

Nanostructures and Nanomaterials: Characterization and Properties

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Lecture - 17

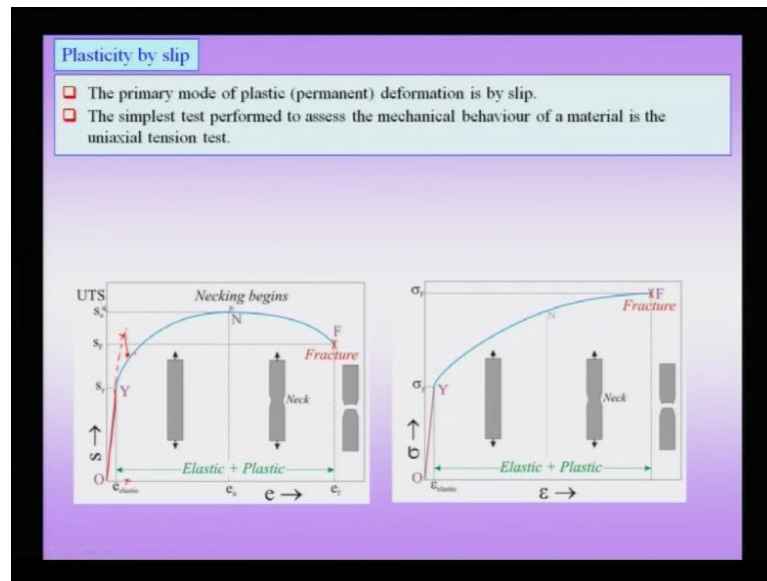
Defect Structure & Mechanical Behaviour of nanomaterials (C3)

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- Weakening of a crystal by dislocations (concept of theoretical shear strength)
- Motion of dislocations and plasticity by slip
- Dislocations in finite crystals: image forces
- Dislocations in nanocrystals
Strengthening mechanisms
- Image forces in nanocrystals: critical size for dislocation free crystals
- Effect of grain size on mechanism of plastic deformation (twinning versus slip)

When we float at tested diagram which is the result of a test we have noted that.

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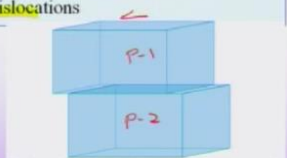


The curve the, this lineal portion of the curve which is from o to y does not continued to straight onward. But actually bends and we said this is, because of plasticity due to slip and I am talking about say a for a room temperature test on a material like a aluminum. And we wanted to understand, how does the slip take place and what is that which is weakening the crystal just in fact, trying to stop this curve from going upward that meant a materials at for instant a strange as this much is not a strong. But it is the actually we curve by this amount.

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Weakening of a crystal by the presence of dislocations

- ❑ To cause plastic deformation by shear (*all of plastic deformation by slip require shear stresses at the microscopic scale**) one can visualize a plane of atoms sliding past another (fig below.**)
- ❑ This requires stresses of the **order of GPa**
- ❑ But typically **crystals yield at stresses ~MPa**
- ❑ ⇒ This implies that 'something' must be **weakening them drastically**
- ❑ It was postulated in **1930s** and confirmed by **TEM observations in 1950s**, that the agent responsible for this **weakening are dislocations**



Shearing of a whole part of a crystal with respect to another

* Even if one does a pure **uniaxial tension test** with the tension axis along the z-axis, except for the horizontal and the vertical planes all other planes '**feel**' shear stresses on them

© By Taylor, Orowan and Polanyi

So, this is the weakening of crystal in the presence of dislocations. Now suppose, I want to understand plastic deformation or permanent deformation I have 2 crystal; 2 parts of a crystal for instance this is part 1 and this is part 2. And I can share 1 with respectively other by applying a shear force. Now, when I apply such a shear force then the crystal may shear.

But if we look that kind of stresses required to cause this kind of a plastic deformation it, if in sourced we of the order of GPa which we will slide again in the next slide and it is the important note that all plastic deformation by slip requires shear stresses at the microscopic scale. You will do any axial tension test at the microscopic level we are actually applying a entail force.

But it is the microscopic level shear stresses are required for plastic deformation to take place by slip. But if we noticed we already seeing that, difficultly crystal seeds of the order of Mega pascals this could be tense of 100s Mega Pascals. So that means, a something's this is weakening the crystal plastically and in 1930s Taylor and Orowan and Polyani consulate that it is dislocations theoretical concept of the stage which is weakening the crystal.

So,, then late tem observations in 1950s proved that is actually indeed dislocations which are weakening the crystal. And which is at part of the plasticity at the micro scale and this important fact the given though and uniaxial tension test as we did before the except for the vertical and horizontal axis all thing in plane feels. So, a vertical or horizontal planes all the other in planes feels actually feel a shear stresses therefore, slip is possible.

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

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

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

Actual shear stress is 0.5 – 10 MPa (experimentally determined)

I.e. (Shear stress)_{theoretical} > (~)100 × (Shear stress)_{experimental} !!!!

DISLOCATIONS

Dislocations severely weaken the crystal

- Whiskers of metals (single crystal free of dislocations, Radius = 10^{-6} m) can approach theoretical shear strengths
- Whiskers of Sn can have a yield strength in shear $\sim 10^{-2}$ G (10^3 times bulk Sn)

Now, if we will got a some of the important things pointed out in the previous slide. This shear modules of crystal is in the range of 20 to 150 GPa and if we use a complete shearing of 1 part of the crystals with respect the others. The maximum shear is required for that composed the order of G by 2 pie which means, it is a range of 3 to 30 GPa and actual in shear stress of the order of 10 MPa order of those that number.

This implies the crystal is actually much weaker compared to the theoretical sharing of the crystal sharing mechanisms which will proposed originally for sharing of the crystal. So, this implies a something dislocation severely weaken the crystal and this is the dislocations which are weaken the crystal. And this also implies suppose, I make a crystal which is completely this is completely free of dislocations.

So, this has been done and this is been done in small cylindrical specimen which are

known as whiskers. And radius of these whiskers in a microns scale, there need a observed that actually you can approach near to the theoretical shear strength. In these case, you load a whiskers what really happens is that dislocations have to be nucleated, and therefore dislocation nucleates then this strangely crystal drastically falls down. In fact, whiskers have strengthen shear of about 10 per minus 2g which is about 1000 times stronger than bulk in crystal. Now, later on the concept of nano crystal we will see how some of these be realized and how the some of these dislocation free concepts comes spontaneously. Then, you go to the nano scale therefore, dislocations are and if there no dislocations to co-plasticity and which I mean plasticity by slip. Then, the crystal can actually be very, very strong.

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Motion of dislocations and plasticity by slip

- ❑ Plastic deformation by slip occurs by the motion of dislocation and their leaving the crystal.
- ❑ Dislocations *may* move under an externally applied stress
- ❑ At the local level shear stresses on the slip plane can only drive dislocations
- ❑ The minimum stress required to move a dislocation is called the Peierls-Nabarro (PN) stress or the Peierls stress or the Lattice Friction stress (*i.e.* the externally applied stress may even be purely tensile but on the slip plane shear stresses must act in order to move the dislocation)
- ❑ Dislocations may also move under the influence of other internal stress fields (*e.g.* those from other dislocations, precipitates, those generated by phase transformations etc.)
- ❑ In any case the Peierls stress must be exceeded for the dislocation to move
- ❑ The value of the Peierls stress is different for the edge and the screw dislocations
- ❑ The first step of plastic deformation can be considered as the step created when the dislocation moves and leaves the crystal
→ "One small step for the dislocation, but a giant leap for plasticity"
- ❑ When the dislocation leaves the crystal a step of height " b " is created → with it all the stress and energy stored in the crystal due to the dislocation is relieved

Move about the motion of dislocations in the chapter on plasticity

Let us, mention take up of few points regarding motion of dislocations and plasticity by slip. Plastic Deformation by slip occurs by the motion and dislocation and their leaving the crystal, it is very, very important that the dislocation actually leaves the crystal. Dislocation may move under an externally applied stress that implies that I can actually move a dislocation, by applying an external force or it may also happen.

There are also, some internal stresses or spontaneous reasons while dislocations may also move. At the local level, shear stresses on the slip plane can only drive dislocations that

mean normal stresses are not responsible for moving dislocations. The minimum stress required to move a dislocation is called the Pearls Navarro stress and sometimes some other context also called Pearls Stress or the Lattice Friction Stress.

