedom which are related to the orientation of one gain with respect to the other. And there are 2 degrees of freedom to specify the orientation of the grain boundary itself.

So thus there are 5 different degrees of freedom by which the grains can move against each other along the grain boundary and hence can significantly control the material properties of a system. Now, how would it actually affect?

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	atures (T < 0.5Tm, where Tm is the melting point), the grain boundaries ng obstacles to dislocation motion giving strength to a material.
	temperatures, they tend to weaken a material as grain boundary sliding r, leading to plastic flow and/or opening up of voids along the es.
	, fine grained materials are stronger than coarse grained ones because more grain boundaries per unit volume .
Grain size	letermination
American So	ciety of testing material (ASTM E 112) method
	$N = 2^{n-1}$
where,	
	number (1-10), which is then compared with standard charts as per ASTM E 112 umber of grains per square inch at a magnification of 100X
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One is that, at temperatures which is actually greater than 0.5 T m, T m is the melting point temperature, then the grain boundaries will actually start to flow. But when it is less than 0.5 T m it will what like an obstacle to the dislocation, the grain boundaries will not allow the dislocation to propagate very easily.

On the other hand, at a higher temperature they will tend to weaken a material why because the grain boundary sliding may occur. Each grain boundary may slide with each other so that may result to a plastic flow or opening up of voids, etc along the boundaries. In general, what we think is that single crystal structures are good.

However, if you have to go for a poly crystal structure, then you should go for a fine grained material which are actually stronger than coarse grain ones why because they have actually more grain boundaries per unit volume, so grain boundaries are actually making the structure stronger. Now, how do we first of all know that what the grain boundary is?

There is a ASTME in a E112 standard of ASTM, which says that the average number of grains per square inch at a magnification of 100 X is related to the grain size by this particular relationship, which is a very useful relationship because in the slide I will show you how to use this relationship.

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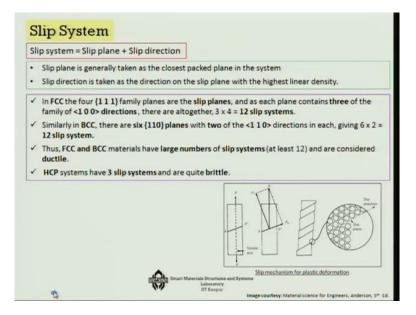
Numerical							
	TM grain size number of a metal specimen if a magnification of 100X ?	45 grains per square inch					
Answer: Using ASTN	Answer: Using ASTM method $N = 2^{n-1}$, n= grain size no., N = grains/inch ²						
Taking logar	thm both sides and on simplifying, we get $n = \frac{logN}{Log2} + 1$						
Therefore,	$n = \frac{\log 45}{\log 2} + 1 = 6.5$						
2). For same specim 85X?	en, how many grains per square inch will there	e be at a magnification of					
Answer: Use equation	n, $N_M\left(\frac{M}{100}\right) = 2^{n-1}$, N_M = grains/inch ² at magn	ification M.					
Substituting	n = 6.5 & M = 85, we get						
	N_M = 62.6 grains/inch ² at 85X						
D ²	Example Smart Materials Structures and Systems Laboratory IT Kanpur	Reference: W.DCallister, 7 Ed.					

So if you look at it that there is this example the 1^{st} one is that you have to determine the ASTM grain size number of a metal specimen if 45 grains per square inch are measured at a magnification of 100 X. So the ASTM standard method is that this N okay is equals to 2 to the power n - 1, where N is the grains per square inch and small n is the grain size number.

Now if you take a logarithm you get a simplified relationship like this, so in this particular case we have said that the capital N is actually 45 that is the 45 grains per square inch okay. And the it is the denominator is log of 2 of course that is fine with us and then there is a + 1 which came from this relationship, so once I know that how many grains are there per square inch, I can actually find out what is the number n that we can find it out.

Similarly, in yet another problem suppose we use this equation where we have the percentage of grains and we have grains per square inch. The n small n is something like 6.5 and the capital M is 85, so if we give out this exercise we will see that N M will come out to be something like 62.6 grains per square inch. As I told you that finer grain structure that is more number of grains per inch is actually good for us if you cannot go for a single crystal structure hence, this determination is very useful for us.

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The second important point here is that there is Slip system. I told the already about the slip plane and slip direction, they together form something which is called the Slip system okay. And in the slip system, the slip plane is generally taken as the closest packed plane in the system and slip direction is generally the direction along the slip plane with the highest linear density okay.

So why are we talking about highest linear density, we have also addressed this problem in the last class when we have said that if there is a high linear density, then it is always easy for many things to happen fast using those items as the pivotal lines okay. I have given you an analogy of ragging a pulling a carpet or rag below if you have certain number of kind of the bearings or balls, then it is much easier for you to pull okay.

So here also the same way if you have more number of slip systems, then actually you if you have higher linear density that would mean, so than you are going to get actually the slip directions along that direction itself. FCC structure for example, it has four 1 1 family and of slip planes and as such this plane contains 3 of the family which are of 1 0 0 with carrot directions and there are altogether 3 into 4 that means about 12 slip systems.

Similarly in BCC structure, there are actually six 1 1 0 planes with two of the carrot 1 1 0 direction in each and that gives us about 6 into 2 that is about 12 slips systems. So what do we conclude from this that FCC and BCC materials both of them have a large number of slip system and that is why they are considered to be ductile materials. Now HCP on the other

hand, okay Hexagonal Closed Packed systems, they have only 3 slip system and that is why they are quite brittle in nature.

