Structure of Materials
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Lecture - 24
Defect in Crystals

Now, we shall take up the important topic of dislocations.

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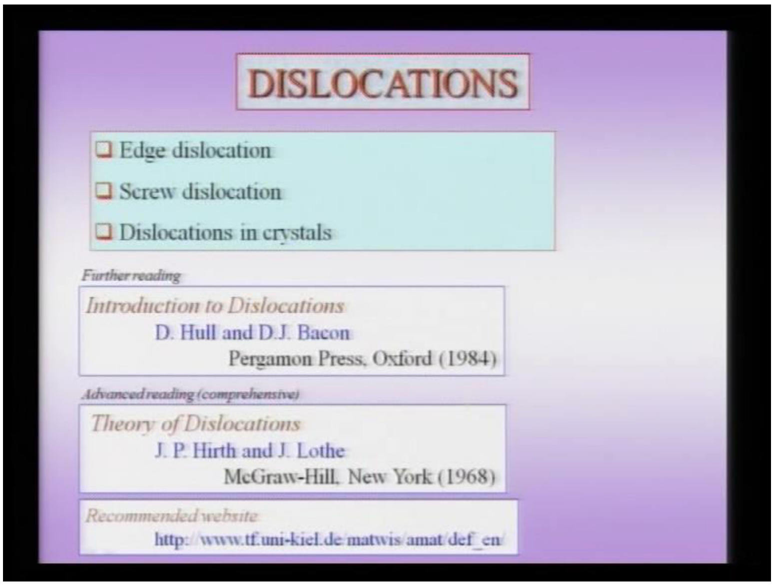

DISLOCATIONS

- ☐ Edge dislocation
- ☐ Screw dislocation
- ☐ Dislocations in crystals

Further reading

Introduction to Dislocations
D. Hull and D.J. Bacon
Pergamon Press, Oxford (1984)

Advanced reading (comprehensive)

Theory of Dislocations
J. P. Hirth and J. Lothe
McGraw-Hill, New York (1968)

Recommended website
http://www.tf.uni-kiel.de/matwis/amat/def_en/

We will take about edge dislocations, screw dislocations, mix dislocations and importance of dislocations in crystals, especially the way they effect the material behavior. There is lot of very good literature on dislocations, nice interesting introductory test would be by Hull and Bacon, which forms a nice interesting reading for people, who are interested in more advanced concepts and especially a comprehensive treatment of dislocations. Theory of dislocations by Hirth and Lothe is a very good text, there are some nice websites also like the one, which is tf uni kiel, which also gives comprehensive information about dislocations.

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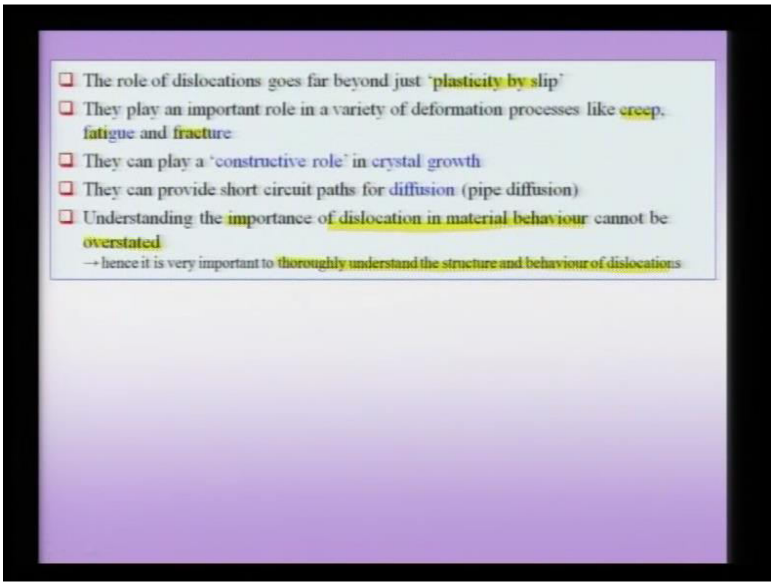

❑ The role of dislocations goes far beyond just 'plasticity by slip'
❑ They play an important role in a variety of deformation processes like creep, fatigue and fracture
❑ They can play a 'constructive role' in crystal growth
❑ They can provide short circuit paths for diffusion (pipe diffusion)
❑ Understanding the importance of dislocation in material behaviour cannot be overstated
→ hence it is very important to thoroughly understand the structure and behaviour of dislocations

The first and fore most important thing, I would like to say about dislocations and we already said that, dislocations are line defects. That means, they can be considered as one dimensional defects is a fact that, their role goes for beyond plasticity by slip. This of course, we not defined what is plasticity by slip, but as we know associate with plastic information, but the role of dislocation goes far beyond that. In fact, they play very important role in deformation processes like creep, fatigue and fracture.

So, whenever people focus on the role of dislocations in plasticity, we should remember that, there is just one important role, but there are many other important roles of dislocation in various diverse kind of phenomena. And in the next slide, we will take up a nice graphic, which explains this overview. Apart from this deformation process like plastic deformation like normal plastic deformation, creep, fatigue or fracture, they can play actually a constructive role in crystal growth.

And typically it is screw dislocations play a very important role in crystal growth and before we will see that, often dislocation is talked about as a defect. But, even though in spite of being a defect, they can actually play an very important and very surprisingly constructive role in the very growth of crystals. So, that is a very important role that dislocations can play and in this context we will say, these are the screw dislocations, which play that role.

They can provide short circuit paths for diffusion and typically the diffusivity, which occurred a core of dislocations that is, through the dislocation region, which is called the pipe diffusion as a diffusivity, which much higher magnitude, higher than the normal latest diffusion. And we will of course, try to understand that, why this is so and this will become obvious by the time we understand the structure of dislocation. And in this context, I would definitely like to say that, importance of dislocations in material behavior cannot be over stated.

The more we try to understand dislocations, the better we try to, our understanding of material behavior will be, especially the mechanical behavior materials. Of course, their role is not just related to mechanical behavior, for instance in electronic equipment and devices, if there are dislocations in the semiconductors for instance then, the material behavior could be adversely affect. And therefore, we need to understand the presence of dislocations, how many dislocations can be tolerated for instance, in an semiconductor device and so forth. And in this context, definitely that we need to thoroughly understand the structure and behavior of dislocations if you want to comprehend the material behavior starting from of course, the microscopic skill. Just to rehydrate the important thing in the slide, that dislocations are very very important and we need to understand them thoroughly.

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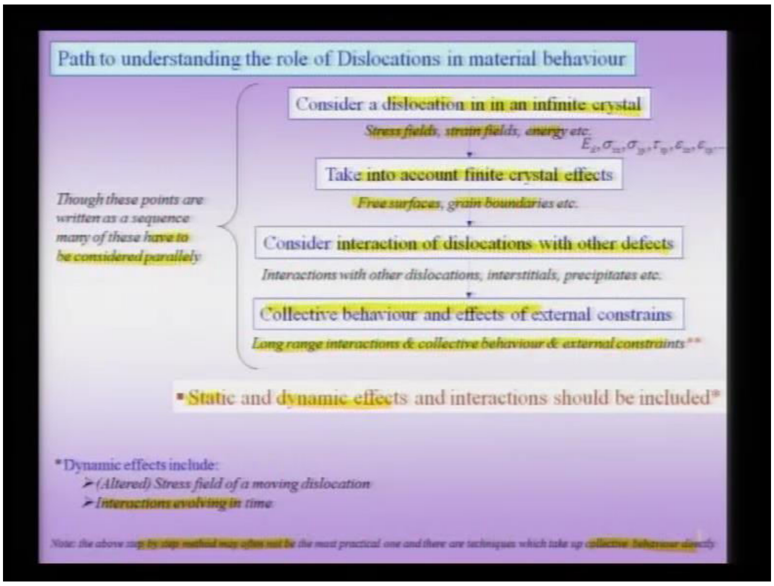

Path to understanding the role of Dislocations in material behaviour

Consider a dislocation in in an infinite crystal

Stress fields, strain fields, energy etc.

$E_d, \sigma_{xx}, \sigma_{yy}, \tau_{xy}, \varepsilon_{xx}, \varepsilon_{yy} \dots$

Take into account finite crystal effects

Free surfaces, grain boundaries etc.

Consider interaction of dislocations with other defects

Interactions with other dislocations, interstitials, precipitates etc.