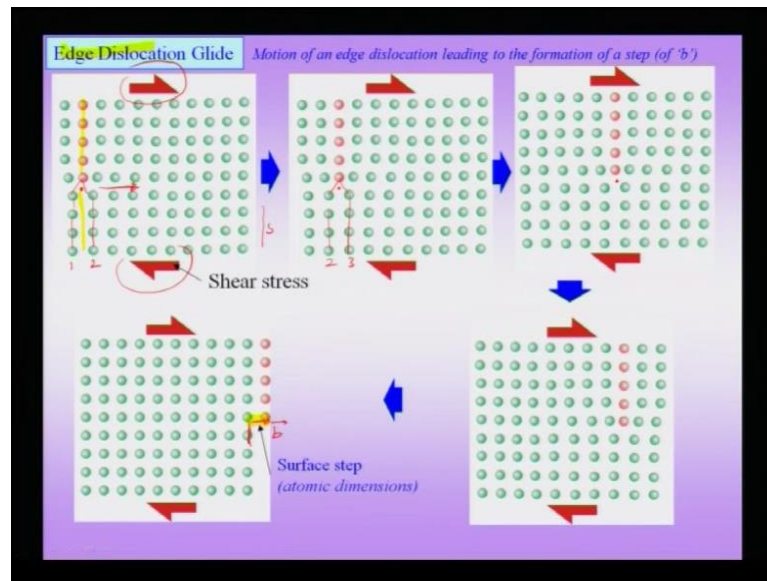
This is the minimum shears stress I have to apply a dormice level on the planes on the slip planes, so that plastic deformation can be initiated. In other words, if I apply on the microscopically off course, I may apply at force. But, then using the split I can actually calculate the shear stress on the slip plane which is nothing, but all resolve shear stress on the plane.

Then, when this resolve shear stress on the slip plane exceeds this Pearls Stress or the Lattice Friction Stress or the Pearls Navarro Stress, then that is location can be move and actually initiate plasticity. This location may also move under the influence of the other internals stress fields like for instance those arising from other dislocations, those arising from coherent precipitates, those arising due to phase transformation, those arising due to thermal mismatch at inter phases etcetera.

So, internal stress may also be responsible for moving these locations, but in any case the pearls stress must be exceeded. If slip has to be initiated at the microscopic scale to value of pearls stress is different from pure edge and pure screw components of a dislocation and this is very, very important. Because, you could have a crystal which is will as we shall see late of free of edge dislocations, but not free of screw dislocations.

The first step in plastic deformation can be considered as the step created when the dislocation moves. And leaves the crystal will have a graphic of this in the next line, but essentially the dislocation has to move and leave the crystal.

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And I am illustrate in this concept for the case on Edge Dislocation and Edge Dislocation can be thought of as an extra half plane in crystal or equivalently. And missing half plane as crystal as below, but never the less it is the edge location itself neither the extra half plane or the missing half plane. It is the reason between its the line between the 2 which have drawing systematically here in this diagram.

So, this is the dislocation going in to the plane of the board and when I apply a sheer force as shown here. And of course, here if you Terrence a region of crystal and then this externally applied or the resulting shier stress on the dislocation can cause it to move. And as you can see here, the dislocation is actually tending to move in this direction and that means, at this point of time you can if you label this plane 1 and plane 2 of these green a tabs below.

Then, this a tab is red plane which is just colored differently for easy identification is bonded to these, but at a later step you can see that it is actually bonded between 2 and 3 planes the green planes. Therefore, its location is moving under the shires stress and as it moves you can see that it is getting closer to this surface or you might call it surfaces. Then finally, you can see that it leaves the surface creating a small step and the value of this step is to burgers vector b which is a mixture of the strength of this location.

Therefore, if I have to cause plastic deformation then this location have to plastic deformation by slip. Then, this location has to move under the shear stress and finally of course, we have to leave the crystal. This is a core the full surface of the crystal of a single crystal, but then in a poly crystal and material it could actually go and reside in a grain boundary or main status looking neighboring grain.

It is important to note that, this is the first stage where all the energy of the dislocation has been dissipated when the step has been created. Because, this dislocation is associated with stress fields and these stress fields cost energy to the crystal. But when these step is formed, all the energy is and only of course, a little extra energy comes because of the formational step here which is in the form of surface energy.

Now, it is important to note that this is 1 small step for a dislocation, but a jointly for plasticity; all plastic deformation this small step which we are considering here when as I pointed out even the dislocation leads the crystallized step of height b is created with these all the energy. And stress stored in the crystal jurisdiction location and therefore, now the dislocation expresses itself as a vector what you might call a vector strength being on this as a surface of the crystal.

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Dislocations in finite crystals

Dislocations are attracted to free-surfaces (and interfaces with softer materials) and may move because of this attraction → this force is called the **Image Force**

$$F_{\text{image}} = \frac{-Gb^2}{4\pi(1-\nu)d}$$

Original Free-surface

Edge dislocation

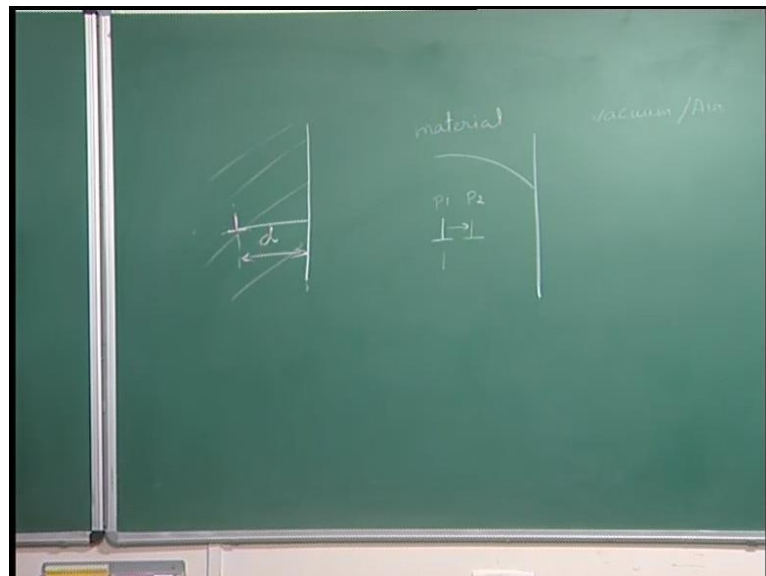
Image dislocation

$F_{\text{image}} \propto \frac{1}{d}$

If you look at dislocations in infinite crystals, then they have a certain stress field. And if I am only talking about a single isolated dislocation in an infinite crystal, such a dislocation feels no forces. Of course, you may want when you apply when you apply external forces that force may translate in to shear stresses at this slip plane level and it may feel illustrations.

But in the absence of external loading such a dislocation would feel no forces, but suppose I consider a dislocation in a semi-infinite crystal, when I mean a semi-infinite crystal I imply that the dislocation.

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So, there is material on the left hand side, there is no material on the right hand side. And the dislocation is positioned at a distance d from the free surface. This implies that this dislocation is not located in a symmetric way with respect to the material there is a certain asymmetry with respect to the right and the left. So, of course I will assume that the top and bottom are infinite for now.

Therefore, such a dislocation is asymmetrically positioned with respect to the material. And such a dislocation actually feels a force towards the free surface and this force is called an image force. And therefore, dislocations in finite crystals feel this can only feel

such kind of forces and this force is called Image Force. Because, to calculate this force what is done is that of course, you have this material here which is in blue color.

So, this is my free surface which is drawn here the original surface, then to calculate the force that this dislocation feels towards the free surface what I do is that I put an additional material on the right hand side; I put a fictitious dislocation exactly at the distance d at the fictitious material. So, of course on the same material or property has the blue material and now because, this is now positive edge dislocation, this is negative edge location.

These positive and negative dislocation feel of course, and that is why this is called an Image Force. In other words, it is the attractive force of a dislocation towards the free surface, and since I used a concept of an image dislocation to calculate the force I call it d Image Force. So of course, the reason that the dislocation feels towards the free surface is that now this is attraction free surface; that means there are no attractions.

Then, it is perfectly a free surface and this is my material and this is my Marque Moral and here is my dislocation. Now, the energy of the dislocation would decrease if it is positioned little closer for the free surface. In other words, dislocation is at position p_1 and it moves to position p_2 then the energy of the dislocation is lower. Because, if I look at the stress feels of dislocation then it is intense closer to the dislocation and it is weaker further away.

Here, the dislocation is closer to the free surface implies that more of the intense region that the dislocation have been revealed; that means, the energy of the dislocation is going to be lower. And therefore, continuously the energy of the dislocation will be lower as I go towards the free surface. And since radiant of an energy is actually the force; that means, the dislocation will free of course, towards the free surface We just called a Image Force.

Now, it is important note that this image force varies as 1 by d the image force here can be written as a function of 1 by b that Gb etcetera. And new are the material properties G is share modules and ratio and b is the strength of this vector. So, image force goes as 1

by d this of course, the classical formulas I will illustrated it for the case of an edge dislocation. But it is essentially to also for a case of screw dislocation it will feel a force toward to see free surface.

However, in the case edge dislocation in though the force this not changed, but there are issued related to cancelation to the fractions when you use an image constructions. So, now we use what we called concentrate on the force and notice that, when a dislocation is positioned in a so main it feels a force towards a free surface which is called an Image Force. And the value of the Image Force get intense and intense because of this course assumed it assumed of the as the dislocation position closer to the free surface.

