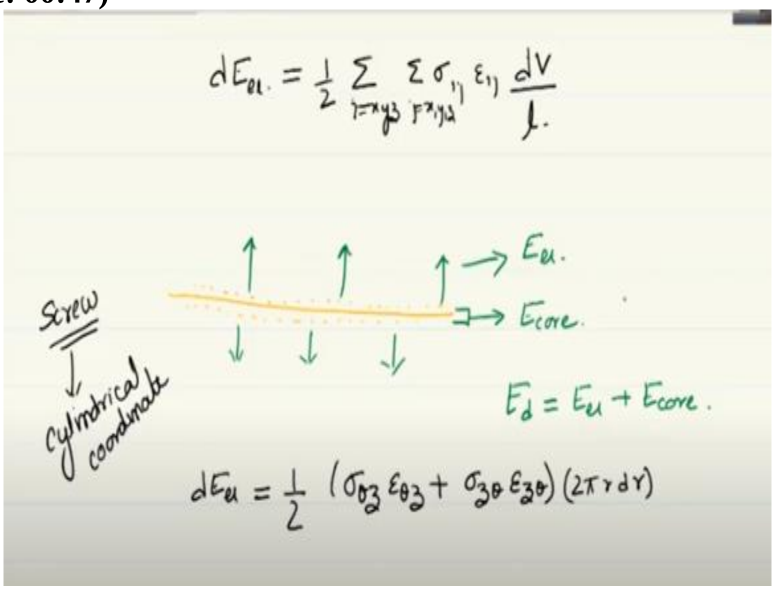
Mechanical Behavior of Materials-1
Prof. Shashank Shekhar
Department of Materials Science and Engineering
Indian Institute of Technology-Kanpur

Lecture - 20
Energy of Dislocations

Okay, so welcome back. Now that we have looked at the stress and strain field for edge dislocation as well as the screw dislocation, we are now in a position to determine the energy of the dislocations. So what we will use is the standard rule, a standard equation for finding the energy if we know the stress and strain which is $\frac{1}{2} d\sigma \times d\varepsilon$ gives us energy per unit volume.

(Refer Slide Time: 00:47)



So what we have here is, so the sigma and epsilon both have several components. So

$$dE_{el} = \frac{1}{2} \sum_{i=xyz} \sum_{j=xyz} \sigma_{ij} \varepsilon_{ij} \left(\frac{dV}{l}\right)$$

The dislocation is whatever energy we calculate it is for the energy per unit length. So if you look at a dislocation it is like this.

And it has some core region where there is lot, very large distribution or difference in the misfit between the atoms. So in that region, we will not have elastic energy. And therefore, when we are using this equation, we will not be able to calculate the energy for that region which would be contributing to the core. So this will be the E core and outside it we have the elastic deformation and here we will have the E elastic.

So this relation that we will be deriving or using to get to the final energy would be only for this part. And this one we will have to estimate from other ways. And therefore, the total energy of the dislocation would be E elastic plus E core, okay. So coming back to this equation, so as this is more like a cylinder and therefore, when we look at it dv by l, so volume of a cylinder so it will be$2\pi r dr$.

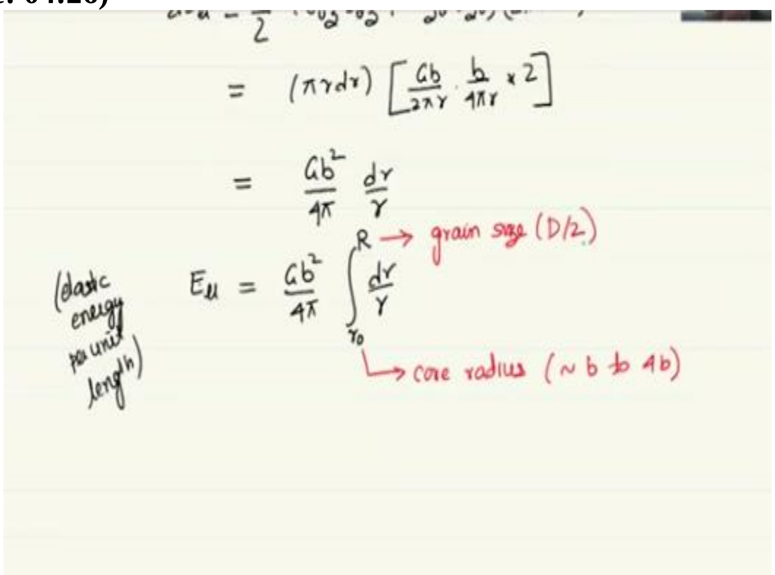
So volume is equal to $\pi r^2/l$, but we already have divided by l because this is the per unit length whatever energy we calculate. Therefore, it is πr^2 and therefore, dv/l becomes $2\pi r dr$. So we have over here and the next thing is that we will first be calculating for screw dislocation, where we have the cylindrical coordinates where the formulation or the equation is much more simpler or easier to deal with.

