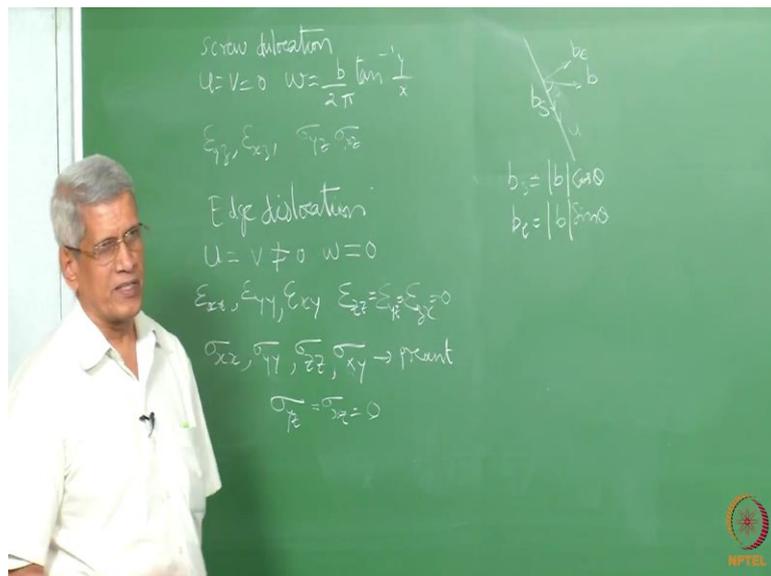


Defects in Materials
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Lecture - 20
Self Energy of Dislocation

Welcome to this class on Defects in Materials. In the last class we have looked at the stress and strain field around here perfect screw and an edge dislocation, but generally the dislocations are not either a perfect screw or an edge dislocation. It is a mix dislocation. So, how do we find out the stress and strain field around the mix dislocation, we will just look at it and all the cases which we are considering is for isotropic case. That isotropic elasticity the; is what we are considering it because for a; is screw dislocation the displacement which is there; u equals v equal 0.

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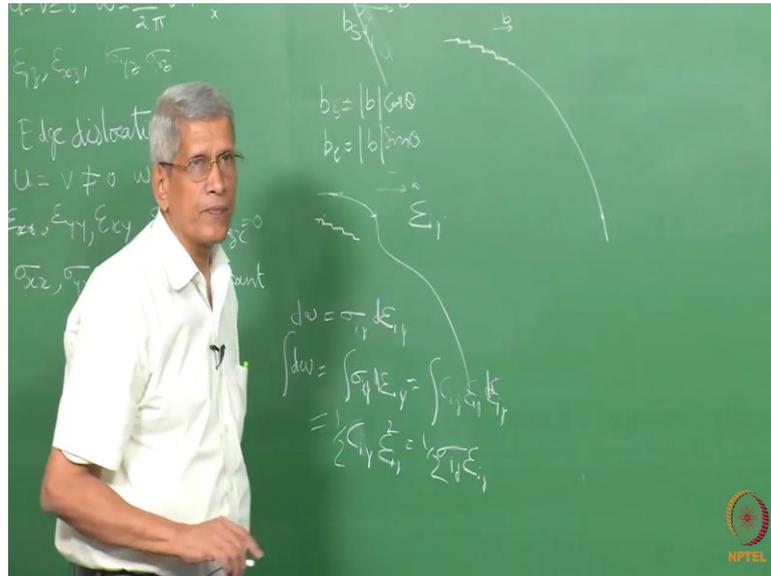
Only the w is going to be there which is d by 2 pi into tan inverse y by x correct and epsilon y is epsilon x is these are all only the stresses which we see and sigma y is a and sigma x is a; are the stress fields which we see around the dislocation. What happens in the case of an edge dislocation? U and v x is; displacement field is not equal to 0 that expression which you had seen in the last class w equal 0, correct and the strains if you look at it epsilon x x, these are all the strain fields are there; equal 0 and stresses if we

look at is σ_{xx} , σ_{yy} , σ_{zz} , these are present σ_{yz} σ_{xz} equal 0, correct, this is how it is. When you look at a screw dislocation and mix dislocation.