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Image Forces in Nanocrystals

□ In nanocrystals more than one free surfaces will be in proximity to the dislocation → leading to multiple images. [1]

Image Force (F_{image}) (Edge Dislocation, Finite Domain)

$$F_{\text{image}} = \frac{-Gb^2}{4\pi(1-\nu)} \left[\frac{1}{d} - \frac{1}{L-d} \right] = \frac{-Gb^2}{\pi(1-\nu)} \left[\frac{2x}{L^2 - 4x^2} \right]$$

Superposition of two images

[1] "Image forces on edge dislocations: a revisit of the fundamental concept with special regard to nanocrystals" Prasenjit Khanikar, Anu Kumar and Asandh Subramaniam, Philosophical Magazine, 91, p.730, 2011.

Now of course, if I want to considered and nano crystals dislocation what will happen if I put this dislocation a nano crystal. In a nano crystal or small size crystal, it is obvious that there are multiple surfaces which are in proximity with a dislocation. Now, suppose this might this dislocation called a then originally edge force there is only 1 free surface here which a called S.

But now we there is a additional free surface in the left hand side, we can see here and this my glide plain of the dislocation where the dislocation came slip the middle plain.

Then, I have I now have 2 surfaces in this case s_1 and s_2 this implies I have to construct 2 images with respect to this free surface to actually calculate my image force. So therefore, there is 1 suppose this is my 1st edge dislocation, there will be 1 negative edge dislocation of this side is the surface at a distance of d . And there will be 1 more image on the left hand side at a distance of a same distance here, this distance is this surface as I called this.

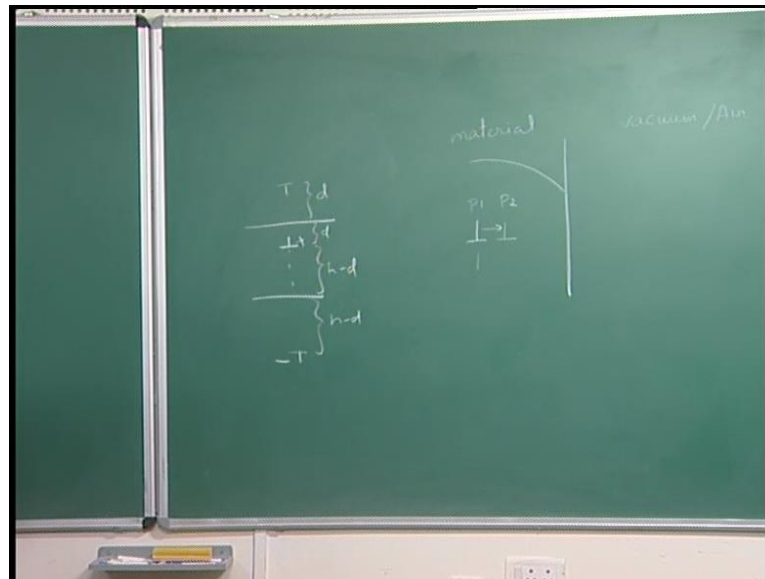
Now, at this x then this is also be x and therefore, I have 2 images and net force can be a thought of as a super position of these 2 forces are a seeing from these 2 surfaces which have parallel to this plane. This force of course, can be calculated by super position by using the formula which we saw and previous slide. And therefore, I can drive the image force $S G \text{ minus } G b \text{ square by } 4 \text{ minus new divided } 1 \text{ by } d \text{ minus } 1 \text{ by } L \text{ minus } d$.

$L \text{ minus } d$ be in this distance the other dislocation dislocated. Now, the minus sign comes in between because 1 dislocation is pulling it to exist surface, the other dislocation pulling in to the left. And therefore, the net will be what you called superposition both negative sign in between. Now, this force I am talking about here is what am I called the glide component of the image force.

Because, now this lies perpendicular to the slip line, but there are 2 other surfaces that means, the this glide force which is coming from each images have a tendency to make the dislocation slip on the slip line. But now, suppose I am talking about reference to these top and bottom surface I got a top surface and I have got a bottom surface.

Now obviously, these is could also constitute a images can draw the diagrammatically this. I like this and one of course, is the same distance here below at a distance this is to be above. So, I can draw images, but this would be called a climb component of the image force, so let me draw on clearly here.

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So, now I have painting of a dislocating here and this is my distance b and this is my h minus d . So, I can construct an image here at a distance of ... So this is a positive this is negative and 1 more at a distance d . If there are 2 images coming again, but this image force will make this dislocation actually claimed that means, it will be particular to it sleepy. And for claim requires actually vacancy diffusion therefore, is not possible normally at low temperatures.

Therefore, to summarize this slide in bulk crystal or in an infinite crystal in a dislocation field low forces arising automatically; that means, low forces in the absence in the single dislocation an infinite body there low forces. If it is a single dislocation in a semifinal body, then you have the image force coming from a single image. If it is a final crystal, then you have multiplied images have just showed you and therefore, if a dislocation position in a nano crystal.

Then, you will have multiple images contributing to the net force on the dislocation. And it is a important note, that in the case of a bulk is the dislocation is far away from the free surface. The force will be too small and I need not will worry about it while in a case of nano crystal, I cannot ignore the images.

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Dislocations in nanocrystals

□ The energy of a dislocation (in bulk crystal) is given by:

$$E_{\text{edge dislocation}} = \frac{Gb^2}{4\pi(1-\nu)} \left[2 + \ln\left(\frac{r_0}{b}\right) \right]$$

- E_{dis} – Energy per unit length of dislocation line
- b – Modulus of the Burgers vector
- r_0 – size of the control volume $\sim 70b$

□ In nanocrystals the energy of a dislocation will be lesser than that in a bulk crystal:

- Due to domain deformations
- Due to smaller amount of material available to be strained

Because, they are located because dislocation is going to in approximately of the free surfaces continue with the topic of a dislocation in nano crystal. If you have noticed the energy of a dislocation goes a Gb^2 square and that means, it is a proportional to a Gb^2 square. Then other in this equation like of course, the certain ratio these 2 coming from something known as Core energy.

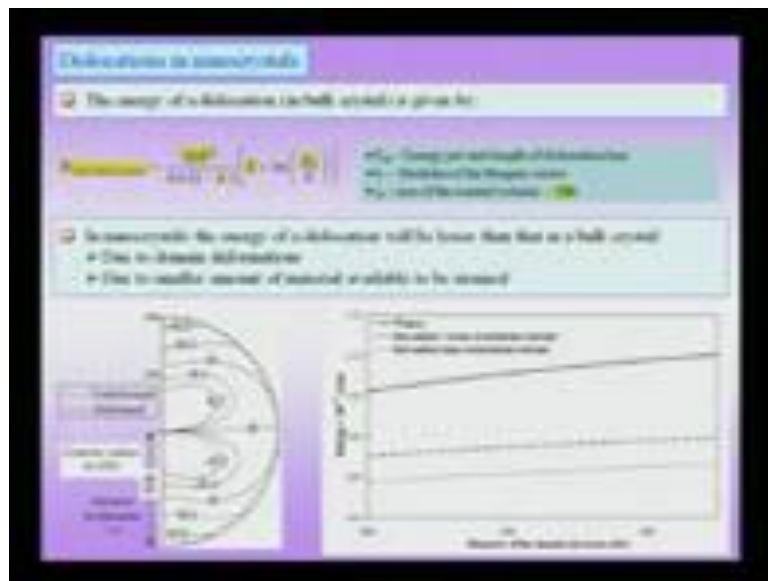
Core is that regional very close to the dislocation line which is where in the theory of elasticity breaks down where in there is an extra free volume there in the crystal. And this come control volume of the volume the crystal we are talking about. And therefore, it will goes the energy goes with the size of the crystal. Typically, in calculations this coma 0 or r is a about take an as about 70 burgers vectors.

But in a case of nano crystal is important of that is energy formula is not valid anymore. Because, the presence of the dislocation get actually be differ to determination of the crystal itself. Because, we noticed before now when I have a crystal edge dislocation glide I can think of it as an extra half plain. This introduction of extra half plain actually introduced, if I am floating my $\sigma \times x$ concludes.

Then, I will noticed that there is compressively reason these are concludes about and

there is tensile stress below. And therefore, to this is compressive, this is tensile and these stresses with lead to the distraction of the crystal. In of course, it is a infinite crystal I do not have to worry about these distraction to the crystal because of that, but in the case of a nano crystal it is clear suppose I am not talking about the syndical nano crystal I have shown below here.