So we will have

$$dE_{el} = \frac{1}{2}(\sigma_{\theta z}\varepsilon_{\theta z} + \sigma_{z\theta}\varepsilon_{z\theta})2\pi r dr$$

So here you said σ_{ij} and ε_{ij} meaning the same sigma should multiply with the same epsilon which is what we are doing over here, only that we are doing it for cylindrical coordinate and for the screw dislocation, we saw those relations were very straightforward and dv by l becomes 2 pi r dr. And these two are same. So basically whatever we write for this will be into 2.

(Refer Slide Time: 04:26)



And therefore above equation can be written as

$$dE_{el} = (\pi r dr)[\frac{Gb}{2\pi r}(\frac{b}{4\pi r}) \times 2] = \frac{Gb^2}{4\pi}\left(\frac{\mathrm{dr}}{\mathrm{r}}\right)$$

And on integrating above equation

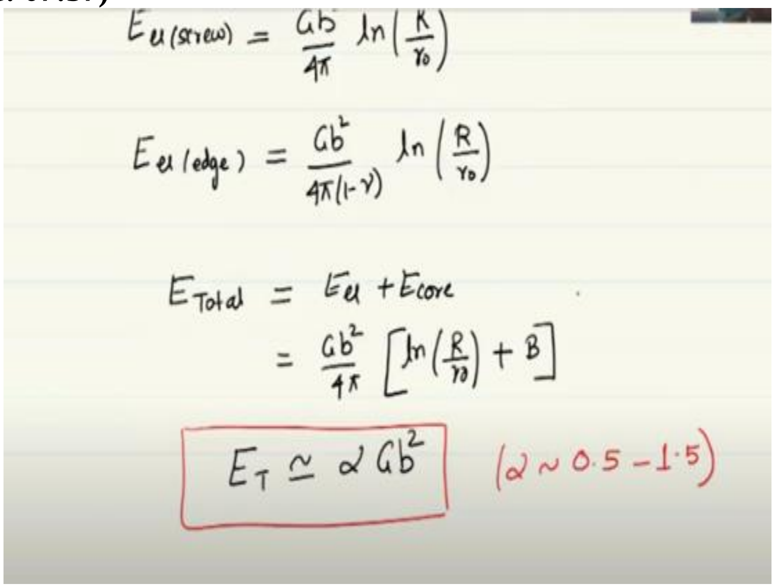
$$E_{el} = \frac{Gb^2}{4\pi}\int_{r_0}^{R}\frac{\mathrm{dr}}{\mathrm{r}}$$

Where r_0 is the smallest value and R is largest value. And at this point again I will like to remind you that this energy that we have calculated is elastic energy per unit length. Now coming back to the right hand side, so we have the smallest r_0 and the largest R. So what is the value of the smallest r_0? Now looking at this equation clearly the diameter of the radius of the core is what will be the smallest r. So this is core radius.

And usually it is taken somewhere from b to 4b. But what about the higher side, upper side. What should be the maximum value of r? Now ideally we would like to go all the way to infinity, but then no material extends to infinity. So should it go up to the dimensions of the component? The answer is no. The actual value up to which r would extend is the size of the grain.

