

Mechanical Behaviour of Materials
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Lecture - 13
Introduction to Dislocations I

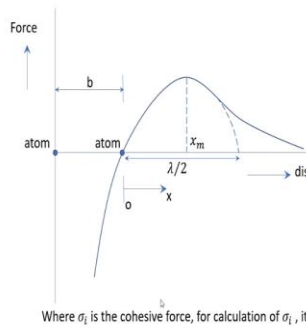
Hello I am Professor S. Sankaran in the Department of Metallurgical and Materials Engineering. Hello welcome back to our lectures and if you recall what all we have seen so far in this course, especially in the last class we discussed about anelasticity that means time dependent elastic behaviour. So, we also looked at some of the examples for this anelasticity nature in terms of thermoplastic effect and diffusion and there is something called relaxation time.

So, all these parameters we will be using it in the material application and it is deformation behaviour and so on. Today we are going to turn our attention to another important concept as the part of introduction and fundamentals to this course called dislocations very important idea or concepts, especially in explaining the deformation behaviour of crystalline materials. As long as you are dealing with the crystalline materials and the deformation is only explained through dislocation mediated plasticity.

And if it is not crystalline material amorphous material that things are different but as far as the crystalline materials are concerned the dislocation concepts are very important. And it is better to spend some time on this as a background before proceed with the course that was the intention I have prepared this kind of lecture.

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An estimate of the atomic bond strength



- The force required to separate two atoms to a distance $x + b$ increases for increasing x until the maximum cohesive force is reached at which total separation results
- The force displacement curve can be approximated by a half sine wave
- Hence, the force per unit area to separate two places of atoms is given by

$$\sigma = \sigma_i \sin 2\pi x / \lambda$$

Where σ_i is the cohesive force, for calculation of σ_i , it is necessary to eliminate λ .



And before I even go into the dislocation introduction and we will spend some more time on an estimate of the atomic bond strength. So, we have already looked at the different types of bond and we also looked at the definition of what is bond length, bond strength and different kind of bonding and etcetera. So, suppose if you theoretically try to estimate how much energy is required to break a bond know they are wrong atom to atom to bond how much it would be?

So, it is theoretical estimation of bond strength and what you are seeing in this schematic diagram is well known to you now because we have enough background for this kind of what is this curve? This is a force versus distance plot several times we have seen this. And the notations are different because I have taken this particular image from the different references. So, do not worry about the different notations but that the meanings are exactly the same.

So, what you are seeing here there are the two atoms atom-1, atom-2 here and the distance between these two normally we denote as the d naught but in this particular figure it is written as b . And this is the force distance curve and it can be approximated as you know sine wave this is that is why this section is given and this is the direction you know the distance from which we are going to pull this atom from its equilibrium position.

And then it when it moves from this position towards the x direction it goes through a maximum and then it comes to minimum. So, what are the points? The force required to separate two atoms

to a distance $x + b$ increases for increasing x until the maximum cohesive forces are reached at which the total separation results. So, $x + b$ so this is b , so this is x so 0 to x so as a start moving from here the force is increasing and it reaches some maximum where the cohesive forces reach this x_m this is the position where it is cohesive forces maximum.

After that the two atoms get separated. The force displacement curve can be approximated by a half sine wave this is a half sine is also here, hence the force per unit area to separate two planes of atoms are determined by

$$\sigma = \sigma_i \sin 2\pi x / \lambda$$

So, the distance here that is half sine wave you know this distance is $\lambda / 2$. And the force per unit area is given by

$$\sigma = \sigma_i \sin 2\pi x / \lambda$$

where σ_i is the cohesive force and we are interested in calculation of this. So, what to do for calculation of σ_i it is necessary to eliminate λ .

(Refer Slide Time: 06:20)

An estimate of the atomic bond strength

For small displacements, $\sigma = \sigma_i \cdot 2\pi x / \lambda$. These small displacements are still **elastic**. The elastic strain is $\epsilon = x/b$ and the stress follows from $\sigma = E\epsilon = xE/b$, combining the above equations

$$\frac{x E}{b} = 2\pi x \cdot \frac{\sigma_i}{\lambda}; \sigma_i = \frac{\lambda}{2\pi} \cdot \frac{E}{b}$$