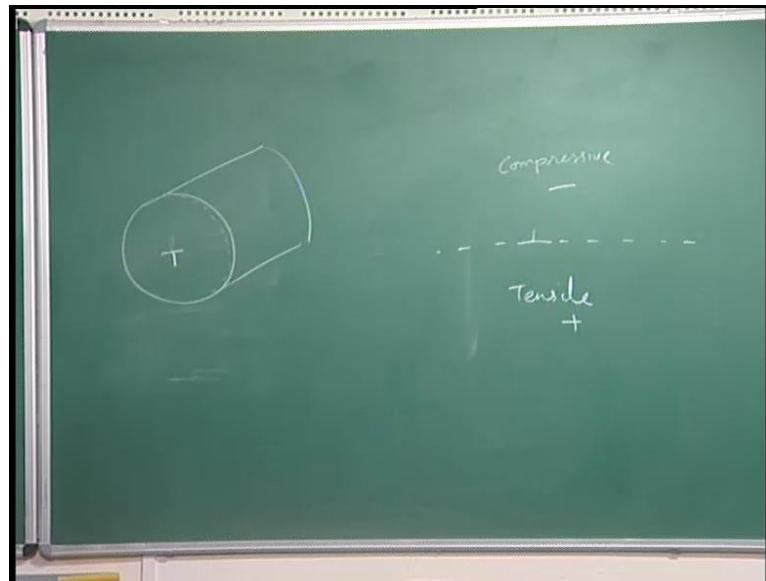
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And this now, my sigma x part of you which has showed you can noticed that these are a sigma x x part of you I can see here, so this is where my extra half plain would be. So, this is where my extra plain should climatically alive and therefore, these are compressive reasons in the crystal. And these are tensile reasons in the crystal, but mere presence of the dislocation you can see is actually distracting the crystal.

So, this reason you can see here is this deformation you have seeing this is the uniformed crystal the dotted line. And defund crystal is by the solid line you can see the crystal is getting d form the entire shape of the crystal getting altered by the mere presence of this edge dislocation. Now, of course to draw these whole body this actually cylindrically dimension.

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So, let me draw the full geometry for you here on the board see got a cylinder showing in the third dimension like this. And mine dislocation is located here to be consistent with the geometry there I will actually do the extra half plain in below. So, these mine dislocation and now my body is getting destroyed in the presence of this dislocation in a cylindrical body.

Therefore, if I now compare my infinite body energy case which is given by the formula here for the large body case the energy with the size with the domain actually goes like this. But you can see that, there is an relaxation in the, and therefore I am taking 2 size of crystal. Suppose, I am taking a small crystal then you can see that this is not my energy float for the free crystal I mean the small size crystal.

So therefore, for a given diameter say about i am talking about 140 burger vector there is a reduction in the energy. And this reduction in energy is coming. Of course, from 2 factors 1 is fact there is lesser amount of materials which has been strained. But additionally, there is actually also an additionally at domain deformation which implies that there is going to be a relaxation an energy.

It is important to note in an infinite crystal the entire hours place about the dislocation

suppose I am talking about infinite crystal. So, this is my dislocation is infinite crystal this going to be an entire half place about this dotted line is going to be compressive and this is going to be tensile. Now, I show compare this the float which have showing you right here, you can see that this is not to any more for a finest crystal.

The smaller the crystal these effects will start to dominate, that actually here even though this reason about tensile here. But if you go further away you see that these are reasons of compression. So that means, these reason about is now compressive; that means, the though the top down symmetric is approximately meant a as in the case for an infinite crystal you see that sign switches as you go to as a top free surface.

Therefore, if the behavior is different from that offer bulk crystal or any infinite crystal were entire half space is purely of on sign. So, to summarize my this slide dislocation in nano crystals have a lower energy is compared to dislocation in infinite crystal. Because of 2 reasons 1 occurred that a smaller amount of material is available to be strained which mean there is not be reduction energy. But also additionally there is going to be domain deformations or which is going to be a relaxation to a strain the energy of the crystal. Additionally, we will also notice that infinite crystal there is actually switch in the sign of the stress field as you go away from the dislocation core.

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- ❑ In nanocrystal one or more free surfaces may be in proximity to the dislocation.
- ❑ As the dislocation is positioned closer and closer to a free surface, at a certain stage the image force may exceed the Peierls force ($\tau_{PN} \times b$)
 - the dislocation can spontaneously leave the crystal without the application of any external stresses [1].
- ❑ In nanocrystals the proximity of multiple free surfaces may lead to all dislocations leaving the crystal when: $F_{image} > F_{PN}$ (for all dislocations)
- ❑ Hence, nanocrystals can become completely dislocation free.
 - For single crystals of Al and Ni this size is the order of a few tens of nanometers.
- ❑ Thus the strength of such a nanocrystal may approach the theoretical strength of the crystal.

$$\tau_{PN} = G \epsilon \left(\frac{2\pi w}{b} \right)$$

- G → shear modulus of the crystal
- w → width of the dislocation !!!
- b → |b|

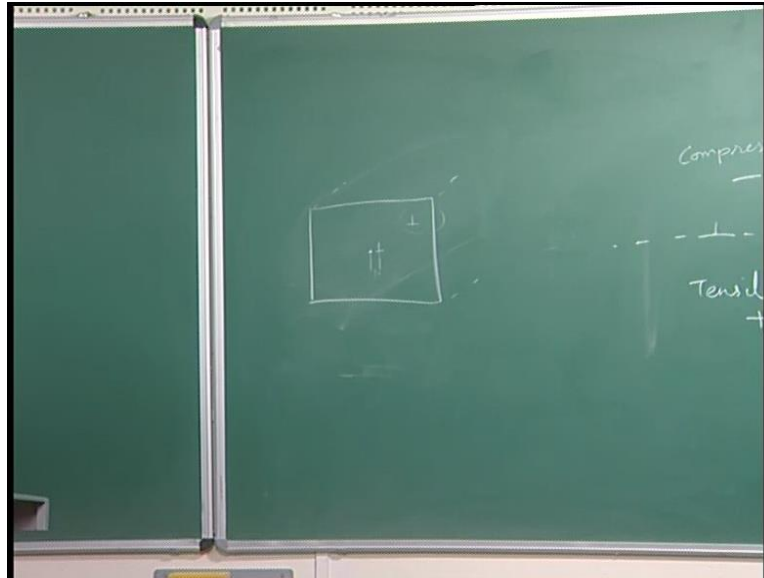
[1] "Critical Size for Edge Dislocation Free Free-Standing Nanocrystals by Finite Element Method"
Prasanna Kumar, Anandhi Subramanian, Journal of Nano Research, 10, p.93, 2010.

We will soon take an extreme example of these kind of devine deformation and interesting effects observed in a specific kind of nano crystals at the coming slide. So, to summarize few the points we just now seeing in a new point in a nano crystal 1 or more free surfaces may be in the proximity to the dislocation, as a dislocation is positioned closer and closer to a free surface, then the image force.

Then, increases at a certain stage the image force may actually exceed the pearls force. Pearls force as we defined before is the inherent for the motion of dislocation and this pearls force can be calculated from the pearls by multiplying the burgers vector. And when this happens it implies that the dislocation can spontaneously leave the crystal without the application of any external stress.

So, this is the very important point that I make a crystals smaller and smaller and therefore, there are proximity a free surfaces which have possible. And the crystal now, have the dislocation will feel a image force which will need the crystal to becomes spontaneously completely dislocation free without application of any extra stresses; when my first stresses exceeded by the or the first forces exceeded by the image force. So this of course, will happens as a pointed out then the image force actually it exceeds the bulk or in a stress for a all dislocation. To make this calculation of course, have to make sure that the list image force it is experience.

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Suppose, I have a I just for a now take a symmetric body like this is crystal goes and take a symmetrical body write the center of the body dislocation will experience to know image force. Because, the 2 all the surfaces are the equally listed, but suppose I considered a dislocation at a distance b from the center. Then, if the force experience because the image forces now you see the image force is gone be very, very weak.

Because, this surface is want very different from this surface, even in this middle weak force can be exceeded by the if this large then pearls stress. Then, all dislocation suppose you considered dislocation here of it closer it will leave. If this is the worst case scenario or near worst case because, center of dislocation of course, feels. If this dislocation came leave the crystal, then I assume that all the dislocation will have left the crystal.

So, this crystal can be come down spontaneously dislocation free. And for aluminum single crystal size have been found it will be of the order of a few 10 of nanometers were and the crystal is found becomes continuously dislocation free. So, still we will have a few more things to say about this coming slides and but the beautiful thing is that now if it becomes spontaneously dislocation from free.

Then, nano crystal may approach the theoretical strength of the crystal; that means, now

we can produce an extremely strong nano crystal nearly. Because, the dislocations are leaving the crystal and of course, I am assuming now these are dislocations which have the ability to move. Then, I can have a dislocation frequently this is extremely strong. A few points have to be told about the pearls of the stress or a pearls stress this occurred the original formula, I am sitting you have to going back to pearls.