So assuming that this dislocation is somewhere at the center, so the radius this r would go all the way up to the half of the diameter. So this will be determined by grain size and if the diameter of the grain size is D then R would be D/2.

(Refer Slide Time: 07:37)

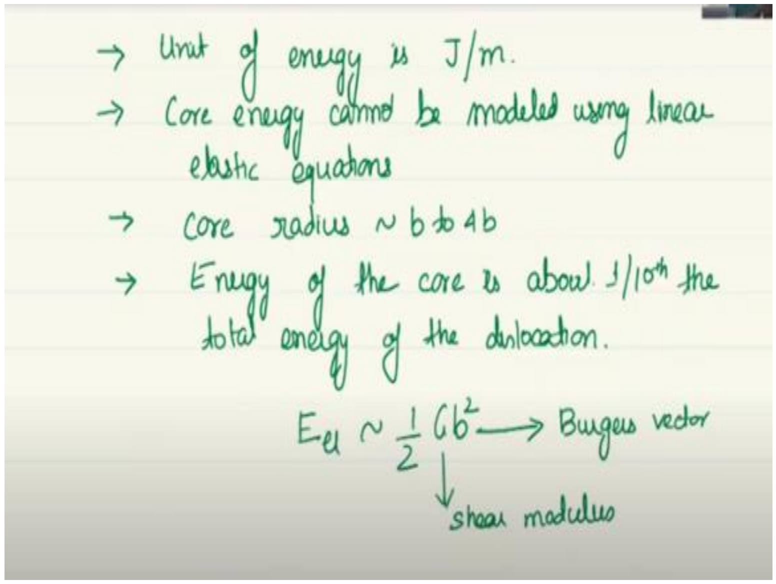


And therefore, what we obtain is for screw dislocation where we know what the values of R and r_0. And if it were edge then there is one slight change from this and it is that there is a factor of 1 minus nu. So this is the elastic energy for the dislocation. This is the edge dislocation and this is the screw dislocation. Now here we have already mentioned that this is the elastic component.

Now if you want the total energy component then we can write it like this. $E_{elastic} + E_{core}$ where we already know the $E_{elastic}$ and let us say we are talking about screw then it is $\frac{Gb^2}{4\pi}\ln\frac{R}{r_0}$ because this is what is varying for G and b would be constant and this is something that would vary from dislocation to dislocation. And let us say for the core component we write the term B.

Now this whole thing can now be approximated as some parameter and usually you can write it like $\alpha G b^2$. So this is a very common relation that is used to describe the energy of dislocations. And hereα is anywhere in the range of 0.5 to 1.5.

(Refer Slide Time: 09:50)



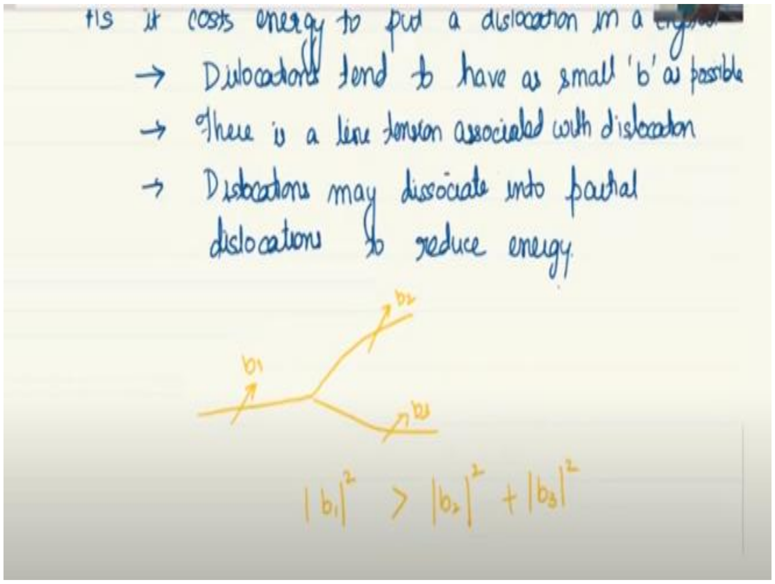
So couple of things are important to note here that the unit of this energy is joule per meter because it is energy per unit length. Another thing that we have already emphasized is that core energy cannot be modeled using linear elastic equations. We have already seen that the core radius is usually taken from b to 4b. It depends upon the model on the researcher.