For a mix dislocation we assume that the way we can look at is one; we can look at the mix dislocation as a mixed one or we can look at it that this is a straight dislocation with the line direction u and the burgers vector is inclined with respect to dislocation that we also we can consider it. Let us just consider this case then this will be b_e , this is the angle θ it next with the line direction and this will be b_s ; the screw component. So, b_s will be equal to $b \sin \theta$, b_e equals into $b \cos \theta$, correct, from this expression now if you look at it you can understand very easily that for a screw dislocation, only the displacement w is there, correct for a any screw dislocation so; that means, that with respect to it for the screw component if we are trying to find out we will be getting expressions which are corresponding to σ_{yz} (Refer Time: 04:38) σ_{xz} is a these are all the stress components; whereas, with respect to edge component after mix dislocation, we are going to get the other stress components right these components are all independent there is no component which is common.

So, what is the advantage of it? We can take with respect to this corresponding to the screw component only thing is that the b has to be taken as the component of b , b_s and here for this u and v the edge component has to be taken then this can be used to describe these expressions give if you find out the stress and strain with respect to taking the component of a b the screw component and the edge component that for mix dislocation all the stress components could be calculated very easily.

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Generally what happens is dislocation are never straight they are always are like this they will be bent like this, then they will have a burgers vector maybe in a specific direction which is depend to slow graphically. So, the line direction here could be in this direction; line direction here could be in this direction.

So, the various ways in which the line direction, actual computation when we have to do what are the options which we have to choose in, one which we can do it is you take a small segment of this to be the dislocation line correct and with respect to this we can find out the screw and the edge component and do the calculation correct other is way of looking at it if that this itself can be considered as a screw. This is the way that is dislocations will have one b that is a screw component and an edge component the dislocation line itself can be that is before dislocation is bent like it. We can assume it to be like this, a small like this we can take it and if the burgers vector is in this direction then this will be a screw component of the dislocation and this will be the edge component depending upon that here, if you commit the edge component will become more, the screw component will become less that like the very this way also we can look at it, both the options are available for computationally determining.

This stress field and strange field around a mix dislocation; there is should do that we out the split them into screw component and edge component either we take the line direction to be the same take the burgers component or keep the burgers component

burgers vector that same and the line itself can be taken to be and edge gender screw both options are available with these we have got expression for the stress field and the strain field around the dislocation when we know the stress field and the strain field around the dislocation.

We can calculate the total energy which is associated with introducing this location in the sample correct. So, if you look at the dislocation energy in doing that we have to keep on point in mind that here also when we have calculated the stress field the code of the dislocation has been omitted because where the elasticity theory is not or we cannot apply the elasticity theory. If you have to find out the strain energy of the dislocation how do we go about and do it.

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Strain energy of a deformed crystal

In an elastically strained material, stress at any point is nearly related to strain at that point and is given by the Hooke's law related to stress

Physical basis of Hooke's law:
For small strains, displacements of atoms are small and the interatomic force separation relationship can be assumed to be linear over such small range

During elastic deformation, internal elastic forces do work which is converted into potential energy and is recovered when the deformation is removed.

The work done by tractions acting on the unit cube within the body is given by $dw = \sigma_{ij} d\epsilon_{ij}$

If ϵ_{ii} is only acting (all other strains zero), then the above equation can be integrated to find total work done

$$w = \int_0^{\epsilon_{ii}} \sigma_{ii} d\epsilon_{ii} = \int_0^{\epsilon_{ii}} C_{ii} \epsilon_{ii} d\epsilon_{ii} = C_{ii} \int_0^{\epsilon_{ii}} \epsilon_{ii} d\epsilon_{ii} = \frac{1}{2} C_{ii} \epsilon_{ii}^2 = \frac{1}{2} \sigma_{ii} \epsilon_{ii}$$


We know that if you take any material the linear elasticity theory we apply it to find out the strain energy that is the Hooke's law is; we can apply it and all these expressions are given here. That is if by applying some stress a small increment in a strain is introduced into the sample, what will be the total increasing in energy which will be taking place in the material because of this strain these we can write it as sigma into to d epsilon which we can write it anyway in the view graph I had given with respect to a tensor notation here I am just writing it as a which I can write it has epsilon i g.