Here you see that, it goes exponentially with the width of a something known as a width of the dislocation and burger vector. There a modified formula and there are automatist calculation which super exceed formula. But a nice physical and it is important note that this burgers vector of course is a result of the Crystallogpy; that means, even if I did not have a dislocation this is the shortest of the crystal.

The width of the dislocation is a measure of the bonding in the crystal; that means, you have a covalently bonded crystal. Then, the width will be small and pearls stress will be large we have metallic crystal then the it will more relax kind of land it. Crystal again, would have a small it expect to a small width. So, this is reflection bonding these are the Crystallography and put together the given you the pearls stress. If a pearls stress is a larger then image forces will find a difficult to overcome the pearls stress.

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Edge dislocation free

| Material | Material Properties Lattice parameter, Slip system, b, G, v | Critical size (nm) |
|----------|--|--------------------|
| Al (FCC) | 4.04 Å, <110>-{111}, 2.86 Å, 26.18 GPa, 0.348 | 36 nm |
| Ni (FCC) | 3.52 Å, <110>-{111}, 2.49 Å, 92.00 GPa, 0.286 | 20 nm |
| Nb (BCC) | 3.30 Å, <111>-{110}, 2.86 Å, 36.23 GPa, 0.38 | 8 nm |
| Si (DC) | 5.42 Å, <110>-{111}, 3.83 Å, 67.72 GPa, 0.219 | < 4 nm |

- ❑ Work done on Ti and Pd thin films show that with grain size in the range of ~6-9 nm the grains are dislocation free [1]. The study also showed that many grains had twins and stacking faults.
- ❑ Additionally, in nanocrystals the partials may leave the crystal leaving a stacking fault.
- ❑ It has also been observed that surface regions of polycrystals can become dislocation free.

Shockley Partial

[1] Interface Structures in Nanocrystalline Materials, Scripta mater. 44 (2001) 1169-1174

So, if you take a metal crystal like aluminum and the critical size respected to be the order of and when of course, here I am sitting not a completely dislocation free crystal. But, then edge dislocation free crystal, because screw dislocations have a higher Peierls stress and additionally if experiences smaller image forces. So that means, you have to go smaller sizes to actually get rid of screw dislocation and you can get an edge dislocation certain larger size.

And for a material like, aluminum it is about of the edge dislocation it will become spontaneously edge dislocation free at the size over 36 nanometer; that means, these numbers lie in the nano scale. For Nickelates even smaller about 20 nanometer, for Niobium Bcc material and therefore, which as an higher Peierls stress. The size is about go to even smaller size its actually make a completely edge dislocation free.

Then, even when Niobium a 8 nanometer is expected to from edge dislocation free, screw dislocation this location will Peierls stress essentially bonded diameter to be structured. It is called a very large Peierls stress and there are no experimental evidence so far to actually determine it becomes completely spontaneously dislocation free.

Work done on Titanium and Palladium thin film, show that with grain size in the range of 6 to 9 nano meter. The grain are dislocation free experimentation the scene that if I taking my in the range of 6 to 9 nano meter then dislocation it become dislocation free. And it also shows, many grains stacking fault we have little more say, about the stacking faults.

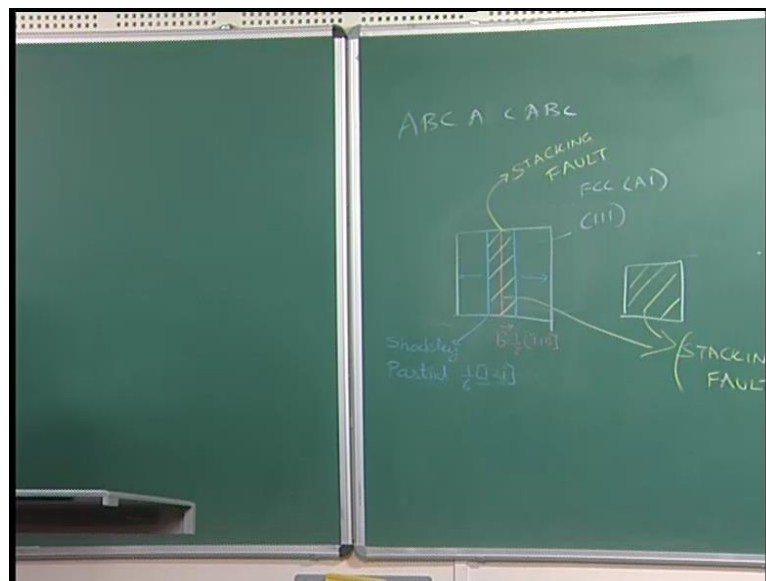
The twin and stacking fault, we have little more say for stacking fault part the twins part is clear that may be the deformation mechanism switching from plasticity by slip to plasticity to by twin; which also we thought about a little more in some of the coming slide. And additional we should note, that regarding stacking fault part that in nano crystals the partials may leave the crystal leaving a stacking fault.

So that means, entire dislocation may not leave the crystal, but actually partial may leave the crystal. And I am talking about the partial, I am referring actually something known as Shockley partials. Because, we know energetically the fundamental satisfaction the say

Aluminum material which is slip plane 111 factor $1\bar{1}0$ line on this 111 plane. Then, such a dislocation can actually lower its energy by splitting into 2 partials both of which lie on the 111 plane.

Then, these partials are of $1/6$ type, so if $1/6$ Burgers vector added to $1/6$ Burgers vector $2/6$, then I get the fundamental dislocation. But these partials lower energy because, I pointed out the energy of dislocation goes as the square of the factor. So, this if in other words I am talking about dislocation $2b$ strength the square of that will be $4b^2$ square will if have that base to be then again b^2 plus b^2 which is $2b^2$ square has lower energy. Now, regarding splitting partials now suppose, I have work list now I am drawing slipping in the crystal.

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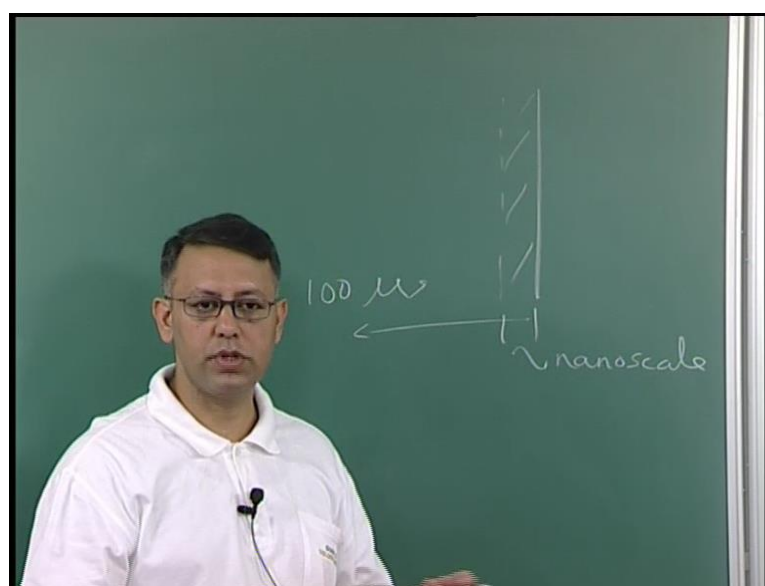
So, this is my crystal and I put a dislocation what might happen now talking about let me now consider this to be the 111 FCC material like Aluminum. Now, dislocation instead of remain like dislocation like split into partial and the region between the 2 partials would be a stacking fault. And therefore, I am in 111 plane of the crystal this is my full dislocation given by this factor b equal to $1/2[110]$ and this is my partial of type I called the Shockley Partial.

So, which is the type 1 2 1 to be 1 bar 2 now, we is partial will also be attracted towards surfaces this to surface and this to this surface. So, in then what might happen that you actually land up in the end configuration as right hand side. So, of course these when this location leave the crystal this partial you will have step created on the partial not of the full dislocation, but I will left with stacking fault.

So, I will left the stacking crystal and this tells me and staking fault as you now is the fault in the stacking sequence you talk about in FCC Aluminum. Then, you know that the shocking sequences ABC, ABC, ABC and suppose the packing sequence change the we becomes ABC, AC, ABC. Then, such a thing called Stacking Fault therefore you consider that in the case of nano crystal the full dislocation will the crystal make it possibility partial.