Depending on other parameters, they may find the radius, core radius somewhere between b to 4b. Another important fact is that the energy of the core is about one-tenth the total of the dislocation. So if you look back into this equation, so what it is saying is this b is approximately 10% and this factor is 90%. So that will comprise the total energy of the dislocation.

And overall we will have the energy as $\alpha G b^2$. So the elastic energy is usually taken as $\frac{1}{2} G b^2$ where G is the shear modulus and b is the Burgers vector. Now since we are talking about energy, so this also means that dislocations will tend to have the lowest energy and when can they have the lowest energy they cannot change G. R and r_0 are not within a dislocation's purview.

What it can change is though the Burgers vector. So a dislocation would tend to have smallest Burgers vector. So if you have possibility of several Burgers vector, the dislocations would only be possible where the Burgers vector is smallest.

(Refer Slide Time: 12:53)



Because it is we are talking in terms of energy as it costs energy to put dislocation in a crystal, dislocations tend to have as small b as possible. Another important thing is that because we are talking about dislocation as a line and because it has energy associated with it, therefore there will also be a line tension associated with the dislocation.

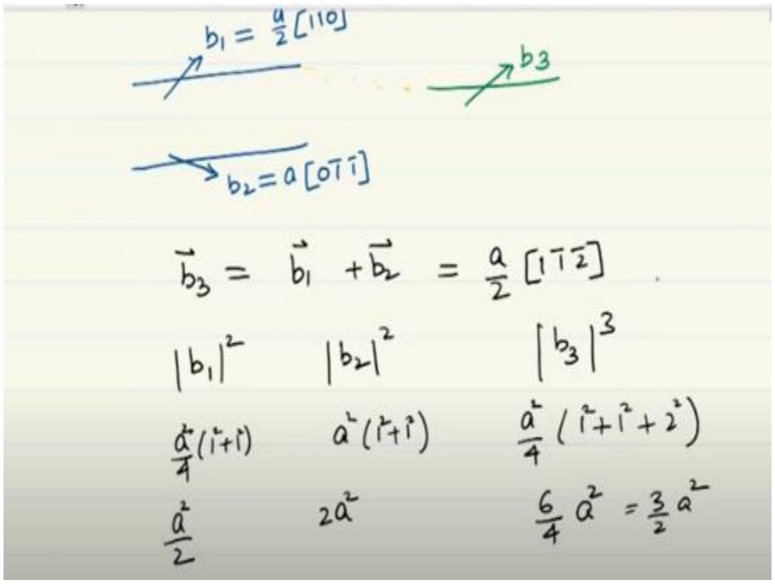
And in order to minimize the energy sometimes the dislocation may dissociate into what are called as partials and the sum of those partials would be less than the energy of the original dislocations. So you may have a dislocation like this and at some point it may dissociate into these two Burger vectors, so these two dislocations. So let us say if this was the Burgers vector b_1, this was b_2 and this was b_3.

So this is favorable. That is this transformation into the partials is favorable only if $b_1{}^2 > b_2{}^2 + b_3{}^2$ because energy is proportional to Burgers vector square. Therefore, we will take the squares of the Burgers vector and compare.

So if ever you have to find out whether this dislocation reaction would be favorable or whether this dislocation would dissociate, you have to just calculate the square and then compare the total energy, compare the values. And then you would know if it is lower, then it means it would be favorable, if not then it would be unfavorable.

So that is how we compare. And in this respect, let us say we are given Burgers vector two dislocations.