Collective behaviour and effects of external constrains

*Long range interactions & collective behaviour & external constraints***

Though these points are written as a sequence many of these have to be considered parallely

- Static and dynamic effects and interactions should be included*

*Dynamic effects include:
- *(Altered) Stress field of a moving dislocation*
- *Interactions evolving in time*

Note: the above step by step method may often not be the most practical one and there are techniques which take up collective behaviour directly

To understanding the role of dislocation in material behavior, of course this is similar to the path we under took for understanding, any kind of defect, but here specifically I have dealing dislocations. So, the first thing we will do of course, is to consider and isolated dislocation in an infinite crystal. So, this is some sort of an ideal description of a dislocation and we really know that, for instance there are no infinite materials.

And often we will always deal with finite sized of crystals and not only a just single crystal, but often this could be even a poly crystal, but we will start with an description of an dislocation in an infinite media. And we will try to understand things like for instance, stress fields, strain fields, the energy of dislocation, etcetera. Then, we will proceed or we should proceed to taking to account finite sized crystal effects like what do free surfaces do to a, for instance stress field of a dislocation, what is the effect of grain boundary on the motion of dislocation.

So, these kind of questions we should ask in this introductive course, of course we will not take up all aspects of dislocation, we just take up perhaps a descriptive sample. And then, the remaining perhaps would be left more advanced course and plasticity or some of those other kind of courses, where in deal with more advanced concepts. Then, after considering finite crystal effects, we need to considering interaction of dislocations and we will of course, considering this course few examples of interactions between dislocations.

And in this interaction, is not only between dislocations, is between between dislocations and other kind of defect in the material. These are the defects could be vacancies, they could be grain boundaries, they could be twins or any other kind of defect. So, we need understand the interaction of dislocations with other defects in the material, this is an important topic.

And then finally, the goal is to understand collective behavior of dislocations and this is the very challenging task of material science, wherein you try to understand that, not a single dislocation, but thousands of them or even millions of them are moving together, interacting with each other, interacting with free surfaces, interacting with precipitate. And finally, all this evolution is taking place in time and under the action of external constraints.

External constraints could be displacement boundary conditions, they could be stresses impost or forces impost on the body. Of course, we could visualize simplest case being and uni action tension test. So, there are these external constraint, which are perhaps driving these dislocations and these dislocations are evolving in time via they are interactions with each other and with other defects in the material. So, this long range interactions and collective behavior is, of course is very challenging problem in material science, but that is the real goal of this whole task of starting from an single dislocation.

Many of this aspects, though they are written separately in a very sequential form, these can also be considered parallely in many of the approaches, actually that is what precisely done. You do not start with the single dislocation and try to evolve entire behavior, but the whole description process starts with a more collective or an average kind of a description of the entire deformation, that dislocation perhaps would give. Not only we need to consist static dislocation, but we also need to take into account dynamic effects.

And that is a very important thing, for instance like a moving dislocations as a altered stress field with respect to a static dislocation. And suppose, the velocity of the dislocation increases, it starts to approach the speed of sound in a material, which is shear velocity in the material. Then, there are serious dynamic effect, which cannot be ignored and these dynamic effects are also involving in time obviously and this makes the problem very complicated.

And this sequential thought process we have evolve now, is more of understanding or didactic thought process and in reality, this step by step method may not be followed and a practical, there may be techniques, which take up the collective behavior directly. So, there are techniques in dislocation plasticity, wherein actually take of large scale descriptive on an average parameter description of these material behavior directly without going through a step by step process, which we have illustrated here for a better understanding of the kind of concepts we will be going through in this elementary course.

Student: ((Refer Time: 08:00))

Yes.

Student: Sir, stress field and strain field are be inter depended to each other or to separate in property material.

Good question, in this case obviously, they are interdependent with each other, because stress filed is related to strain field via the material properties, that is very clear in this case. But, as a macroscopic case as we know that, for instances you could have stresses without strains and strains without stresses, so that is macroscopic. Like suppose, I take a rod and put it between two rigid walls and heat the material then, the rod is not allow to expand, but stress is to develop in a material, but this is now stresses without strains.

Either extreme example would be the same rod, which I just allow to heat, in that case it just freely expands in the medium. In that case, there is strain, but there is no stresses, because now all the stresses is relieved by the expansion of the rod. So, that is a macroscopic description, in this case stress field and strain fields are ultimately associated with the each other.

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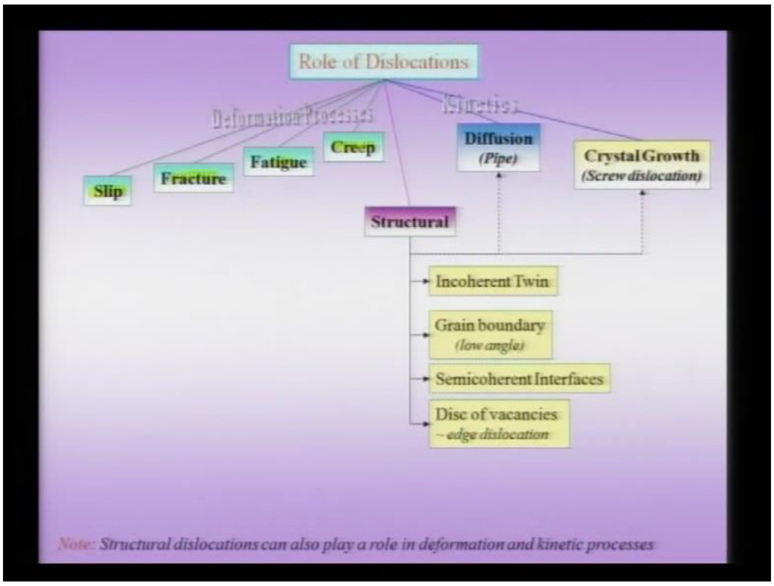

Role of Dislocations

Deformation Processes

Slip

Fracture

Fatigue

Creep

Kinetics

Diffusion
(Pipe)

Crystal Growth
(Screw dislocation)

Structural

Incoherent Twin

Grain boundary
(low angle)

Semicoherent Interfaces

Disc of vacancies
~ edge dislocation

Note: Structural dislocations can also play a role in deformation and kinetic processes

Now, I was talking about the roll dislocations in materials and advent that, though plasticity by slip, the one which is first in the slide, is an very important aspect of the behavior of dislocations of the role of the dislocations, but this role goes far beyond and all these aspect put together, is what we need to keep in mind when we are trying to understand dislocations.

They play very important role in various deformation process like I mentioned, they play a role in normal plastic deformation, in fracture, in fatigue, in creep. For instance, when I am talking about fracture we will see that, if I have a sharp crack in a material, like the one I draw in the board.

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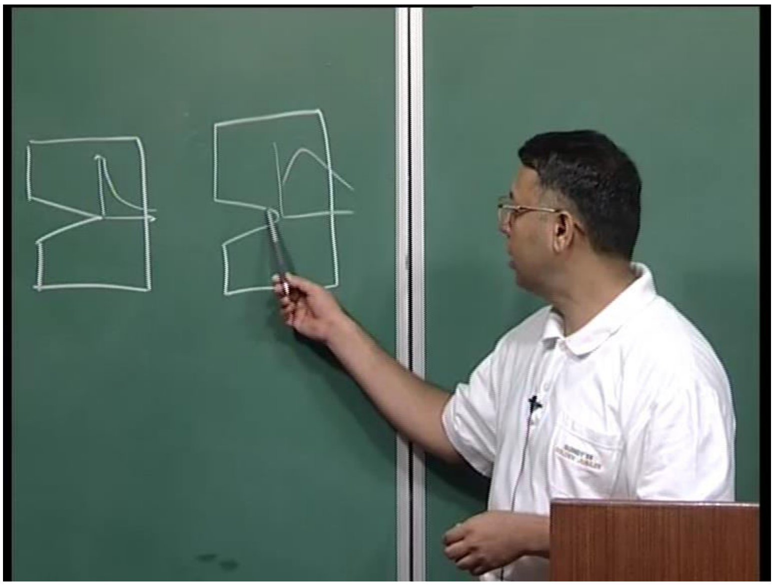

And this kind of sharp cracks typically are in brittle material, so I have material like this and now, a sharp crack. So, this is the brittle material suppose, I had a ducktail material then what would happened, the sharp crack would actually blunt and this blunting process is aided by the presence of the plasticity by dislocations. So, because of this blunting now, there is for instance, if I had a sharp crack then, I would have a singularity in the stress field that means, the stress field would blow up at the crack tip.