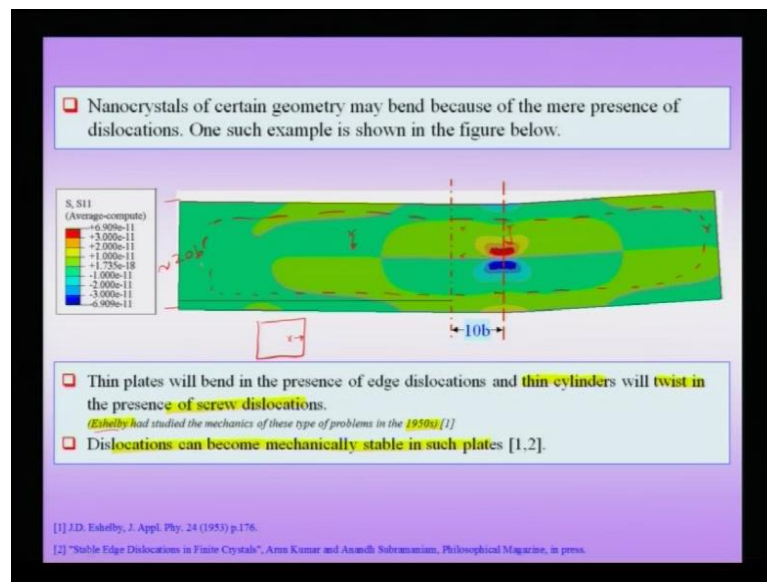
Therefore, you left the stacking fault in the material and this is been observed actually experimentally Titanium and Palladium by and published 2001. So, in addition up course it is obvious based on the argument just I have made. But suppose, you 1 if I have single material is surface region the poly crystals can become dislocation free. So, close to the surface region suppose have crystal.

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And I have surface region both there will be a small region close to the surface where the is existed. So, this crystal it is self could be of the order of microns 100 microns, but this region in the nano scale actually becomes spontaneity dislocation free. Because, the so there are important. So, you are working bulk crystal there is some important image. But this is region is very small compare to the whole crystal we tent ignore this region. But defiantly case of nano crystal we cleared that I cannot ignore image forces and beautifully we show that.

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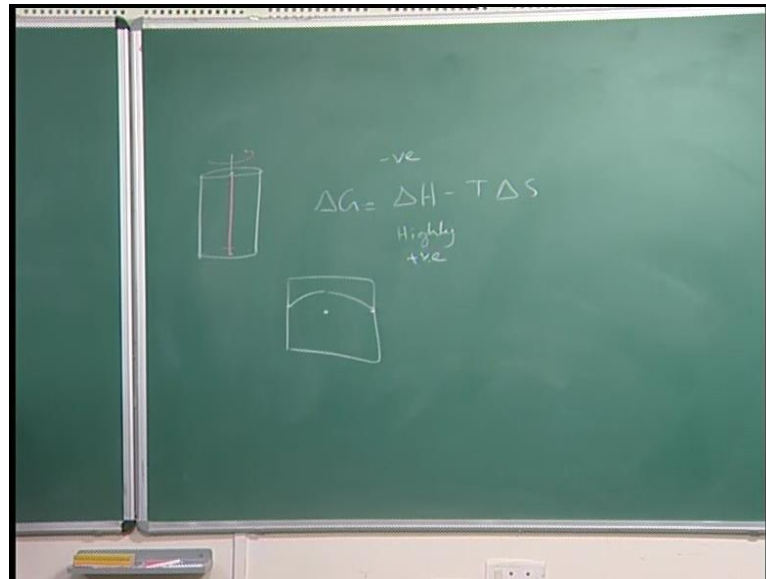


Now, can recover me theoretical dislocation may spontaneously illegal crystal making it completely dislocation free and give me the theoretical see as strength. We are mentioned before, that when you talking about nano crystal then I cannot ignore domain information. Now, will take up esteem example domain deformation and this work theoretically goes back to the 1950s were in talk about dislocation in thin plate.

And there domain deformation cannot ignore and they became significance part of entire structure. And here if look thickness of the plate it is order of the board vectors. So, this thickness of so the order of 20B thinner plate bend more, thicker palate bed less, in the presence of an dislocation it is important note that originally up course also study dislocation thin cylinder.

If in and what the dislocation he talked about was actually screw dislocation thin cylinder. And these cylinder will actually 10 to twice in presence of screw dislocation. Now, there are 2 type of the domain possible I can talk about dislocation in plate like this.

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So, 1 as I can talk dislocation cylinder and now talking about 2 dislocation in the middle of the cylinder. Now, in the process this dislocation actually that do mine will actually twist the cylinder will twist. Therefore, in nano crystal there are important affect we coming because of the presence of the dislocation. Now, the important thing up course note is that the energy of the plate is going to be considering relaxed or will be reduction the energy because of the process dislocation.

Then, see you consider trust value also relaxed and we talk about interesting effect also come about because of the presence of the dislocation. Now, if you talk about the dislocation in bulk crystal we saw that the energy actually decreases as the dislocation goes to of the free surface. This implies the dislocation is going to be unstable, now I am talking unstable, now I am talking mechanical un stability.

Because, dislocation any of the unstable dislocation reason dislocation are un stable is

because we know the criteria of stability of in system constant temperature is the energy. Now, putting dislocation actually cost it energy and therefore, the entire of the system is going to increase. But never the less putting dislocation gives the crystal configuration benefit, even those this term is highly positive; this term be negative.

So, there is going to be enter benefit, by putting and dislocation we would assume there is going to be temperature T as this terms can be asked by this term. And the overall energy is negative in the presence ΔG negatives in the process of an dislocation. But unfortunately this temperature happens to be about the melting point of all non crystal and therefore, dislocation un stable defect.

But the other point talking about here is mechanical stability which means, the energy of the dislocation actually decreases when we go towards the free surface. So that means, crystal and dislocation here the energy decreases as go towards the free surface and therefore, they are mechanically unstable of course, here in this stability ignoring the factor.

There is pulse oscillation sitting on talk about because, I know that dislocation sense sit in energy. And if ignore that, then I talking about the including the pulse value of mate stable otherwise it is mechanically unstable. But it interesting note that, dislocation can be actually become thin in this thin cylinder and thin plate they can actually stable. So, that shall be shown as 1950s that is screw dislocation is can be stable in an cylinder it is very interesting point mechanically stable thin cylinder.

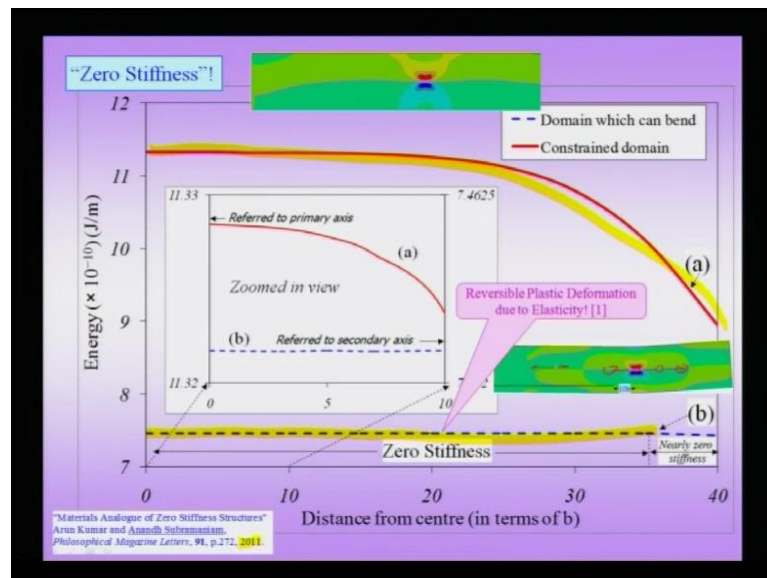
Now, of resent time we also shown that dislocation can be mechanically stable in plate like this. So that means, irrespective dislocation in the center of the plate I can put it here or here and there is the reason stability with dislocation of course, it is very close to the free surface it again the mechanically un stable. But there could be region stability of the dislocation. In other words, dislocation position here center and not that is an interesting point.

So, I have dislocation in normal crystal suppose normal like this you dislocation here will feel words the free surface. But here, is put a dislocation some were here than it

actually feel center of the domain rather than the center domain free surface. And of course, this you demarked region were this is table it is non that entire crystal stable. But never the less important point a note is that d special nano crystal these special nano crystal.

So that means, having at special geometry dislocation can be mechanically stable. So, this is very interesting that in bulk crystals dislocation are always mechanically unstable of course, want very, very technically correct mate stable. But here, in these crystals we can actually see that we can mechanically stable thin plates and thin cylinders.

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Now, an additional interesting thing is that now normally as we pointed out in the previous case that when you have a dislocation. Then, it feels an image force towards the free surface; that means, suppose I take a crystal and plot the energy of the crystal as such dislocation its position towards a free surface. The energy would decrease as shown by a curve like this. So, it is decreasing always and finally of course, it will increase the crystal it creates a step.

Now, if you talk about a dislocation in a thing in a thin cylinder like this and I am positioning the dislocation for instance here then I move it to a next position here then

here. And or in the left or the center of the domain and I track my energy of the crystal now, then it would seem that the energy practically does not change. That is this material now, is some kind of an analog of a nucleus it is and it exists in a state of a neutral equilibrium.