(Refer Slide Time: 16:32)



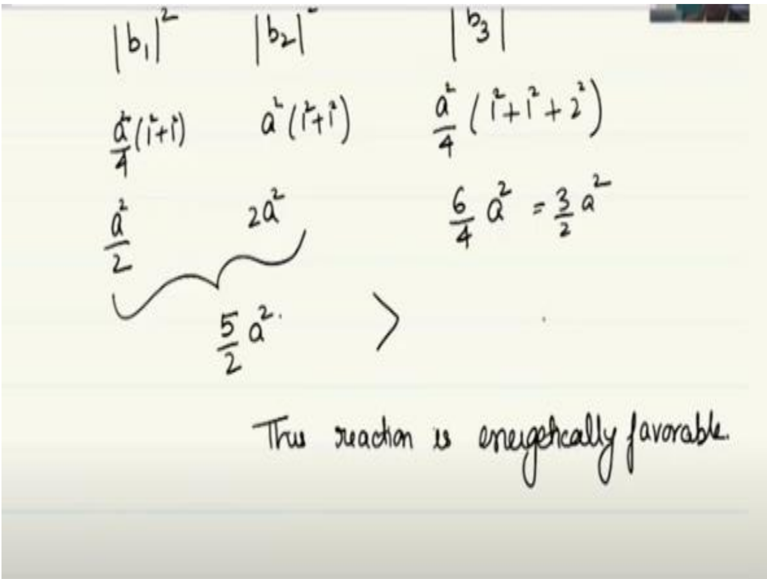
So let us say this is one dislocation, which has some Burgers vector, which is $\overrightarrow{b_1} = \frac{a}{2}[110]$. And there is another dislocation, which has Burgers vector $\overrightarrow{b_2}$ and this is a purely fictional case, because usually you do not have this kind of dislocations. So $\overrightarrow{b_1}$ and $\overrightarrow{b_2}$ are there and it is given that these dislocations combine to form one dislocation which is $\overrightarrow{b_3}$ Burgers vector.

So first thing is to find out what is that $\overrightarrow{b_3}$ Burgers vector. Now $\overrightarrow{b_3}$ Burgers vector would be equal to $\overrightarrow{b_1} + \overrightarrow{b_2}$. If we add these two what we get is a/2. So you can take it as a/2[0 $\bar{2}$ $\bar{2}$]. So now we add a by 2 1 plus 0 is 1 0 and 2 bar is 1 bar and this is 0 and 2 bar. So this is 2 bar. Now how do we calculate the energy?

So on this side you have $\overrightarrow{b_1}$ and $\overrightarrow{b_2}$ and on this side you have $\overrightarrow{b_3}$. So we will take the squares of these. So

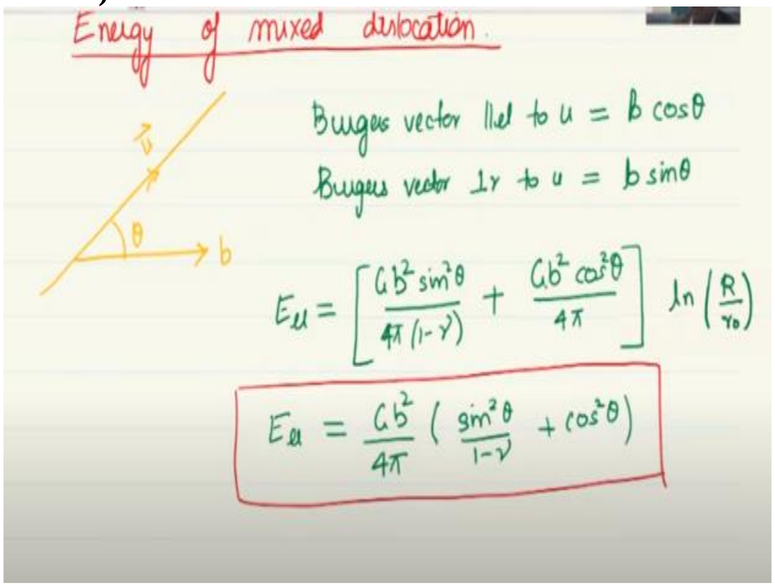
${b_1}^2 = a^2/2$ ${b_2}^2 = 2a^2$ and ${b_3}^2 = 3a^2/2$

(Refer Slide Time: 19:01)



On the other hand if we sum these two what we get is $5a^2/2$. Therefore, this energy is greater than this and therefore what we understand is, what we now know is that after reaction it will have lower energy and therefore this reaction is energetically favorable. Now the next question is that we have already seen the energy of edge dislocation, we have seen energy of screw dislocation. How do we calculate the energy of a mixed dislocation?