But, in this case, because of the blunting of the crack, the stress field will not blow up and actually, you draw stress field, which actually goes up and comes down. That means now, that there is a very important role of dislocations in causing, which is a very intimated relationship with fracture. Suppose, if I had a specimen like this then, this would fail by brittle fracture and in this case, because ((Refer Time: 10:31)) blunted, there would be actually reductility in the material.

They also play a very important role, for instance in nucleation of a decracks and in fatigue loading, is when we have a oscillating sort of stress field that means, it changes sign or could actually go through an up and down. And in that case, dislocations could move and come to the surface, cause surface steps, which actually could act like surface intrusions, surface extrusions, which would actually act like cracks. So, in other words, the very process of dislocation motion, which is of course happening by slip at the microscopic level, can give rise to a macroscopic kind of a crack. Or as slightly largest scale microscopic kind of a crack, which is related to fatigue cracks then, also play a important role in a creep and related phenomena.

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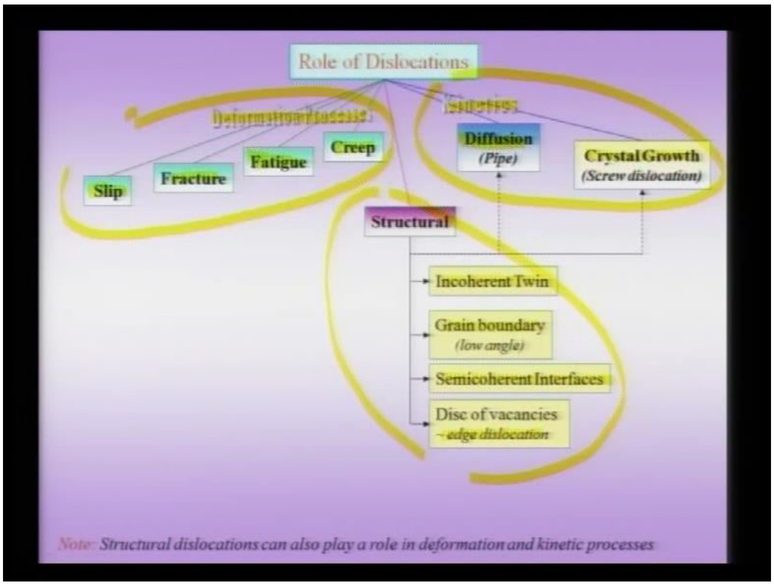

Role of Dislocations

Slip

Fracture

Fatigue

Creep

Diffusion
(Pipe)

Crystal Growth
(Screw dislocation)

Structural

Incoherent Twin

Grain boundary
(low angle)

Semicoherent Interfaces

Disc of vacancies
~ edge dislocation

Note: Structural dislocations can also play a role in deformation and kinetic processes

So, dislocations have obviously a very important role in deformation process, but we should also know that, for instance they also play very important role in kinetic process. Like for instance, in diffusion and validly talked about these aspects, the diffusion and crystal growth. So, they can actually as we saw, perform a constructive role like in crystal growth. As you said, defects can be classified as structural and non structural defects or statistical defects.

Structural role of dislocations are also very important, for instance they can play structural role in coherent twins in a low angle grain boundary and there are two kinds of low angle grain boundaries, as we shall see in the next chapter, which will be on surface defects like they will be the tilde boundary and twist boundary. And in both these cases, they are dislocations are responsible for that tilt on the twist, they play very important role in semi coherent interfaces.

And as usual see for instance, when you have a disk of vacancies on a slip lean or a certain crystallographic plane then, they can be thought of as an edge dislocation. So, we can see that, not only dislocations have very important role in deformation processes like in the left of the slide, they have very important process in various kinetic roles and they have very important role in structure of material, the structural role. And some of these examples of the structural role, we will actually take up during these set of lectures.

Yes question.

Student: ((Refer Time: 12:49))

Good question, we will perhaps come to little later, this question of what role they play in cell growth. Yes, they can actually, because when edge dislocation leaves a surface of crystal for instance then, they can provide high energy side perhaps, which would be good for an add attempt to actually add ((Refer Time: 13:09)) to. But, that role is much limited as compared to the role of screw dislocation and crystal growth, but they clearly provide the very preferred side for the add attempt to attach to.

So, in this case, screw dislocation is very clear, but dislocation is also could provide a high energy area, where heterogonous nucleation could actually take place of the add attempt that means, the nucleation of the surface step could start over there. But, of course, we should note that, when they are defining certain kind of dislocation, structural dislocations, these dislocations also can play a role in deformation and kinetic process, that should not forgotten.

This visualization or this classification is for better understanding of these kind of defects in their various roles. But, even suppose, there is you had a low angle grain boundary, wherein array of dislocations, some of dislocations also could leave the grain boundary and play a role in plasticity or these grain boundary could pick up more dislocations than actually increase the tilt angle. So, both these cases are possible in other words, their role would extend beyond just being a mere structural unit.

So, this over view slide I would have told you, the importance of dislocations in diverse kind of material behavior and material structure. So, that is what is a key, perhaps is most important slide in this whole, what do you mean course and this overview slide has to kept in a mind when you dealing a dislocations. Now, we had mentioned that, dislocations play a very important role in plasticity that means, suppose I take a rod of copper and bend it, so it bends easily.

And if I take a rod of steel and bend it, I will find it is little more difficult to bend a rod of steel. So, for the questions I can ask is, first of all is that, why this is so, but the kind of deformation that means, irreversible deformation. That means, when I remove my stresses, the deformation, the bending is still remains and that is what I call plastic deformation.

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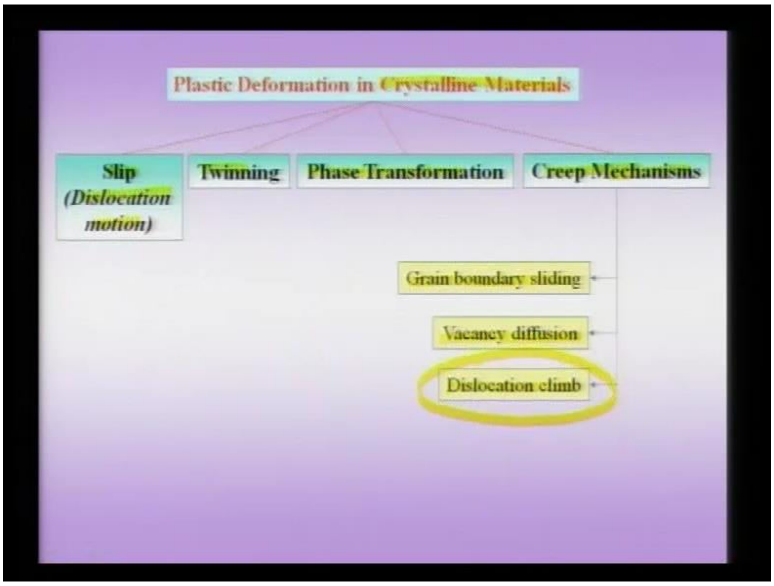

Plastic Deformation in Crystalline Materials

Slip *(Dislocation motion)*

Twinning

Phase Transformation

Creep Mechanisms

Grain boundary sliding

Vacancy diffusion

Dislocation climb

And the primary agent responsible for most of the cases for plastic deformation is dislocation motion or motion of a large number of dislocation and this is called plasticity by slip. But, we should not forget that, even though this might be there common mechanism in our many other cases we often consider, that there other mechanisms plastic deformation, which could play a, for instance predominant role under certain circumstances.

And these includes twinning, phase transformations and there are many creep mechanisms, which also can lead to permanent deformation, which we can call plastic deformation. And this is what, we may call the plastic deformation material of crystalline materials, could have a whole set of plastic deformation mechanism for partially crystalline materials or even amorphous materials. For instance, I am taking about BCC material at very low temperatures then, plasticity by slip could be very limited.

And in those cases, twinning plays a very very important role in giving rise to whatever deformation that I observe, so twinning can play very impotent role in plasticity. Phase transformation for instance, again as you know, can even play very important role in actually strengthen materials, inhabiting the role of cracks in materials, but they also can be responsible for the plastic deformation. Suppose, I had a single crystal, which course from cubic face to a tetragonal face then, this would be obviously be accompanied by a certain shape change and this would be permanent irreversible plastic deformation.