We all know that to take a ball the ball and put it on a plane, then this ball is in a state of neutral equilibrium. Now, exactly equivalent to that this dislocation now is residing in a state of neutral equilibrium with respect to its position in a thin plate like this. So, this is an nano crystalline plate which has certain dimensions as we have seen here before that that when this out of the 100 buggers factor and the thickness of the 20 buggers factor.

In such a thin plate, not only do the dislocation bends the domain not only there is a slight relaxation with respect to the energy in a bulk crystal because of this bending the additional in addition to the fact that the amount of material strain is more. But more interestingly, so that the crystal the dislocation. Now resides in a state of neutral equilibrium with respect to its configurations and this has been termed as Neutral Equilibrium Material Structures.

These are very special structures which were discovered very recently. Therefore, you can see that there are important effects coming because of the presence of the dislocations in nano crystals; that means, in bulk crystals dislocations have certain characteristics. But when we go to nano crystals there are additional effects that come in and which have to be taken in to account.

A few of this we have already pointed out like the case of the image force, the case of the domain bending. And very interesting case of for a given, specific geometric case of what you might call Neutral Equilibrium. And even more interestingly suppose, I now have to move a crystal move the dislocation along the slip plane which is now my central plane. This central plane I move the dislocation, then I can introduce the concept known as Reversible Plastic Deformation Elasticity, because now this resides in state of neutral equilibrium therefore, if I move my dislocation from point to point.

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So, I have a thin crystal here and the thickness is order of the 20 buggers vector then my dislocation is positioned in different places. Then, the energy does not change, but you know the crystal bends differently that means, because of the précised dislocation you have got now plastic deformation plus. What is plastic deformation? Plastic deformation is, deformation in the absence of externally applied forces.

Here, even in the absence of any externally applied forces we see that I am exaggerating here the picture the crystal actually bends because of the dislocation that I showed you. And this implies and this bending is permanent, I do not have to apply any external stresses this is merely because of the presence of the dislocation it is permanent, therefore we can call it plastic deformation.

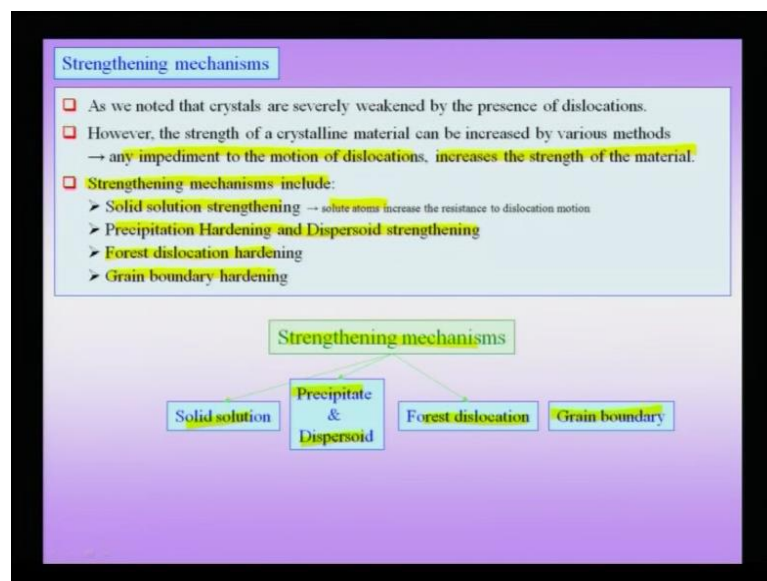
So, this plastic deformation changes differently as I move the this dislocation suppose I have been trying to put it in the middle of the plate. Then, I need to bend a little differently compared to the case where it is positioned towards a free surface. Therefore, this explore the various configuration and this is permanent deformation. But since it applies it is existing without change in energy.

Therefore, you can call it reversible that means the 2 states are equivalent in terms of energy. So, it is strictly reversible and it is plastic and this essentially deformation is coming from the trust fells dislocation. So, it can come of the strange effect like as the now the plastic do not go a handing hindering. In fact, plastic but you get very interesting effect like reversible plastic coming because of I am talking about dislocation and thin plates.

So dislocation may crystal, but then I am varied I am talking about dislocation in nano crystal. There interesting effect which some because of the presses dislocation nano crystal. So, we that if dislocation can be weaken crystal, then we can ask obvious question how can crystals. And 1 mechanism we already seen that, remove the dislocation then the crystal becomes strong.

But this is not practical approaches, so we saw that we only make crystal ache things about microns in diameters which are actually we can maid dislocation free. And additionally dislocation always nuclear during loading, therefore this is not a practical solution to strength on a crystal.

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There are other mechanisms which can actually increase the strength of the dislocation and these arise from the fact any impediment to the motion of dislocation increases the strength of the material. So, if you can stop this dislocation from moving freely, you make the dislocation less mobile. Then, you would actually increase the strength of the crystal. So, what are the mechanisms you have got for increasing the strength of crystal?

Few of them stand here, solid solution strengthening; that means, you have an impurity in solid and then you can have substitution or interstitial and this will actually increase strength in some sense, inherent to most dislocation leading to the increasing strength of the material. So, more impurities you can have, the greater the strength of the material. Further, precipitation hardening and dispersed strengthening can actually increase strength of the crystal.

Noted that, dispersed strengthening can also be achieved by high temperature increases strength of the material; for dislocation mechanisms another mechanism is work hardening which we can increase strength of the material. This essentially implies if you increase dislocation density and which automatically happens when you have plastic deformation that implies during plastic deformation dislocation actually multiplies.

Therefore, the density is increasing, but surprising when there is only one car on the road, you can drive to the road, but many cars cause a traffic jam. Similarly, if you have many dislocations, one dislocation actually moving and cutting across other dislocations present and this would raise the hardening effect coming from dislocation density. And finally, the grain boundary hardening is a very important effect and in this context is taken up a little more later.

We will talk about the relation and more importantly to break down the relation especially in nano crystals. So, the important strength mechanisms are solid solution strengthening where you can use an interstitial like carbon or substitute solid solution like Nickel in Aluminum, Nickel in Copper. You can do precipitation and dispersed strengthening with very large precipitates and dispersed.

Finally, distributed can give raise to impede the motion of dislocation giving strengthening I can use forest dislocation strengthening. So that means, increase dislocation or I can make fine grain material.

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Twinning versus slip

- ❑ Twinning readily occurs in low stacking fault energy materials like Cu and Brass. In high stacking fault energy materials like Al twinning is difficult.
 - Twinning can occur either during annealing or during deformation.
 - Twinning is an important mechanism of plastic deformation and can give ductility to materials wherein slip may be limited. In BCC metals (e.g. Fe) at low temperatures, twinning may become the dominant mechanism of plastic deformation.
 - TWIP (twinning induced plasticity) steels have been developed keeping this in view.
- ❑ Process parameters (temperature, strain rate) and material parameters (stacking fault energy, grain size) determine the mechanism operative for plastic deformation (between slip and twinning).
 - For a given strain rate, at higher temperatures slip would be favourable as compared to twinning (as slip is thermally activated, while twinning stress is essentially constant with temperature).
 - On increasing the strain rate the stress required for both slip and twinning increase and the transition temperature (from twinning to slip) is shifted to higher temperatures.

Because, grain boundary is a finally, dislocation a exists, of course it when dislocation grain boundary it may be observed by the grain boundary or may become dislocation grain boundary or it slip in the next grain ad joining grain. So, in which case it continue slip through the poly crystal. And alternative mechanism, which also can give plastic deformation which note that common as normal slips suppose, I take rode Aluminum bended normally I am expecting that the plasticity.

I am absorbing room temperature the permanent deformation I am getting is because of slip. But then suppose I deform BCC low temperature, then there dislocation by slip become difficult an actually which predominate. Twinning typically occurs in low stacking fault for materials like cu and brass. Suppose, I looked micro structure of cu and brass, I would actually absorbed board of twins.

Then many of this, we absorbed optical micro scope a striate line a stranger really sharp. In high stacking fault energy material like, Aluminum twinning actually difficult; the

reason being that, in if looks at twine and I am talking about mirror twine. Then, the second nearest neighbor surface are affected. And if the second nearest the first nearest neighbor as the same in either side of the twine boundary, but second nearest surfaced is affected.

So, with case of the stacking fault therefore, the stacking fault energy then aspect essay twinning. Twinning can occur either during annealing in which case they are calling annealing or they can occur during deformation and. In fact, they can occurring reason for actually giving arise plastic deformation in which case called deformation twins. Twinning can become important mechanism of plastic deformation and can give ductility to material wherein slip may be limited.

Then, once again example I said you was case of be what is that BCC metals at low temperature. In fact, there a been example like the twip steel which is called twinning induce plasticity. Twinning induced plasticity at twinning steel have been develop keeping this the twinning accept in the focus. That not only slip; that means, dislocation activity then give plastic deformation, but twinning is also important mechanism by which we can get actually some plasticity.