(Refer Slide Time: 19:51)



So let us say you have a dislocation going like this so that we are looking at a segment, which is straight and therefore the line vector is like this, but the Burger vector is given like this so that this angle is theta, which means that the Burger vector component parallel to u is equal to $b \cos \theta$ and the Burgers vector perpendicular to u is equal to b sin θ.

So effectively now what we have is that we can consider it that there is edge dislocation and a screw dislocation superimposed onto each other and we know the Burgers vector for both of them. So what we all we need to do to calculate the elastic energy is to use the equation that we have for screw dislocation and edge dislocation.

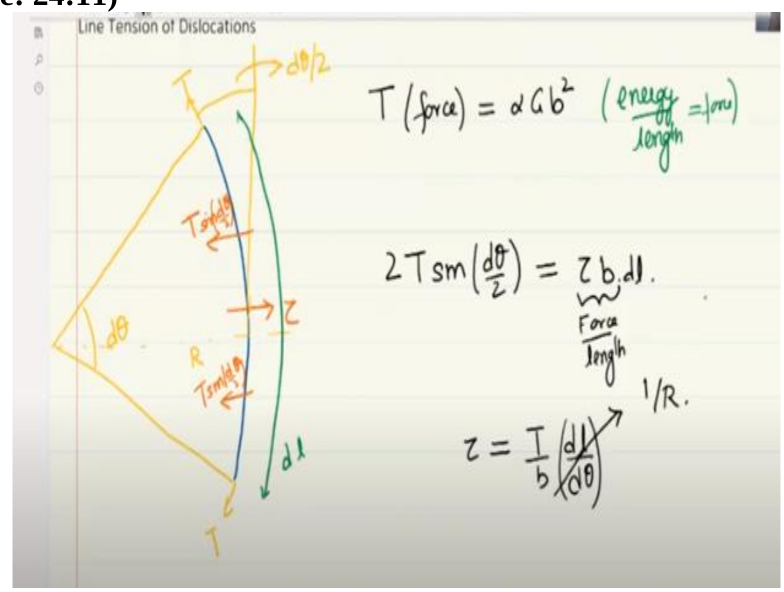
So for the edge dislocation, where we have $\sin\theta$ as the Burgers vector, so we take $Gb^2(\sin\theta)^2/4\pi(1-\nu)$ and for that screw dislocation we have $Gb^2(\cos\theta)^2/4\pi$. And therefore we can take some of these quantities outside and we have a simpler relation $\frac{(\sin\theta)^2}{1-\nu} + (\cos\theta)^2$. So this gives us the relation for the energy of mixed dislocation.

And we have also seen how to compare the energy of the dislocations to find out whether a reaction would be favorable or not. And another important thing that we have mentioned and we will utilize later is to is that there is always a line tension associated with the dislocation and these are the energy of the dislocation, the elastic component and the core component. So that brings us to the end of this lecture.

And we will in the next topic will explore more about dislocation motion. We talked about energy of dislocations. Now related to this is a very important concept about dislocations, which is the line tension. So if you want to increase the length of dislocation, it would basically mean you will have to increase the energy of the dislocations and which as any system would like to minimize.

And therefore, there will be a force tension which will try to disallow it from increasing. And therefore, if you want to or any internal or external stresses wants to cause a curvature in the dislocation, it would mean that it will have to overcome that line tension. So in this particular topic, we will look at the relation between the shear stress required to create a radius of particular curvature against the line tension in the dislocation. So let us begin.

(Refer Slide Time: 24:11)



So let us say that this is a dislocation which has been curved because of some shear stress. So now, I will show the shear stress like this. Shear stress is acting like this τ and there is also line tension, okay. So the line tension will be acting along the line direction at that particular point. So this is assuming a very small region and so we will assume that this is a very small segment which is $d\theta$.

And which would mean that this would also be $d\theta/2$. And this line tension is T and this line tension is also T. So a component of this line tension T is acting in this direction, which is trying to reduce the length or get rid of this curvature. And a shear stress is acting, which will try to create this curvature which has a radius r.