What we are doing? It is we assume that it is only this component is being applied in only one direction that is a small increment if the total strain changes from 0 to some

particular value take it to be ϵ_{ij} then if you integrate this, we can find out ϵ_{ij} correct, this itself can be returned as the stress can be written as $C_{ijkl} \epsilon_{ij}$; ϵ_{ij} correct, this way we can write it. This will turn out to be C_{ijkl} can finally, to turn out to be half $C_{ijkl} \epsilon_{ij}^2$ it will turn this will be nothing, but half $\sigma_{ij} \epsilon_{ij}$ correct this is how, now we know that stress we know that the stress and strain are consist there are 9 components associated with it if you take a small volume of a crystal and then apply some displacement that will result in stresses and strains.

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For a generalized stress field, the stored energy per unit volume is

$$w = \frac{1}{2} (\sigma_{xx}\epsilon_{xx} + \sigma_{yy}\epsilon_{yy} + \sigma_{zz}\epsilon_{zz} + 2\sigma_{xy}\epsilon_{xy} + 2\sigma_{xz}\epsilon_{xz} + 2\sigma_{yz}\epsilon_{yz})$$

In terms of strain only, the equation becomes

$$w = \frac{1}{2} [(\lambda + G)(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})^2 + 2G\{(\epsilon_{xy}^2 + \epsilon_{xz}^2 + \epsilon_{yz}^2) - 2(\epsilon_{xx}\epsilon_{yy} + \epsilon_{yy}\epsilon_{zz} + \epsilon_{zz}\epsilon_{xx})\}]$$

In terms of stress only, the equation becomes

$$w = \frac{1}{2G} \left[\frac{(\lambda + G)}{(3\lambda + 2G)} (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})^2 + \frac{1}{2} \{(\sigma_{xy}^2 + \sigma_{yz}^2 + \sigma_{xz}^2) - 2(\sigma_{xx}\sigma_{yy} + \sigma_{yy}\sigma_{zz} + \sigma_{zz}\sigma_{xx})\} \right]$$

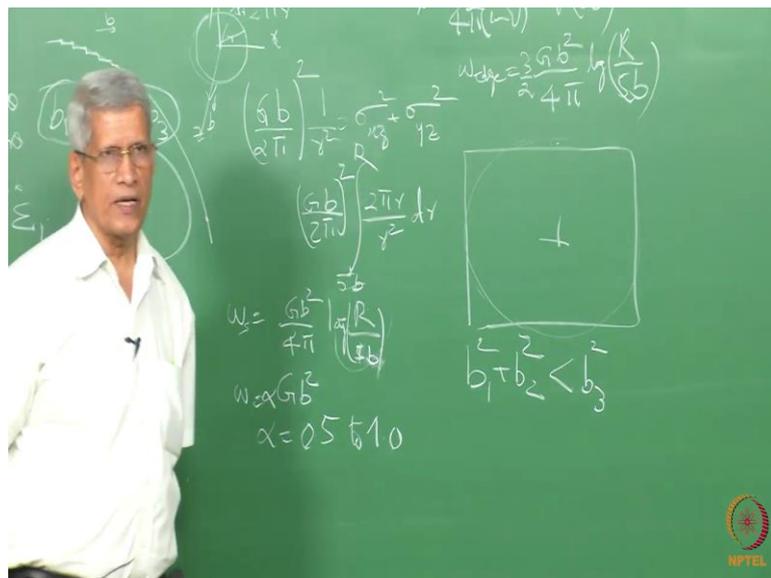

Then the total increase in energy is given by this formula w equals half into all the components here the twice which it has been taken because we know that the stress and strains 9 components are going to be there.

So, this is these components with repeated that is weight twice it comes. So, you now if you look at it total 9 will be there using Hooke's law. We can write this same expression in terms of either strain or in terms of stress correct. So, if we write it in terms of strain then this expression turns out to be in terms of λ and G . This is the way the expression turns out to be and if it; write in terms of stress only then also this equation turns out to be some square terms of stress and then some product terms. But in both the cases if you can see the we can see that essentially it is strain squared will be coming in all the terms are the product of 2 strains are there that is equivalent if they are the same

this to be square term that is how these values turn out to be this is what a general expression when all the components of the stress and strains are present.