And this could even be caused by temperature as you know, so we need to keep this other point in view, because often we will be talking about plastic deformation as if it is synonymous with slip. That means, the role of dislocation would be perhaps the most important one we will considered to often. But, we should not forget that, there other mechanisms of plastic deformation and these other mechanisms could actually play a very important role in certain other circumferences.

And these other mechanisms just for a revision are twinning, a phase transformations and creep mechanisms and these creep mechanisms could involve grain boundary sliding, vacancy diffusion and dislocation climb. And so, you can see that, even with in creep mechanism, there is a role for dislocations with regard to, the way the creep takes place. So, with these two important over view slides, first the role of dislocations and the various plastic deformation mechanisms.

We are in a position to actually take up the most important question perhaps, which or the most important mystery that actually dislocations let to solve. So, let us consider to understand this role of dislocations, they let us consider plastic deformation by shear. So, as I was defining, plastic deformation means, permanent deformation which remains in the material, when external stresses or external forces have been removed. So, in the absence of external forces, whatever strain remains in the material, that is the plastic strain.

So, typically for instance, suppose had a rod of metal, I pull it then, if I release the external load then, what would happens that, some of it would recover back, which is call the elastic deformation. But, the remaining of the rod would remain in the extended state, which is because of the plastic deformation. Under most circumstances, under normal circumstances as I pointed out, it is role of dislocations which causes this kind of plastic deformations.

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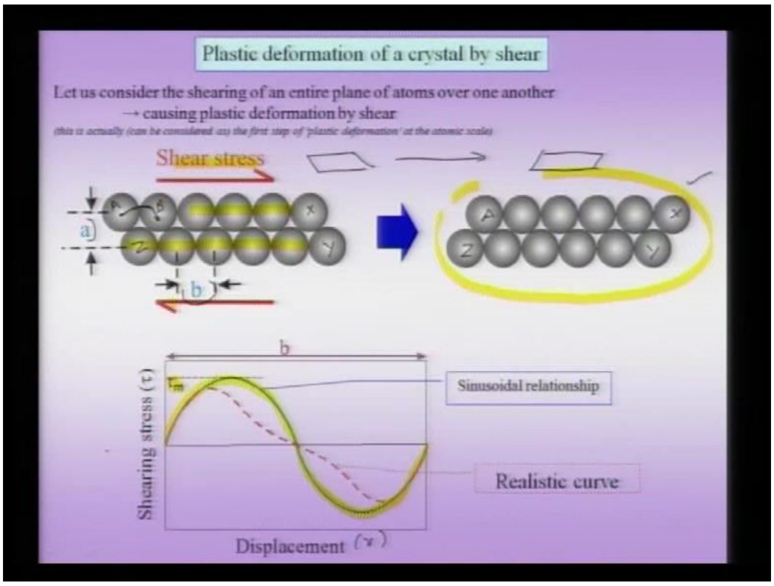

Plastic deformation of a crystal by shear

Let us consider the shearing of an entire plane of atoms over one another
→ causing plastic deformation by shear
(this is actually (can be considered as) the first step of 'plastic deformation' at the atomic scale)

But, going back historically, saying putting us backward 100 years back or 80 years back, it is a simplest way a plastic deformation can be conceived is actually, suppose you had a row of atoms as shown here and you apply some shear stress. So, what would happen is that, this row of atoms would slide into the new position, which is shown on the right hand side. In other words, this atom would actually climb and get into this new position.

So, this is an equilibrium position of this atom A for instance and this can actually climb over the other atom and get into equilibrium position, which is B. Means of course, as far as the macroscopic feature was identical, configurations of the crystal. But, the end suppose, now I consider my configuration is A X Y Z then, this new position would be A X Y Z. So, you can see that, this is been sheared, the shape has changed to this new kind of a shape as compared to this old shape, which was these two atomic planes.

So, if we have many rows of atoms then, this would go from this shape to this shape, so this can be thought of plastic deformation or if we want more accurate, more descriptive, this is actually the first step of, what we meant called a gross microscopic shape change or plastic deformation. So, if I want to consider the plastic deformation, wherein I am just shearing in one row of atom over another row of atoms, leading to a stable configuration as on the right hand side.

So, this is my stable configuration on the right hand side, wherein atoms are not going o further deform, but to go from configuration on the left hand side to the right hand side, I need to apply shear stresses. And we shall see this thing that, shear stresses play very important role at the macroscopic scale in causing plastic deformation. Now, if the spacing between the atoms, that inter planar distances a and now the inter atomic spacing along the direction is b then, you can see that, both of them remains same after the deformation has taken place.

Now, I can think of a force displacement curve or a shear stress displacement curve and displacement of course, in this case is being x then, I can think of shear stress displacement curve, which has a some sort of sinusoidal kind of shear. More realistic calculations are shown, actually it is not truly sinusoidal, but it is got a more complicated shape, but now we will assume sinusoidal kind of shape to illustrate a very important point.

So, that is my blue curve, which you can see here blue curve, this is the curve which is of course, in a sinusoidal fashion. important point we noted in this curve is that, initially we need to apply increasing amount of stress and afterwards, actually the whole process take place down here. And after some time as you know, it takes a negative value, in other words the system actually tends to fall into an equilibrium position after it has reached a maximum.

So, the important quantity in this entire deformation process is the maximum shears tau m, which I need apply so that, this configuration on the left hand side goes to the configuration on the right hand side. So, if I applied tau m shears then, I am guarantee, that the configuration on the left hand side goes to the configuration on the right hand side. So, assuming a sinusoidal kind of a relationship in the stress displacement and of course, I am taking about shear stress displacement relationship.

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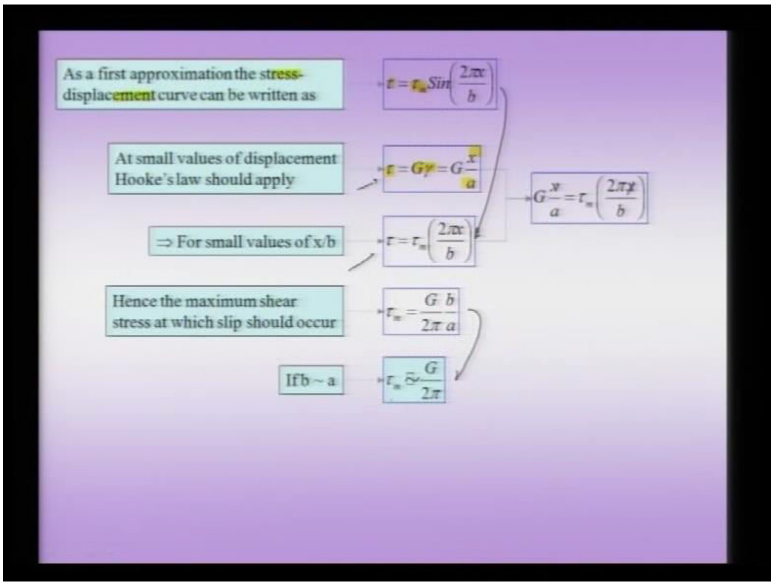

As a first approximation the stress-displacement curve can be written as $\tau = \tau_m Sin\left(\frac{2\pi x}{b}\right)$

At small values of displacement Hooke's law should apply $\tau = G\gamma = G\frac{x}{a}$

⇒ For small values of x/b $\tau = \tau_m\left(\frac{2\pi x}{b}\right)$

$G\frac{x}{a} = \tau_m\left(\frac{2\pi x}{b}\right)$

Hence the maximum shear stress at which slip should occur $\tau_m = \frac{G}{2\pi}\frac{b}{a}$

If b ~ a $\tau_m \approx \frac{G}{2\pi}$

Then, as to our first approximation, I can write the stress displacement curve as a sinusoidal function. That means, tau which is the shear stress I need to apply, is a function of tau m sin of 2 pi x by b, where b as pointed out is distance between the atoms along the direction of shear and x is the displacement, which I am talking about. So, I can write tau as tau m sin 2 pi x by b. At small values of displacement, I can assume that, Hooks law actually applies and I can write tau as G gamma, gamma being the shears strain.

And since gamma is again small, I can write it as x by a ((Refer Time: 22:27)) and X as you know, is a displacement and a is a inter planar spacing. Therefore, I can write, constructing a triangle in this direction for instances now, so this is my a direction, I can construct a triangle and it is my shear strain gamma and this is my X and this is my A. So, I can actually write it as G gamma, which G is x by a, for small values of x by b, which is what again I am talking about small stress strains that means, that this relation of the top can be reduced to the relation at the bottom, where tau is equal to tau m 2 pi x by b.