The area under the curve is the work required to separate the planes of atoms. Hence, the area represents twice the true surface energy, γ (2 new surfaces)

$$2\gamma = \int_0^{\lambda/2} \sigma_i \sin \frac{2\pi x}{\lambda} dx$$

$$= \frac{\sigma_i \lambda}{2\pi} \left[-\cos \frac{2\pi x}{\lambda} \right]_0^{\lambda/2}$$

$$= \frac{\sigma_i \lambda}{2\pi} [-\cos \pi + 1]$$

$$= \frac{\sigma_i \lambda}{2\pi} [2] \text{ or } \lambda = \frac{2\pi\gamma}{\sigma_i}$$

$$\sigma_i = \left(E\gamma / b \right)^{1/2}$$

Elementary Engineering Fracture Mechanics, David Broek, Springer, 2012

For many materials, $\gamma_s = E b / 40$, $\sigma_{th} = \frac{E}{6}$

For mild steel, $\sigma_{th} = \frac{2800}{6} = 33 \text{ GPa}$



So, how do we do that let us look at what are the simple terms available with us for small displacements

$$\sigma = \sigma_i \sin 2\pi x / \lambda$$

this is valid. These small displacements are still elastic; please understand we are still talking about elastic deformation only. The elastic strain is $\varepsilon = x / b$ we are interested in moving the atom to the position of x and then the actual displacement original displacement this b .

And the stress follows from $\sigma = E \varepsilon$ and we can replace the ε with x / b then you get $\sigma = xE / b$ is supposed to be combined these two equations for σ then we get a different formula

$$\frac{xE}{b} = 2\pi x \cdot \frac{\sigma_i}{\lambda}; \sigma_i = \frac{\lambda}{2\pi} \cdot \frac{E}{b}$$

So, this is one expression and we need to eliminate λ . So, we will go to the other part of the calculation.

The area under the curve is the work required to separate the planes of atoms. Hence, the area represents twice the true surface energy γ , you see when you create or when you break a bond or a plane we will see this in much more detail in fracture mechanics we will bring this concepts when you separate these two you know when you break an atom you are essentially creating two surfaces. So that is why it is given and it is surface energy γ is being considered

$$2\gamma = \int_0^{\lambda/2} \sigma_i \sin \frac{2\pi x}{\lambda} dx$$

So, we can just solve this it is a simple integral, so what you get is

$$= \frac{\sigma_i \lambda}{2\pi} \left[-\cos \frac{2\pi x}{\lambda} \right]_0^{\lambda/2}$$

suppose if you substitute this limits then we get this. So, we get finally

$$= \frac{\sigma_i \lambda}{2\pi} [2] \text{ or } \lambda = \frac{2\pi\gamma}{\sigma_i}$$

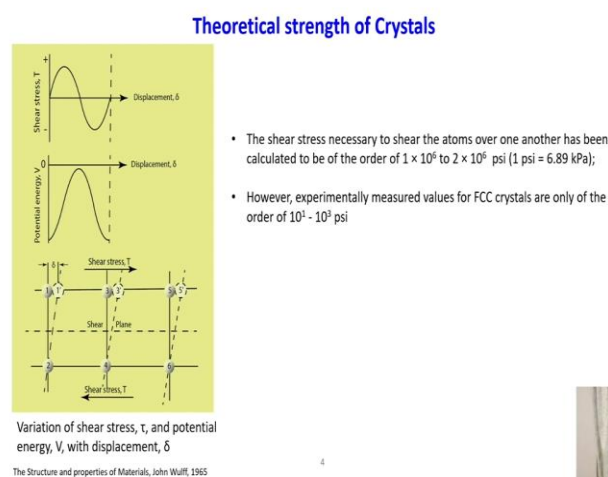
Suppose if you compare this equation with this equation and combine compare and combine what we will get? We will get something like

$$\sigma_i = \left(E\gamma / b \right)^{1/2}$$

So, this is the expression for the cohesive force for separating the two planes of atoms theoretical value. So, for many materials surface energy γ_s is given by $E_b / 40$.

And then the theoretical strength σ_{th} is about $E / 6$, the problem is this value of $E / 6$ is very high for example E normally measured in GPa. But in practice most of the engineering materials or any common material called mild steel even if you calculate the theoretical strength it is $200 / 6$ approximately it is 33 GPa which is phenomenally high far away from what we get in a simple tensile test. So, this is one big discrepancy.

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Similarly another example same idea we are trying to give suppose if you take this lattice and then the shear stress applied in both directions just imagine that because of this shear stress the atom one most from the new question one prime and making a displacement δ still it is within the elastic deformation, please understand we are talking only about elastic deformation. Suppose if you consider this one prime atom comes to somewhere in between here between the two and four some little way that means the atom has reached a meta stable position.