Now, we have looked at the dislocation where it has a stress and strains are present around the dislocation, but we know only if few components are there then we can find out, what will be the strain and the stress around the dislocation then whatever the components which are there we can substitute it and find out what is the total energy which is generated in the sample due to the creation of a dislocation in the material here. Again when we consider the strain energy of a are the this energy could be called as a strain energy which is generated in the material you to dislocation are this is called also as the self energy of the dislocation both that terms are being used to represent thus energy the total energy.

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Now it comes of 2 terms one is called the, is the core elastic that this core is the region where we cannot apply their Hooke's law linear elasticity theory cannot be apply.

So, if you look at it, the stress and strains what we had calculated is also outside of the core this will give rise to the elastic displacement this part of the core energy this tells about how the energy is varying within that is small core where the displacements are very large generally this energy has been seen to be rather very smart the core energy. But what is essentially important is that this core energy can change as a function of position as the dislocation most in the material this is what each responsible for lattice

friction stress, because we see that the friction stress varies as the one item moves over the other like a sinusoidal wave that comes that happens in the case of a core energy how do we calculate that elastic energy.

Let us take the case of a screw dislocation which is very easy to do in the case of a screw dislocation essentially around the dislocation, we choose a coordinate system x y is a burgers vector b is in this direction.

So, at a distance r from the core of the dislocation, if you look at it the stress field which is presently sigma y is z and sigma x is z correct, these are all the only 2 stress fields which are present. So, what will be the total energy that we can calculate in this formula? If you see that all other terms turn out to be 0. It is only this term which is going to be their sigma y is squared plus sigma x is square.

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Self energy of dislocation

Two contribution: $W_t = W_{\text{core}} + W_{\text{elastic}}$

$$\sigma_{xz}^2 + \sigma_{yz}^2 = \left(\frac{Gb}{2\pi}\right)^2 \frac{1}{x^2+y^2} = \left(\frac{Gb}{2\pi}\right)^2 \frac{1}{r^2}$$

Screw dislocation

$$W_{\text{el}} = \frac{1}{2G} \left(\frac{Gb}{2\pi}\right)^2 \int_{5b}^R \frac{2\pi r dr}{r^2} = \frac{Gb^2}{4\pi} \log \frac{R}{5b}$$

Edge dislocation

$$W_{\text{el}} = \frac{Gb^2}{4\pi(1-\nu)} \log \frac{R}{5b}$$

Core energy of screw dislocation $\sim 0.2 Gb^2$ per unit length for NaCl

Core energy of screw dislocation $\sim 0.1 Gb^2$ to $0.05Gb^2$ per unit length for glide in close packed planes



That is what essentially is calculated here taking the appropriate expression this turns out to be G b by 2 pi the whole square this is one by r square correct this equals sigma x is z square plus sigma y is z square what this tells this tells the energy at a distance r. What if the total energy suppose you want to know; the total strain energy, we know that the displacement is taking place, suppose we take a material like this, the dislocation line is being percent like this one, so throughout the sample displacement if they are.

Now, we have to calculate what is the total energy strain energy at every point on that sample and add them together then only we get the total energy that in this case, this we can take it to be of circumference $2\pi r$ into a small distance dr . This is the increase in area then what we can do it? We can integrate it these into dr and there integrains from $5b/2$ or which is the out of most radius of the sample when we do this, this value will turn out to be $G b^2$ square by 4π into logger them up r by $5b$, this $5b$ we have chosen because we said that that is the maximum where the size of the core radius depending upon what the value is we have to choose that appropriate value.

So, now what we have caught, it is an expression for the total strain energy which a dislocation is introduced in the sample are what? The same which we call it as the self energy of the dislocation that by introducing a dislocation what is the energy which increase which has taken place in the material similar expression we can get it for this is for screw for edge dislocation if we do it this will turn out to be though a similar methodology, we can adapt for try to adapt for an edge dislocation. But it is much more complicated there are many yeah, but finally, the expressions are essentially the similar one (Refer Time: 19:53) either 1 minus new comes in the Bata.

Looking at this expression there are some few points which become very clear that is value of new at the Poisson ratio is around on by 3. If you take this value input a then what is essentially is going to happen if there the strain energy of screw dislocation is less than that of an edge dislocation that is because here it will be that is the $w_e h$ will be equal to $G b^2$ square by 4π this new equal this will turn out to be 3 by 2.

If we compare this expression with this expression you find that the edge dislocation has got the self energy which is much higher than that of a screw dislocation, is this clear? What will be the consequence of that?