So, sin theta is been approximated to theta, putting these two relation together, one is coming of course, from Hooks law and other coming from the sinusoidal kind of behavior, which we assume for the stress displacement relationship. We can actually write the G x by a is equal to tau m 2 pi x by b, that is what I have done here, G x by a is equal to tau m 2 pie x by b. So, we can obliviously cancel out the x s on both the sides and we can write tau m is equal to G by 2 pi into b by a.

Now b is obviously of the order of a and therefore, since we are, in this whole calculation we are worried about an order of magnitude calculation, we are not interested in the details of the actual numerical values. So, I can actually replace, I can cancel out or we can make this approximately tau m, the maximum stress required for causing plastic deformation is G by 2 pi. Remaining also againm tau m is the maximum stress I required, I did not need to worry about other part of the curve, because after that it is spontaneously go downhill in stress.

Therefore, tau m is equal to G by 2 pi or I can approximate it even further and say that, tau m is of the order of G, where G is the shear modulus of the crystal. So, by considering shearing of two planes of atoms, which is giving me plastic deformation and by assuming as sinusoidal stress displacement relationship, I have would seen that, the maximum stress required to cause this plastic deformation, is of the order of the G.

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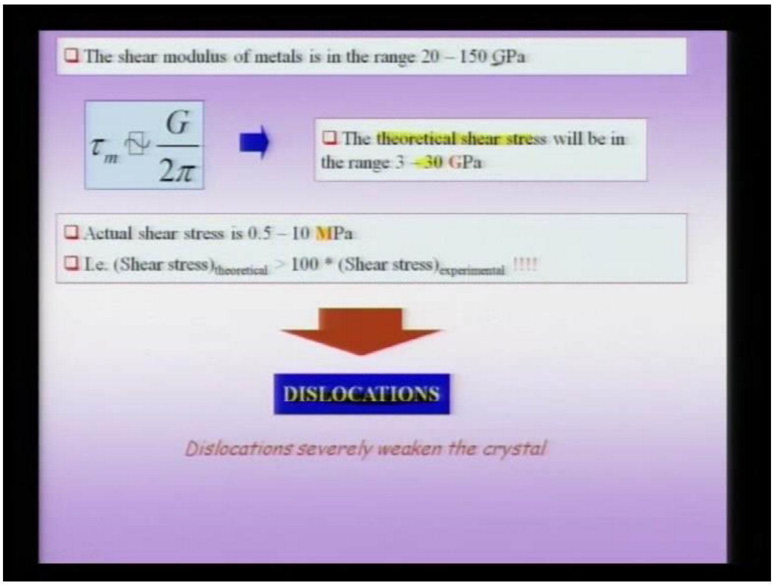

☐ The shear modulus of metals is in the range 20 – 150 GPa

$$\tau_m \approx \frac{G}{2\pi}$$

☐ The theoretical shear stress will be in the range 3 – 30 GPa

☐ Actual shear stress is 0.5 – 10 MPa

☐ I.e. $(\text{Shear stress})_{\text{theoretical}} > 100 * (\text{Shear stress})_{\text{experimental}}$!!!!

DISLOCATIONS

Dislocations severely weaken the crystal

The shear modulus of metal is typically of the order between 20 to 150 Giga Pascal and the important thing I need to note is the word Giga Pascal, so it is of the order of 10 power 9 Pascal, so 20 to 150 into 10 power 9 Pascal. Now, given the fact that, tau m is G by 2 pi, this theoretical shear stress will be of in the range of three3 to 30 Giga Pascal. Why do we call this theoretical shear stress, because the keyword here is theoretical shear stress, because I have theoretically calculated the shear stress required to cause plastic deformation by shear.

And now, this is in a perfect crystal in the absence of any kind of defect, that is obviously. I know I am not introducing any kind of defect in the material, I am actually shearing a crystal purely by applying shear stresses. So, the theoretical shear stresses now to cause this kind of plastic deformation, would be of the order of 3 to 30 Giga Pascal, so of the order of I would assume that it is about 10 Giga Pascal if you want. But, the key thing to note, it is of the order of Giga Pascal, so that is the key thing.

Now, when I do a measurement of actual shear stress of materials and low on behold, that the actual shear stress required to cause plastic deformation. Suppose, take a rod of aluminum or take a rod of copper or take a rod of iron and try to cause plastic deformation then, the shear stress comes out of the order of mega Pascal. So, clearly crystals are weaker at least by 2 to 3 orders of magnitude, as compared to the theoretical shear stress or the theoretical shear strength predicted.

So, often you notice that, the word strength and stress are used synonymously, whenever we say strength of material, we mean it is in the stress units, Newton per meter square. So, theoretical shear strength or the theoretical shear stress is of by at least 2 to 3 order of magnitude, as compared to the practical value that means, the experimentally measured value. For a long time, this is a begin mystery, long time meaning until the early 1930s, that why were crystals so weak.

Why is that, when I metaic make theoretical calculation, I get these shear stress out of the order of Giga Pascal. But, when I actually make a measurement of the shear stress required to cause plastic deformation, I find it out of the order of mega Pascal, clearly crystals are very weak. So, this mystery was finally solved in the 1930s as we shall see by Terror, Taylor, Coravan, Poliani. And of course, independently they have solved this mystery and the reason for behind the weakening of, this severe weakening of crystals is the presence of the defects, which we called dislocations.

So, the first and foremost most important role we need understand dislocations in materials is the severe weakening of the crystal in the presence of dislocations. And this is not just a mere factor of two weakening, it is a weakening by few orders of a magnitude, so that is what an important. And we note that, the shear stress theoretical is more than 100 times the shear stress experimental and dislocations are severely weakening in the crystal.

That means, that if I made a crystal without any dislocations, I would able to retrieve very high strength in the crystal. Of course, if I try to apply very stress of the order of Giga Pascal, what would actually happen is that, these stresses would actually nucleate dislocations in the material will lead to finally weakening of the crystal. But, even then, that the stress is required to nucleate dislocations are much higher than the stress is propagate them, which is the propagation of the dislocation, what causing plastic deformation.

Therefore, since an stresses for nucleation are much higher than the stress is required to move dislocations, which is giving me my plastic deformation, crystals without any dislocations are much stronger than crystals with dislocations. And actually crystals without dislocations have been formed and these are called viscous, very thin filaments which have absolutely no dislocations. And therefore, they actually very strong and we could actually go to very close to the theoretical shear strength of materials.

So, the first and foremost important lesson, which we have learnt is that dislocations severely weaken the crystal, of course this is a bad thing or is a good thing is a different question altogether and good or a bad depends on the context here. As usual, see suppose, I am one into form a component, I want to take a metal which is in the form of sheet and form it into a cup, so I am using a metal forming operation.

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For this kind of a metal forming operation, say semantically let me draw this, suppose I had a sheet here, sheet of metal and I wanted to form it in the form of a cup. So, this could be a, suppose slightly larger cup or of course, I could draw more schematic cup like this, so I need a dye and of course, I will punch this to form this cup. And in this case, I do not want to crystal be too strong, because I want to deform it at lower stresses. If the stress required to cause deformation is very large then, what would happen is that, of course, there would be other competing mechanisms like fracture.

So, the material will fracture actually, before it actually plastically deforms of course, even if no fracture, if the stress required is very high to cause this deformation then, I need to buy presses which are much higher in capacity, which is going to cause lot of money. And the tools will bear out much faster and therefore, in this context actually the weakening of the crystal is actually good. So, leaving aside the issue that actually is weakening of the crystal is good or bad, the fact we need to note is that, dislocations severely weaken the crystal and as we noted, they are the primary agent responsible for plastic deformation.