But in this meta stable position from here the atom can move either to this direction or this direction either both ways are possible. So, because at this mid position we see that the potential energy is almost zero, it has nothing to do we can go this way or that way. So, if you assume that

the displacement or the external force applied the shear stress applied is good enough to pull this 1' atom to the next position that is four above four.


Then the 1' atom will have a new neighbour nearest neighbours it may restore the original position locally but ultimately what happens is that will result in a slip crystal will result in slip because this will move here and this will go here and this will move here like that. So that is exactly as shown here. So, then also so that is a variation of shear stress τ and a petition of V with a displacement δ .

So, this is all nicely shown here, here again the shear stress necessary to shear the atoms over one another has been calculated to be of the order of 1×10^6 to 2×10^6 psi pounds per square inch which is $1 \text{ psi} = 6.89 \text{ kilo Pascal}$. So, we use this units normally this is taken for very old text. So, they use this kind of unit system but again they experimentally measured values for FCC crystals are only of the order of 10^1 to 10^3 psi.

Which is very low as compared to what is being shown theoretically. So, what happens is these are the discrepancies in terms of strength what we actually calculate from theory and what we observe in practice. So, there is a discrepancy.

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Dislocations



Introduction

- The stresses required to cause slip were measured by tension tests of single crystals.
- G. L. Taylor, M. Polanyi, and E. Orowan independently postulated that pre-existing crystal defects (dislocations) were responsible for the discrepancy between measured and calculated strengths.
- Slip occurs by the motion of dislocations.
- Many aspects of the plastic behaviour of crystalline materials can be explained by dislocations.
- Among these are how crystals can undergo slip, why visible slip lines appear on the surfaces deformed crystals, why crystalline materials become harder after deformation, and how solute elements affect slip.



So, in order to solve this discrepancy people introduce the concept called dislocations. So, what are dislocations? We will see now the stresses required to cause slip were measured by tension test of single crystals. G. L. Taylor, Polanyi and Orowan independently postulated that pre existing crystal defects called dislocations were responsible for the discrepancy between measured and calculated strengths.

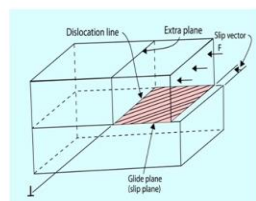
So, this is a postulation by these three scientists and they kind of prove that their dislocations are responsible for the measured low strength values in single crystal. So, they said that the crystal slip occurs by motion of dislocations and many aspects of plastic behaviour of crystalline materials can be explained by dislocations, among these are how crystals can undergo slip, why visible slip lines appear on surfaces of deformed crystals, why crystalline materials become harder after deformation and how solute elements affect slip. So, these are some of the questions they try to explain.

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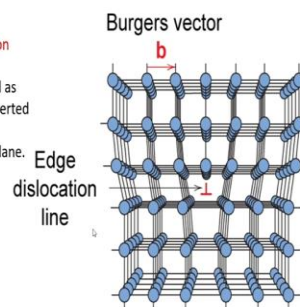
THE GEOMETRY OF DISLOCATIONS

Edge dislocation:

- One special form of a dislocation is an *edge dislocation* sketched in Figure.
- The geometry of an edge dislocation can be visualized as having cut part way into a perfect crystal and then inserted an extra half plane of atoms.
- The dislocation is the bottom edge of this extra half plane.



Fundamentals of Physical Metallurgy, John D. Verhoeven, John Wiley, 1975
Callister's Materials Science and Engineering, Adapted Version, R. Balasubramanian, John Wiley India (P) Ltd, 2007



- Extra half-plane of atoms inserted in a crystal structure
- $b \perp$ to dislocation line



Looking at the dislocations behaviour so that is why studying about dislocation is important as long as you deal with the crystalline materials deformation behaviour. So, now we will slowly see what is a dislocation? And first we look at the geometry, geometry of dislocations. So, this is the nice picture of I mean the schematic of dislocation which is called edge dislocation you see that you have the view of atom columns and it was looking at from the front.

And what you see is these are all atom columns they are all connected by the kind of springs and you have the extra plane for inserted in the middle and this is called edge dislocation this kind of geometry is called edge dislocation. One special form of dislocation is in edged dislocation shown here. The geometry of an edge dislocation can be visualized as having a cut part away in a perfect crystal and then inserted an extra half plane of items.