So slip system plays a very important role to actually define the nature of the particular material. Now what we will say is that what is the a very special case of Twinning that you will see in terms of the grain structure, when particularly you will see that this is happening with a symmetry line like this okay.

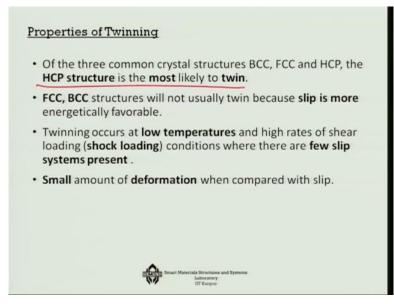
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• Sp	ecial type of grain boundary – mirror lattice symmetry.
	curs on definite crystallographic plane & specific direction – crystal structure dependent.
	The second secon
	oduced by Mechanical twin (Shear forces) ✓ Occurs in metals with BCC & HCP crystal structure.
ь)	Annealing twin (Deformation due to annealing) {Annealing - heating material followed by slow cooling to remove internal stresses and toughen it;
	✓ Occurs in metals with FCC crystal structure.
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So with a very definitive way that these kind of symmetric lines are going to actually, for example this particular case, this is the symmetric line, this is going to move the atoms in a flip flop condition. This flip flop condition I have given you earlier an example of Shape memory alloy, I will come back to it at a later stage. Now this can be in the form of mechanical twins, which occurs generally in BCC and HCP crystal structure.

Or you will see the annealing twin in which the deformation is due to the annealing itself okay. So annealing is actually heating the material followed by slow cooling to remove the internal stresses and toughen it and this occurs mostly with FCC crystal structure. So that is about the twinning, now twinning plays a very important role because those crystal structures which can twin more like FCC structure can actually twin more.

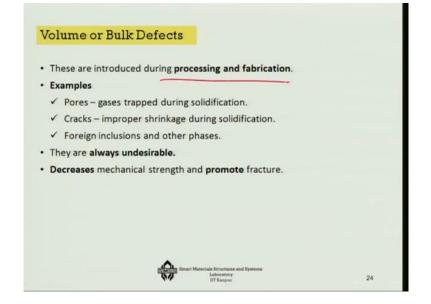
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And out of the BCC and FCC both of them are fine, but BCC actually twins more. But those which can actually twin, they can be used for phase transformation. So FCC, BCC structures will not use any twin because the slip is more energetically favorable. And this twinning generally happens at low temperature and at high rates of shear loading like shock loading, there are few such slip systems, which are present in the system.

And there is a small amount of deformation okay if you consider it in comparison with the slip. In fact, memory effect is one of the most prominent examples of this kind of twinning, but we will talk about it at a later stage. Finally, we will talk about Volume and Bulk defects okay. So we have talked about Point, Line, Surface, now then the volume.

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This happens mostly during the processing and fabrication like the pores come okay, so that is a defect or cracks is a defect, foreign inclusion and other phases, these are all defects. They are always undesirable, 1st thing without defects. And it decreases the mechanical strength and promotes the fracture, so that is what is the kind of flip side of a bulk defect. Now let us try to draw a kind of a summary of what we have discussed today.

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ry S. No	. Type of defect	Properties affected	Applications
		Solid-state diffusion	Annealing
1	Vacancies	Mechanical creep	
2	Substitutional	Electrical conductivity	Semiconductor diodes and transistors
		Mechanical strength	Solute hardening of alloys
		Magnetic coercivity	Strong permanent magnets
3	Interstitial	Dielectric strength	Capacitors
		Optical transparency	Coloring of glasses & plastic
4	Dislocations, Twin boundaries	Plastic deformation (ductility)	Strain hardening
	Grain boundaries	Dislocation movement	Mechanical hardening
5		Electrical resistance	
		Magnetic coercivity	Strong permanent magnets
		Optical transparency	
-	Stacking faults (interruption in stacking sequence)	Mechanical strength	
6		Electrical resistance	
		art Materials Structures and Systems Laboratory ITT Kanpur	

So we have talked about various kinds of defects 1st of all, Vacancy, Substitutional, and Interstitial if you remember. That the properties which are affected are the solid-state diffusion, mechanical creep, conductivity, then the magnetic coactivity, dielectric constant and optical transparency. The way you can remove these kinds of point defects are age old the traditional processes through the Annealing, we call it heat, beat and treat system.

Other than that, the other ways are like semiconductor diodes and transistors okay and solid hardening of alloys where you can apply strong permanent magnets, developing capacitors, coloring glasses and plastic, we can actually apply this presence of defects by converting it into what you call the (())(32:05).

The edge location or similar type of other Screw dislocation, etc, they are actually plastic deformation and they have applications in terms of strain hardening. The grain boundaries okay so they affect the dislocation movement, electrical resistance more than grain boundary, you have more resistance, magnetic coercivity, optical transparency, et cetera.

And the applications are in terms of mechanical hardening or strong permanent magnets. Then of course there is the stacking faults, which is generally it affects the mechanical strength and the electrical resistance itself. So this is where we will put an end in the next lecture we will learn metals like ferrous alloys, their properties and classification, thank you.