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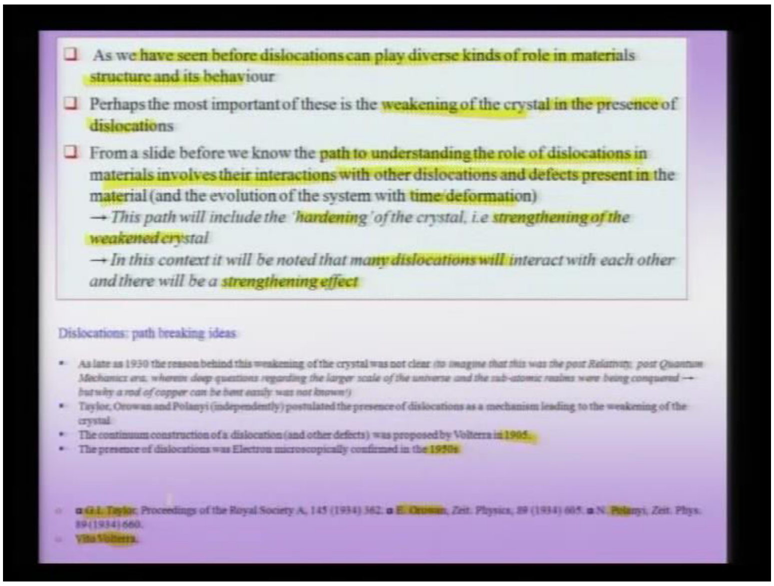

- ❑ As we have seen before dislocations can play diverse kinds of role in materials structure and its behaviour
- ❑ Perhaps the most important of these is the weakening of the crystal in the presence of dislocations
- ❑ From a slide before we know the path to understanding the role of dislocations in materials involves their interactions with other dislocations and defects present in the material (and the evolution of the system with time/deformation)
  → *This path will include the 'hardening' of the crystal, i.e strengthening of the weakened crystal*
  → *In this context it will be noted that many dislocations will interact with each other and there will be a strengthening effect*

Dislocations: path breaking ideas

- As late as 1930 the reason behind this weakening of the crystal was not clear *(to imagine that this was the post Relativity, post Quantum Mechanics era, wherein deep questions regarding the larger scale of the universe and the sub-atomic realms were being conquered → but why a rod of copper can be bent easily was not known!)*
- Taylor, Orowan and Polanyi (independently) postulated the presence of dislocations as a mechanism leading to the weakening of the crystal
- The continuum construction of a dislocation (and other defects) was proposed by Volterra in 1905.
- The presence of dislocations was Electron microscopically confirmed in the 1950s

G.I. Taylor, Proceedings of the Royal Society A, 145 (1934) 362. E. Orowan, Zeit. Physics, 89 (1934) 605. N. Polanyi, Zeit. Phys. 89 (1934) 660.
Vito Volterra.

So, to proceed to the next level, we have seen that, dislocation can play a diverse kind of roles in material structure and it is behavior. And structural role of course, we will take up little more later on and the most important of these you noted is the weakening of the crystals in the presence of dislocations, so that is an important thing we noted. We also noted from the previous slide, that the path to understanding dislocations in materials involves their interactions with other dislocations and defects present in a material, so these are the important thing we are noted so far.

And the evolution of the whole defects structure with time and with deformation. So, it is not like a defect structure is constant, dislocations are moving, they are leaving the crystal, their interaction between dislocations and their fresh dislocations being created, there are other kind of point defect being created, so the whole dynamic picture is evolving in time and obviously, this time is a time scale of the deformation.

In this whole process, we will see that, actually the material gets harder, so there is something known as strain hardening that means, crystal gets harder and harder, as you cause plastic deformation. And this itself is actually very surprising aspect, though perhaps you will not take up this point in this course. And this hardening is very interesting thing, because when you had a single dislocation, the crystal became weaker or a few dislocations of material, the crystal became weaker.

And as plastic deformation proceeds that means, you say for instance, there is a tensile rod, you pulling at and you causing larger and larger plastic deformation then, you would notice, that the crystal actually, the material actually gets stronger and stronger and this effect is pronounced in poly crystalline materials. Now, this hardening of materials is, because of more and more dislocations are being generated during the deformation. That means, the dislocations density is increasing and we know the units of the dislocation density, it is length of dislocation line in a volume of material.

So, as the dislocation density is increasing, the interaction between dislocations becomes more frequent, the interaction of dislocations with point defects with grain boundary and other defect become more frequent and this process leads to actually the strengthening of the crystal. So, a single or few defects is bad for crystal, it causes weakening, but we could when this thing was further, actually you see there is a strengthening of the crystal by the presence of many dislocations.

So, this good analogy perhaps or a some sort of crude analogy for this would be, suppose you had a road and few cars, these cars can actually escape very fast, they can drive very fast on the road, but too many cars, there will be a traffic jam. So, something like that, when there are too many dislocations, they interact with each other. This actually leads to the strengthening of the crystal and actually this is one of the techniques, in fact used for strengthening of a crystal, which is the method of work hardening or work hardening of the material by plastic deformation.

So, this hardening effect is coming by the interaction of multiple dislocations and this is one of the reason, why we want to consider the collective behavior dislocations and their interactions. So, before we proceed to the next slide, as I pointed out, there was some many impotent path breaking ideas, which came with the proposed dislocation theory. So, but the most surprising thing was that, the whole idea of that dislocation came with Taylor, Coravan and Poliani in the 1930s.

And this of course, I am talking about the concept of crystal dislocations, which came of course, considerably after the concept of something known as continue dislocation, which came from Vitovaltran in 1905. And we will take up that concept little later, but the surprising thing is that, till 1930s which is of course or the early 1930s, wherein people understood contribution of quantum mechanism.

They understood the sub atomic relb, they understood the revolution of galaxies, they understood relativity, they could in predict, what was the beginning of the universe, but they could not understand, why a rod of copper could be bend so easily. Because, we saw that, theoretically calculations tell you, that the rod of copper is much weaker in practice, as compared to a theoretical calculation and this was not explained for a long time. So, this is very surprising, but these three scientist came up with the model of the dislocation in 1930.

And in 1950s, this concept of dislocation was electron microscopically confirmed, the presence of dislocations were confirmed it using an electronic microscope. So, some of the path breaking ideas on dislocations came between about 1930 and 1950. And this include the concept of crystal dislocation, but we will also consider something the Volterras dislocation, which is a continuum concept of a dislocation.

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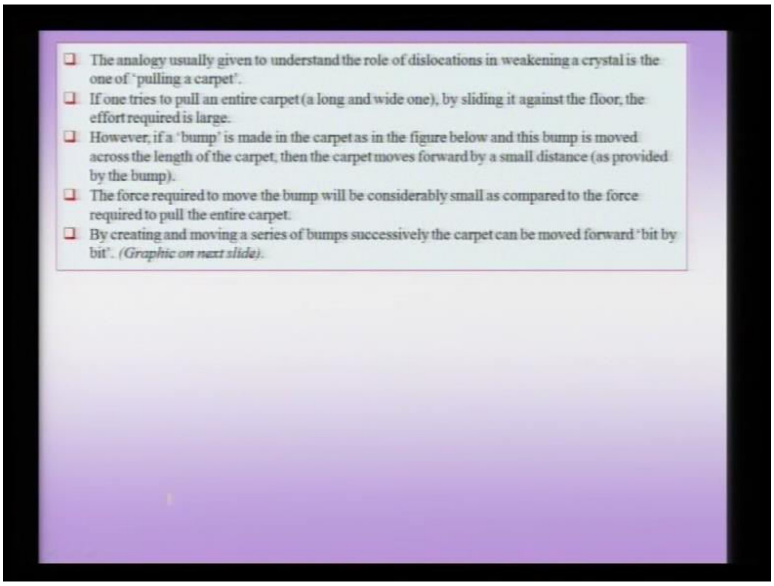

- ❑ The analogy usually given to understand the role of dislocations in weakening a crystal is the one of 'pulling a carpet'.
- ❑ If one tries to pull an entire carpet (a long and wide one), by sliding it against the floor, the effort required is large.
- ❑ However, if a 'bump' is made in the carpet as in the figure below and this bump is moved across the length of the carpet, then the carpet moves forward by a small distance (as provided by the bump).
- ❑ The force required to move the bump will be considerably small as compared to the force required to pull the entire carpet.
- ❑ By creating and moving a series of bumps successively the carpet can be moved forward 'bit by bit'. *(Graphic on next slide).*

So, how do I understand in a more common sense way, the weakening of a crystal in the presence of dislocations. So, that is the first question I am asking myself, that of course I know that, crystal is being weaken by the presence of dislocations by comparing the theoretical result with the external result. But, the common analogy, which is given to understand is weakening of the crystal is the one of a pulling of a carpet. So, suppose I have carpet, which is a two dimensional carpet and I assuming a very large carpet and it covering a large surface area and I am trying to pull this carpet.

So, if I pull it by sliding along the floor then obviously, the friction between the carpet and the floor is going to give me some resistance. So, the effect, if the carpet is pretty larger, assuming the carpet as thick carpet is as large as a room or bigger than a room then, the effort required will be pretty large.