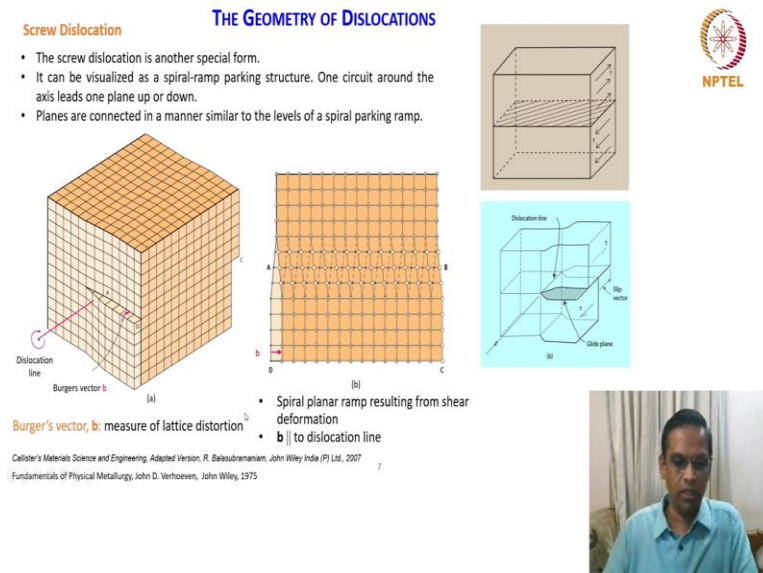
So, what it means is it looks as if this particular plane was cut from somewhere and got inserted from the perfect lattice it gives an impression like that. The dislocation is a bottom edge of this extra half plane. So, this is an extra half plane and this is where the dislocation core is there and this is a bottom edge the other schematic shown here is also showing the edge dislocation only but it is a little more information, what are the other information there is something called b here.

That something marked b here and there is a symbol for this dislocation edge dislocation. So, the edge dislocation line is here so we will see what is this line so because we are seeing it from the front and this picture shows much more detail even though it gives a similar information but more details can be found here, what is the more detail you have to see? So, this extra half plane is inserted here this is a hole crystal.

And this extra half plane is moving in a plane called a glide plane or a slip plane, this is a plane and then you can see that this symbol is edge dislocation symbol is here over here that means this whole block is tilted here and then you are seeing the dislocation line. So, the dislocation line is going through the plane of this slide, it is going perpendicular inside. So that is what is shown here that is called dislocation line.

And this is an extra half plane and this where ever that crystal got slipped to a distance which is b called by Burgers vector also called slip vector is shown here. So, extra half plane of atoms inserted in a crystal structure is a typical description of edge dislocation. The other important observation is b is perpendicular to dislocation line. So, in this geometry the Burgers vector is perpendicular to dislocation line. So, you can see that this is b here and this is a dislocation line so this is perpendicular to this. So, these are all the very important characteristics of edge dislocation geometry.

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The next one is screw dislocation so you can see the nice schematic here the huge block was slipped and what you are seeing is that both of them are same but one is in the side view, the other is in the top view. So, you are looking at from here and we are looking at one this is from here the side view and this is from the top view. So, as the name implies the crystal block has you know what displaced in a kind of screw access here.

I will explain this in much more simpler way in a couple of slides, so here the displacement is measured again by your Burgers vector b . And then here you see that it is the crystal has slipped whatever the b here this more to come out of the other end. And you see the dislocation line is here it is shown here and for the better view the b is shown here and I will explain this a little more by taking up this additional schematic.

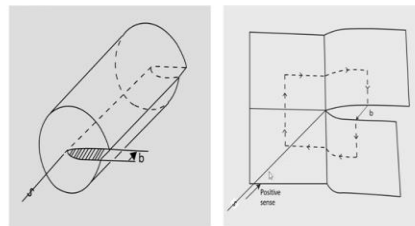
This is an unslipped crystal unit and this is a slipped crystal unit exhibiting at dislocation line. So, here we see that this is a shear stress applied in the top and bottom and as a result to the crystal as slipped and you see that the slip factor is here which is calling to Burgers vector b and this is a glide plane we just compare this glide plane with what is shown in a edge dislocation and this is the dislocation line.

So, the dislocation line is here which is with respect to b it is parallel. So, this is one of the characteristics here. So, screw dislocations can be visualized as a spiral ramp parking structure. So, it is some analogy parking structure it is a structure you can example one circuit around the axis leads to one plane up or down whether it is a positive screw or a negative screw, planes are connected in a manner similar to the levels of spiral parking ramp.