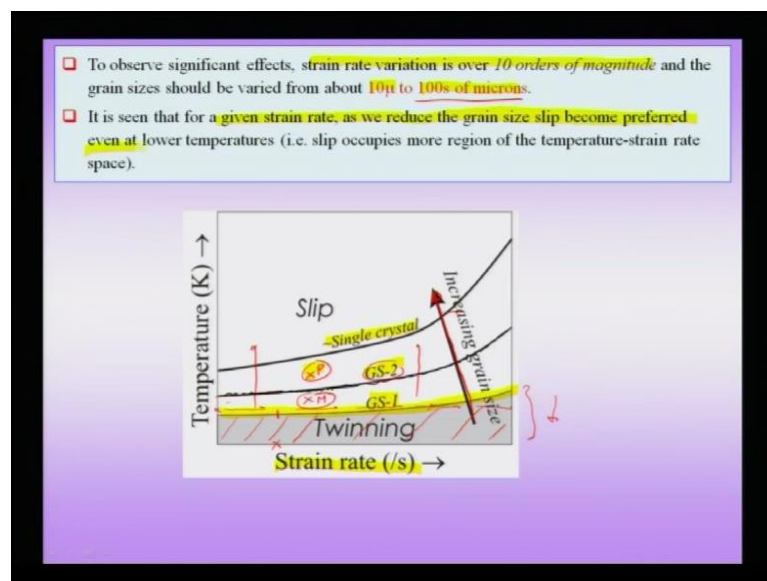
So, though this usually is much smaller compare to dislocation activities for suppose, I get 20 percent because slip. Then, typically the twinning value would be 1 2 percent this much smaller than that by what you met call by slip. Process parameter like, temperature and strain rate and material parameter like stacking fault energy, grain size etcetera determine the mechanism operative for plastic deformation.

So, I here only contractive 2 mechanisms some take I not taking the all the mechanism stated before. I am taking between twinning and slip, then had to look at process parameter like temperature strain rate and I look out material parameters like stacking fault energy and grain size determining which mechanisms going to be predominant in given material .

For given strain rate, at higher temperature slip would be favorable as compared to twinning and the reason that slip is thermally activated. In suppose, I do plastic

deformation slip is mechanism talking about at higher temperature my dislocation actually can jump from 1 pulls validity to another by thermal activation. So, that means I need to apply lesser trust causes plastic deformation and therefore, slip would be profile higher temperature slip. On increasing the strain rate which means, that there is less time was stress and temperature and thermal activation. Then, the stress required for both and twinning increase, but the transition temperature from shifted to higher temperatures.

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So, we will see this effect as the graph below and here I am talking about strain rate variation is over 10 orders of magnitude. So that means, strain rate not merely 1 per second to 2 per second is variation stranded if I have to change I can actually see transaction. And grain sizes here I am talking about variation grain size also in addition to the temperature strain rate and here up there is the case of single crystal.

There is large grain size material, which show of the order of about 10 microns and there is the small grain size material, which is also order about as suppose this is 100 micron and this is 10 size microns. That means, I now in a single diagram and trying to study defer making mechanism; competing defer mechanisms slip, twinning with as a function of the temperature of the strain rate.

Now, it is seen clearly from this graph that for a given strain rate as we reduce the grain size slip becomes preferred, but before we let us understand for single grain size let me take a grain size like GS 1. And tracking this curve like this here, now what is seen below this curve the region below this curve is a region, where I would observe twinning. And the region above this curve, all this region of space of curve I would actually observe slip.

In other words, suppose I am operating strain rate here which could be 10^2 and I actually heat the crystal. Then, I would observe that a cross this line here that the mechanism changes from twinning to slip; that means, at a higher temperature you observe slip at lower temperature you observe twin. Now, for given strain rate suppose I am get given temperature and increase might strain rate.

Which means, that I am actually giving lesser time for thermal activation to take place, then you observe the mechanism changes from slip to twin. So, for other grain sizes so if increases strain rate then you cross line and that means, you actually go from slip to twinning as you increase the strain rate. Now, so you understand 2 effects: the effect of strain rate, the effect of temperature for given grain size.

So, that means increase my strain rate I switch from slip to twinning I increase my temperature I switch from twinning to slip. So, this is basic mechanism, but what happens when I reduce my grain size. Reduction in grain size which is of course, in the opposite direction of this arrow, because this is increasing grain size the arrow shows, then this is increasing grain size of decrease might grain size this is some sense like, decreasing, increasing temperature.

So, decreasing in grain size some in some viewing point we can actually think of it as an increasing temperature. Because, now suppose I take a grain size 1 material which could be of the order of 100s of micron, so I am sitting here. Now obviously, mechanism at point p is point to be slip because it is above this curve now. So, I am specifically tracking 1 curve here which this curve I would call slip curve on this.

So, I am talking about grain size 2 and with respect grain size 2 talking about point p. So, all points like above this here to line are actually points where slip would take place. So,

at point p were accept slip would take place for this givens strain rate and temperature. Now similarly, if I am talking about grain size 1 on the other hand this point say I call it point n for grain size 1 would show slip.

Because, it above grain size 1 curve in other words if for grain size 2.10 is going to between because it slice below the curve what for grain size 0.1 n is actually going to show. So that means, at prosing condition temperature and strain data usually going to if for grain size 1 give raise to actually slip. In other words, when I am decreasing my grain size which are actually increase temperature that means, mechanism is switching from twinning to slip.

So, point 10 would been twinning for grain size 2, but is actually slip for grain size 1 which means, that decrease y grain size the mechanism switches from to twinning to slip. So that means, that it is a function of I just pointed out which mechanism this system chooses is function of the process parameter which we just now consider curve. But additionally also of the material parameter like grain size I am stacking fault energy.

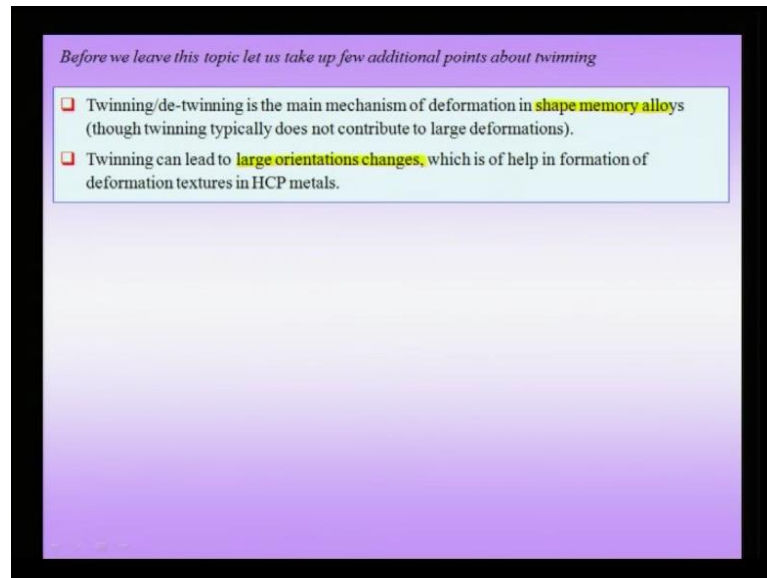
Obliviously, the stacking for energy increases then the region of twinning which is shows here the zone of twinning increases; that means, I have to go to twinning would be less preferred and this region would decrease. And therefore, I would observes slip in materials I stacking fault energy this region would go down this curve would go down correspondingly.

So, the summaries it seen for given strain rate as we reduce the grain size become preferred event at lower temperature slip; that means, slip occupies more region of the temperature strain rate space. So, summaries these slides that we have 2 important mechanism, so plastic deformation twinning and slip; wherever because of low temperature high strain rate slip is suppress.

Then, we have twining typically slower plasticity, then but there are special steel like twip steels which I have developed twinning aspect of plasticity. We have to note that, it is the combination now process parameter like temperature and strain rate and material parameter like stacking fault energy and grain size which tell you, for given strain rate

temperature what kind of mechanism would you observed. The next we will talk about some these accept twinning later on when you take up some example. But we will some basic about some phenomenon like, super plasticity and also about before proceed further.

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We had seen the important of twinning in the context of plastic deformation especially at low temperature and strange. Before we leave the topic of twinning let us, take up few additional point. Twinning d twinning is the main mechanism of de formation in shape memory alloys and has you now shape memory alloys. Now a days have been investigated for very importing application in diverse fields including biometrical application.

We also have noted already that typically does not contributed to large deformation, but twinning can lead to large orientation changes. And this is particular help in the formation of deformation textures which is observed when we deformed HCP materials like magnesium etcetera. So, summaries this slide though twinning typically does not give large deformation it may help by giving large rotations which place and important role in the formation of textures of HCP materials. And additionally, in important

material of not only good academic interest, but also of in terms application they play an important role in the deformation of shape memory alloys.