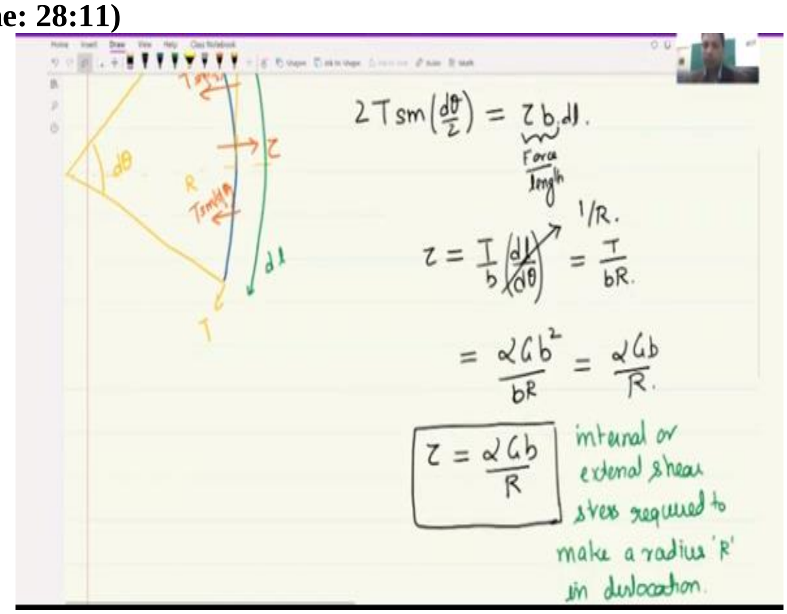
So now, let us look at what is the line tension which is force is basically related to energy and it can be directly given as $\alpha G b^2$. So why it is $\alpha G b^2$? Because $\alpha G b^2$was actually the energy per unit length which is nothing but force. So it is also acting as a force, this energy per unit length.

Now if we take the component which is acting in this direction, so we have T $\sin\frac{d\theta}{2}$. So the component in this direction is $T\sin\frac{d\theta}{2}$. Similarly over here $T\sin\frac{d\theta}{2}$. So there are two of these. Therefore, it means that the total force acting in this direction trying to get rid of this curvature is $2T\sin\frac{d\theta}{2}$.

On the other hand the shear stress that you need to apply is tau which will have to translate it to force where this is the force. So τb let us say this length, overall length is dl. So τb (dl). And you can clearly see this is force per unit length. And into dl which makes it total force. So this is left hand side is force, right hand side is force. So dimensionally we are correct.

And now, when we relate it what we see is that τ is equal to T/b and we will take theta so small that $\sin\frac{d\theta}{2}$ becomes $\frac{d\theta}{2}$. Therefore, this becomes T/b. So this when you $\sin\frac{d\theta}{2}$equal to $\frac{d\theta}{2}$, that 2,2 gets cancelled and what we have $Td\theta$. So τ is equal to$\left(\frac{T}{b}\right)$ $(\frac{dl}{d\theta})$. But $(\frac{dl}{d\theta})$ is nothing but curvature which is equal to 1/R.

(Refer Slide Time: 28:11)



And therefore, this relation translates to T/bR. And T we know is nothing but the $\alpha G b^2$. Therefore this becomes $\alpha G b^2/bR$ which is equal to $\alpha G b/R$. Therefore, you need a shear stress equal to $\alpha G b/R$ with this can be internal or external, internal or external shear stress required to make a radius R in this location.

So this is the effect, side effect of energy that is associated with dislocation which leads to the line tension and which leads to the fact that you must apply at least this much tau to create the right kind of radius. So if you have very small radius you can see that you need a very large shear stress because very small radius means you are creating a very small or you need to create a like a small loop.

Therefore, you need a very large shear stress. On the other hand, a very small radius which means that the curvature is very or the center of radius is very far. In that case you need a very small shear stress. So this is clearly in sync with what we know about dislocations and gives a relation between the shear stress and the radius of curvature. So we will end this topic here. Thank you.