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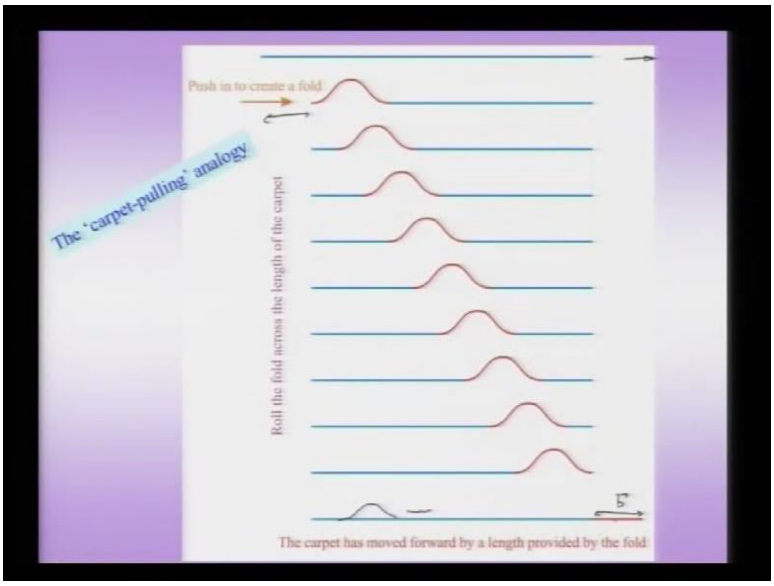

The 'carpet-pulling' analogy

Push in to create a fold

Roll the fold across the length of the carpet

The carpet has moved forward by a length provided by the fold

Now, so the first thing is that, I have a carpet and I am trying to pull this carpet on to the right hand side. So, I am trying to do pull this carpet on the right hand side and I would found, find that the stress required is very large. In the alternative, is to actually create a small fold, which you can see, as which is shown in the red. And then, this small fold or a bump and is can be moved across the length of the carpet and at any point of time, you would notice that, I am not pulling the entire carpet, I am just moving the bump along with the carpet.

So, I take bump in the carpet and this small bump, I slowly moved forward and you notice that, if I try to do this, at each point of time, the stress required to move this bump is actually much smaller than to move the entire carpet. So, when I move this bump across the carpet and finally, when the bump leaves a carpet on the right hand side, I get a little extra length, which is because of the fold, which was originally created, so I have a length which is moved to the right.

In this process of course, I am not moving the entire carpet in one step, but has broken down the problem moving a carpet into small steps of creating bumps and rolling the bumps over to create the small steps. Later on we will see that, this has very close analogy with dislocation motion and this later on, this step which is been created, would be called burger vector. So, later on we will see this, now suppose I have moved the carpet little distance and this is now be, I can do the process again, I make another fold in my carpet and move that forward and slowly, I can move the whole carpet forward.

But, the whole process now takes much less effort from you, as compared to a single effort of moving the entire carpet. So, this is the common analogy given between, how dislocations weakens a crystal and how for instance, pulling of carpet can be done with a less effort in the presence of these bumps, which are roll forward. So, before we actually take up the dislocation in a crystal, just of course, is a most important what you meant call consideration here, we will take up a continual description of a dislocation.

So, this was done as a pointed out in 1905 by Vitovaltran and this is called the continuum concept of a dislocation.

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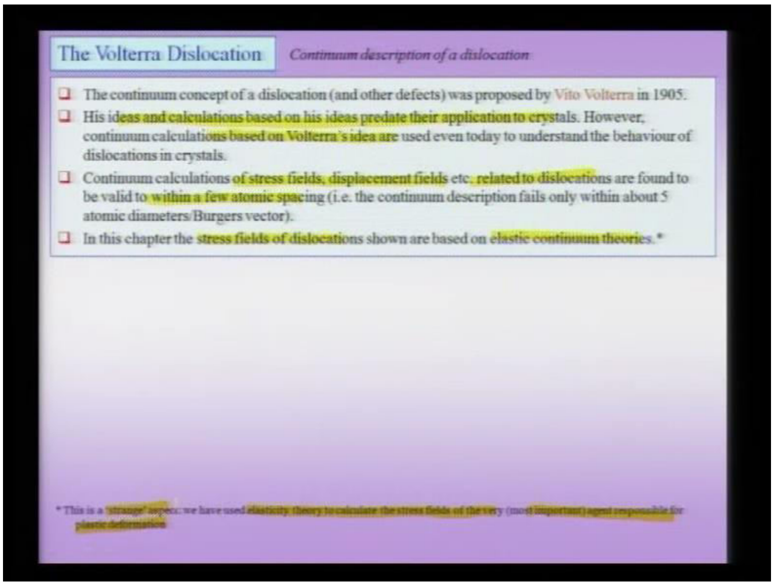

The Volterra Dislocation *Continuum description of a dislocation*

- ❑ The continuum concept of a dislocation (and other defects) was proposed by Vito Volterra in 1905.
- ❑ His ideas and calculations based on his ideas predate their application to crystals. However, continuum calculations based on Volterra's idea are used even today to understand the behaviour of dislocations in crystals.
- ❑ Continuum calculations of stress fields, displacement fields etc. related to dislocations are found to be valid to within a few atomic spacing (i.e. the continuum description fails only within about 5 atomic diameters/Burgers vector).
- ❑ In this chapter the stress fields of dislocations shown are based on elastic continuum theories.*

* This is a 'strange' aspect: we have used elasticity theory to calculate the stress fields of the very (most important) agent responsible for plastic deformation

In this case, there are no atoms, there is no crystalline order, which we are considering, it is just a material, which is a simple smooth continuum. But, the important thing to note is that, his ideas and calculations and many of the things, which we are proposed actually which predate their application to crystals. But, even today, the continuum calculation based Volteras ideas are very important for us to understand stress fields and the behavior of dislocation in crystals.

So, some other behaviors of dislocations and often the collective behavior of dislocations is that, these stress fields and displacement fields etc, which are related to dislocations, are found to be valid within a few atomic spacing or to be precise within a few burgers vectors and the continuum theory only breaks on very very close to the dislocation line. So, even though we know that, dislocation resides in crystal and it is a crystallography defect, but continuum ideas can give us a very important understanding of dislocations, especially the stress fields or motions and even their collective behavior.

And the continuum theory only based on very very close to the dislocation line and which is about 5, some people said 5 and some people it may considered it 1 burgers vector, but a few atomics spacing from the dislocation line. So, and you will notice that, the stress field which will be coating in this chapter are actually derive based on the elastic continuum theories. So, and this is a very very strange aspect as we shall say, because we used, the elasticity theory has been used to calculate the stress fields of the most important agent, which is responsible for plastic deformation.

So, we are using elasticity theory to calculate the stress fields of a dislocation, which is the agent primarily responsible for plastic dislocation. So, this is a very strange, but important defect.

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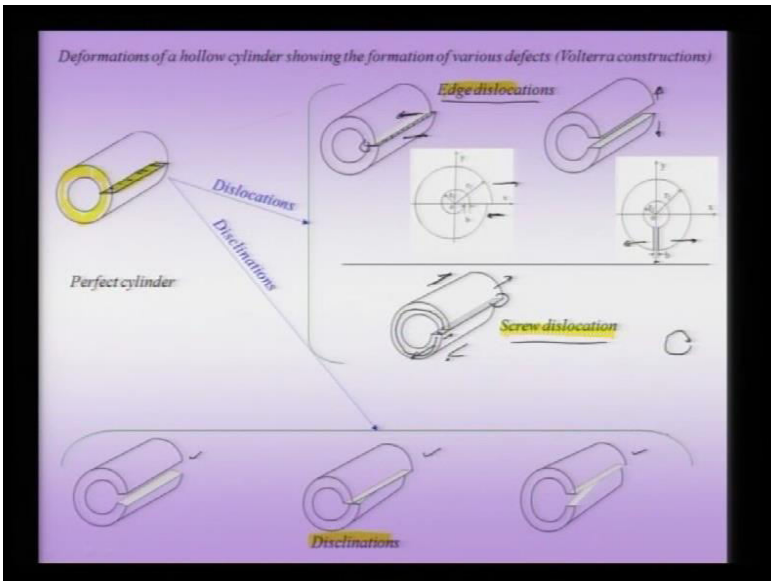

Deformations of a hollow cylinder showing the formation of various defects (Volterra constructions)

So, what is the Volteras picture of dislocation, in Volteras picture you take hallow cylinder that means, take a cylinder wherein, there is a material here and I try to make a cut in this cylinder, which is shown by this grey area. So, this my grey area, wherein I make cut in the cylinder, so this hallow cylinder, which I make a cut. And after making the cut, I make various deformations to the cylinder and swill only consider the important ones from this perspective dislocations, in fact you can actually produce edge dislocation, screw dislocation and declinations based on the idea of Voltera.