And of course this spiral plane or ramp resulting from a shear deformation the burghers vector b is parallel to the dislocation line can we check this? So, what is the dislocation line here? So, this is dislocation line and this is slip factor this is parallel to this. So, b is parallel to dislocation line in a screw dislocation geometry b is perpendicular to the dislocation line in an edge dislocation geometry these are the important points to keep in mind. So, Burgers vector b is a measure of lattice distortion so this is also it is a measure of lattice distortion, not just describing individual dislocation alone.

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Why the name screw dislocation?



The helical displacement produced by screw dislocations, A Burgers circuit for a screw dislocation

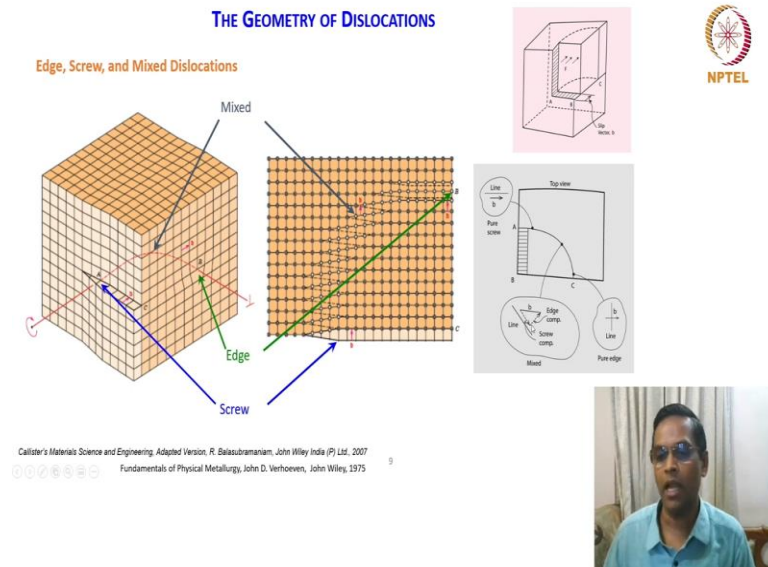
Fundamentals of Physical Metallurgy, John D. Verhoeven, John Wiley, 1975



And why the name screw dislocation? Because yeah as I just mentioned in the previous slide if you take this cylindrical body and what it is shown here is the screw dislocation with a Burgers vector b here and suppose if you try to continue this displacement here as per the screw it will go in a positive direction of make the cylinder as a screw completely it will become screw the path of this glide will be in a spiral way and it will this rod will become like a screw.

So that is why it is called screw dislocation and similarly so this what is this around this? This is called Burgers circuit how do we do that we will see in a minute and we do it in a clockwise direction. So, it is a positive sense and we can also do it in a anti clockwise then it will be a negative sense, so this is called Burgers circuit.

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And what is the next edge, screw and mixed dislocation. We are not just going to stay with edge as screw geometry alone we are also going to have a mixed dislocation. If you look at the schematic here it is nicely shown that this is a screw dislocation in this end and this end it is edge dislocation. So, edge character and it is screw character completely 100% and what about the mixed one where do you find somewhere in the middle? How do we understand this?

So, you look at this top view again this is a pure screw dislocation and this is a pure edge dislocation here and somewhere in between because b still it is very difficult to understand from this image because it is the displacements are not they have shown here but not clearly we will take up some assistance to explain this a more schematic. So, what you are seeing here is this is the crystal which has slipped here in this direction A, B, C.

And the forces applied in this direction so the coastal part of the crystal flips here and then it has both screw as well as edge. So, if you look at from the top so this is how it will look like so this schematic will be very simple to explain now imagine that this is the AC line which is marked in

a dotted line here which is now should drawn as a full thick line. So, A, B, C so if we compare this geometry here in a 2D plane that is top view.

And what you see here is dislocation line is curve like this, so this is screw dislocation which is parallel to b and this is a dislocation line which is also parallel and it comes on the ends here the dislocation line is perpendicular to the b that is edge character but somewhere in between it will be a mixed dislocation. So, how this b and line will collide? Obviously when you say mixed you should anticipate that the b should have some angular relationship with the dislocation line.

So, how do we understand that? So, this is the dislocation line and this is a Burgers vector so if you just take the two components the angular components it will have some angular relationship, so one is edge and another is screw. The screw will be suppose if you make this triangle and this is an α angle and then it is $b \cos \alpha$ has screw components or $b \sin \alpha$ is an edge component. So that is how you should look at it that mixed that is dislocation will have both the characters of edge as well as screw dislocation I mean characteristics and that can be understood by this.