Student: (Refer Time: 21:13).

Suppose we have there dislocation which is a mix dislocation the dislocation will always tries to reach a configuration which is a screw configuration. So, that the energy is less correct that is one what is another consequence of this formula suppose I take a edge dislocate screw dislocation, I apply a stress and try to bend it and what happens there will be an increase in energy. So, it is very difficult to bend a screw dislocation suppose I take an edge dislocation, I try to bend it then what is going to happen it develops a screw

component energy gets lowered. So, it is very easy to bend a edge dislocation. So, bending a screw dislocation is very difficult, but energy of screw dislocation is very small the self energy of an edge dislocation is high you understand that.

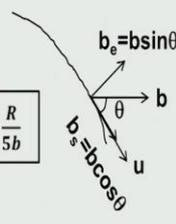
So, these consequences you can understand that from this self energy itself these are all the consequences of having different self energy for screw and an edge dislocation as I mentioned earlier, the core energy of the dislocation screw or a an edge dislocation that core energy is rather a constant value which is a small fraction may be less than 10 percentage of the total energy of the dislocation. And here when we have a dislocation which is present in a sample, how do we calculate that core energy with respect to the total not the core energy the elastic strain energy are the self energy of the dislocation we find out around the radius R which is in this particular case of to end up the sample we have to do the calculation, since this term which corresponds to the distance comes in a large scale if it changes from R equals 1 to 100 or R equals 10 to 100, the value will be this value can turn out to be from 1 to possibly to maximum, correct.

So, it is on a large scale only the increase is going to take this because of that we find that changes are not much as the large volumes are being taken that is one, another factor also which we have to take it if that since it does not increase very largely, we can assume it to be in many cases to be equal to some (Refer Time: 24:16). Generally it is approximated to that equals $\alpha G b^2$ this not of an expression which is being used where this value of α can change from 0.5 to 1 because the rest of the terms are assumed to be not much of a change which we can these an approximation only is a clear, if you try to look at what will be the self energy of a mix dislocation.

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Self energy of mixed dislocation

$$W_{el} = \frac{Gb^2}{4\pi} \left[\cos^2\theta + \frac{\sin^2\theta}{1-\nu} \right] \log \frac{R}{5b} = \frac{Gb^2}{4\pi(1-\nu)} (1 - \nu \cos^2\theta) \log \frac{R}{5b}$$



Self energy of dislocation loop

Stress field of a loop decreases faster than that of a straight dislocation as r increases

$$W_{el} = \frac{Gb^2}{4\pi} \log \frac{R}{5b}$$

R - radius of dislocation loop

$$W_{el} = \alpha Gb^2 \quad \alpha = 0.5 \text{ to } 1.0$$

$$b_1^2 + b_2^2 = b_3^2$$

$$? = \nu$$

Elementary dislocation theory by Wertman and Wertman
NPTEL

Then we can take because as we have seen that since the displacement fields are different in these 2 cases. We can find out that component separately and add them together for the screw and the edge component then we get the expression corresponding to the self energy of a edge dislocation of a mix dislocation. But we know that there is locations need not exist at screw are an edge are a mix dislocation, but sometimes they can be in the form of blue pursue well correct. In the case of a loop also their expression for the elastic the self energy the contribution to self energy from the elastic displacement is given by this formula $G b^2$ squared by 4π into $\log r$ by $5 b$. But essentially this stress field decreases much more rapidly in a screw dislocation than in the case of an edge dislocation here what is R? This r is nothing, but the radius of the loop it is not the dimension of the sample which you are chosen.

So, that is the only difference which one has to understand that and the consequences of for this formula approximating to this value is generally used to find out whether a dislocation reaction will occur or not suppose the dislocation has go to burgers vector b one on another as go to burgers vectors b 2 assume that they interact and producer dislocation which is b 3 that is whether b 1 plus b 3. This reaction will occur or not how do we decide is that if we take if it is in the same material G remains that same, we can find out the b squared value. So, add them together. So, it will be b 1 square plus b 2 square whether it is less than b 3 square, if that is the case then the reaction is possible. This approximation we had this is what we use the rule to find out for the dislocation

reaction is going to occur or not, but this essentially comes from this condition that is what happens to the self energy of a dislocation.