So, how can edge dislocation be made, if when actually slide push in one part of cylinder with respect to another part of the cylinder. So, I can push in this part, so how did you do that, since now the cut has been made. So, you can push in this part, the upper part with and pull out this part and you will make a small step, which is step here and this is one way of creating an some sort of an edge dislocation. Other way of creating edge dislocation is actually pull this through apart, so you will get an edge dislocation.

So, in the two dimensional picture you can see that, in this case, you actually pulling apart and we creating a small displacement b between the two, five sides of the cylinder. And in the case of the other case, actually you are pushing in this part, for instance this is of course, inverse of this picture which is shown in above. But, any other, the concept is same, we pull out this part and pull in this part and therefore, you create an edge dislocation.

And correspondingly, the inner part also will move, the inner free part also will move and which will create a step inside. In the case of screw dislocation, so you do not push and pull the weights done here, you actually slide one part that means, you pull the upper part and shear the lower part, so it is some sort of sharing motion. So, you apply a shear on the cylinder, one of the top and the bottom, to actually create a step, now which is here then, correspondingly there will be a step in this side also.

So, I am using a cylinder, making a cut and after the cut has been made, I slide one part of the free surface with respect to the other and that is done by shearing force. So, I can create things, which we shall see have an analogy in crystals, but this is basically the continuum edge dislocation and the continuum screw dislocation. So, let we go, where this slide, because this is perhaps often not discuss in detail in the crystallographic or crystal description of a dislocation, herein we start up perfect cylinder and perfect hollow cylinder, in this we make a cut here in separate out the two phases.

So, I made cut here and therefore, now I have got two free surfaces here, after wards I do deformations to the cylinder, either by pushing in the top with respect and pulling the bottom to create a step along the length of the dislocations. So, I got a step here or I can pull apart the two phases like this, to create a opening and it is clearly seen in the two dimensional version of the figure, wherein we pulling apart these two to create a opening here and these two correspond to edge dislocations.

If you want to make a screw dislocation, you actually you shear forces and why it is called as screw dislocation, because of the way the planes are or suppose, when you actually uses screw driver to thread in screw, you notice when you go in a clock wise direction, you go one plane inside. So, that is what is happening here, you start from this point and after the deformation is done, as you go round, you land up not in the same place, but deform, there is a small displacement with the original.

So, actually if we take in your slices of the this planes, they will go spirally inward, so this is what we meant called a right handed screw, we could of course create a left handed screw also. So, there other defects, which you can create using Voltera construction and these are the disclinations which are shown briefly here, we will not take up these in this case, but in the context of crystallographic defects, we mention that, these desclinations are associate with rotational symmetry.

So, we can see that, it not only create dislocation, but you can also create these kinds of disclinations in using the Voltera cylinder.

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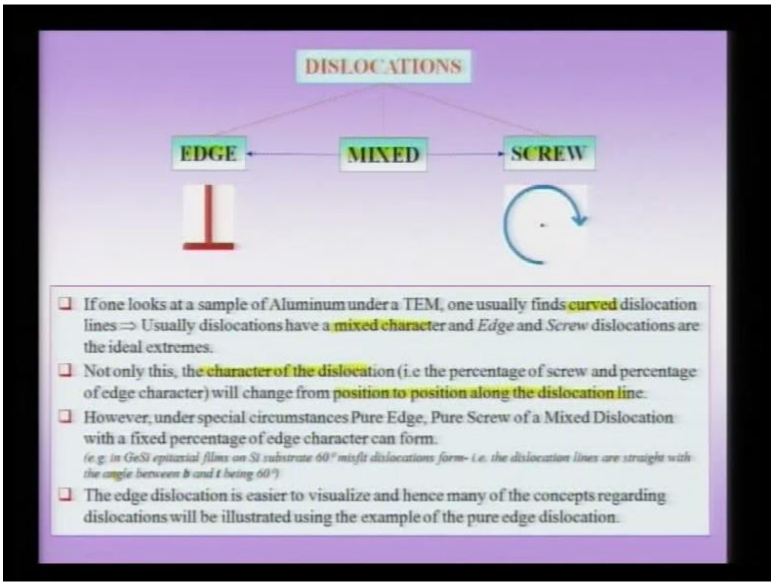

DISLOCATIONS

EDGE ← MIXED → SCREW

- ❑ If one looks at a sample of Aluminum under a TEM, one usually finds curved dislocation lines ⇒ Usually dislocations have a mixed character and *Edge* and *Screw* dislocations are the ideal extremes.
- ❑ Not only this, the character of the dislocation (i.e the percentage of screw and percentage of edge character) will change from position to position along the dislocation line.
- ❑ However, under special circumstances Pure Edge, Pure Screw of a Mixed Dislocation with a fixed percentage of edge character can form.
  *(e.g. in GeSi epitaxial films on Si substrate 60° misfit dislocations form- i.e. the dislocation lines are straight with the angle between **b** and **t** being 60°)*
- ❑ The edge dislocation is easier to visualize and hence many of the concepts regarding dislocations will be illustrated using the example of the pure edge dislocation.

Now, we come to the most important part of this whole lectures, which is the dislocations in the crystallographic crystal, which is we shall see two type basically, the edge dislocation and the screw dislocation and which bare close resemblance to the edge and screw dislocation as described by Voltera. And we had mention that, if we do a Voltera construction actually, which is now continuum construction, we could actually get and try those constructions to actually calculate the stress field and strain fields.

You can actually get the stress fields and strain fields in the crystallographic dislocation or the crystal dislocation. And of course, I told you that, these calculations we valid within a few burgers vector, which is very close to a dislocation line. So, dislocations suppose, I typically look at a sample of aluminum, I take a material aluminum and I thin it down to less than about say about 1000 angstroms and look under transmission electron microscope.

So, typical sample of aluminum will consist of lot of dislocations and you notice that, these dislocations are not straight, but actually they are curved, so typically these dislocation lines will not be straight and they will be curved. So, these curved dislocation lines are nothing, have a mixed character that means, they are neither pure edge or nor pure screw. So, the ideal description of a screw and edge dislocations are nothing but, extreme descriptions and in most cases, you will actually find only mixed dislocations.

So, the norm is the mixed dislocation, the ideal ends, the edge on the screw or the way is understanding is mixed dislocation, based on these extremes. But, in this course, we will spend lot of time and trying to understand the edge dislocation, which is easier of the two to understand. This screw dislocation slightly more difficult to understand and we will have models to actually show, how the displacement field of these dislocations are, how the planes are, but nevertheless the screw dislocation is more difficult to understand, as compare to the edge dislocation.

And once I understand these two extreme forms of dislocation then, we can make an attempt to understand this more complicated version of dislocation, which is the typical mixed dislocation. And why do you need to understand in this mixed dislocation, because typically you find that, any dislocation of any material will have mix character and not only that, any curved dislocation will have this character changing from point to point.

In other words, from position to position on the dislocation line, the character of the dislocation will change that means, how much edge character it has got, how much screw character it has got, will keep on changing, as you go from point to point along the curve dislocation line. There are special circumstances, in which you will actually find a fixed character of a edge or a screw or even a pure edge or a pure screw.

And this of course, can be found in pure tilt boundaries, wherein you see that, the pure tilt boundary, small angle tilt boundary can be visualized, which we will do of course, later in this course, can be visualized as an array of edge dislocations. And a pure screw dislocation can be found in a twist boundary and similarly, for instance, if you want a fixed character of a edge and screw. And this can be found in an epitaxially grown GSI film on silicon substrate, wherein you find 60 degree mixed dislocations.

And this straight dislocations and the edge character, is what is been describe by the 60 degree, as we shall see later. So, you can have the special circumstances, pure edge, pure screw or what we might call a mixed dislocation of a particular character of edge. But, under normal circumstances, you will find that, the character is mixed and not limits, it is varying from point to point along the dislocation line.

So, we will take up the edge dislocation first, we considered it in detail, before we take up the screw dislocation. Because, many of the simple concepts can be understood using the edge dislocation, but this screw dislocation is slightly more difficult to understand.