So, for what, we have considered in these cases is essentially with respect to only a single dislocation all these formula correct and here we talked about the 2 dislocations are present are 3 dislocations are present. So, if more dislocations are present how do we calculate the self energy of the dislocation then we have to define this radius r . So, what is generally taken if that if many large quantity of dislocations are present in the sample then what we do it is that find out the average distance between the dislocations separation between the dislocations take half of this to be the r that is how this self energy is calculated quite often, what it can happen if that some of the dislocations can have positive and some can have negative. But producing all of them the energy has to be that same correct we will come to later some of this depending upon the nature of the force some of these dislocations can interact and annihilate these aspects will consider in the later classes.

So, from this, we can understand that there is an energy and this energy whatever we have calculated derived all these expressions or for per unit length of the dislocation right is it clear. The same self energy is used to represent and another important property associated with a dislocation which we call it as a line tension like I mentioned that, if I take an edge dislocation you try to bend it then we try to bend it that can be an increase in the dislocation line length correspondingly an increase in energy and take place.

So, essentially then we can write the force can be defined at $d \times$ correct increasing length we can write it these force this is per unit length if you take it what it happens increase in energy per unit length which turns out to be the force are which call it as a line tension like a soap bubbled then we take it, it has some area associated with it like to shrink. So, we the same energy which we use it as the surface energy of the bubble itself it try you see to represent the force also line has surface tension also correct, the same thing which is being done in the case of a dislocation and the line tension is defined as the increase in energy per unit length of the dislocation. That means, that the same expression gives can be considered as a force correct, how we can do that per a unit length if you take it? This is a constant value this term if you tried to look at it what it turns out to be? This is nothing, but your force n a dimensionally it is a force.

So, that we also we can understand that it represents of force that a g is a Newton per meter square into that b squared you put it, so it becomes dimensioned a force, one minus nu it has to be. That was put us nu I suddenly now I find that I think in that symbol something has happened its put as a question mark what are return was that allowed to correct it I will do that.

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Line tension

Line tension T is defined as the increase in energy per unit increase in length of dislocation line

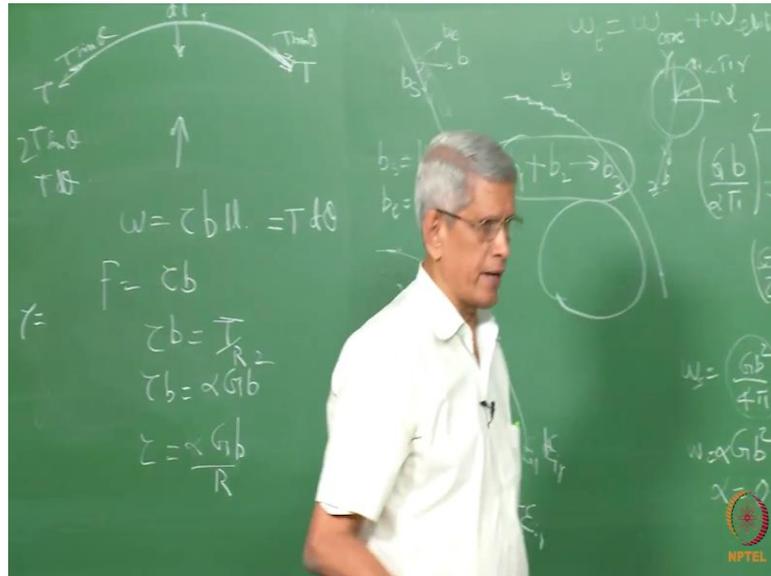
$$T \approx \frac{\mu b^2}{4\pi} \log \frac{R}{5b}$$

$$2T \sin(d\theta/2) = T d\theta$$

$$\tau_0 = \frac{T}{bR}$$

What is the consequence of a line tension? We know that the line tension is similar to suppose we have a thread which he for a (Refer Time: 32:05) you put it in home when we put a cloth on it what happens? So, were because a line intention did not increase, it just drops down, exactly a similar thing will happen with respect to a dislocation.

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So, we assume that dislocation is bent into and t and if you take that tangent which is going to be $T \sin \theta$ here also, T is the line tension the tangent to θ which will come to a line is $T \sin \theta$ it is going to be and this force if we look at it, $\sin \theta$ is the one which will be together (Refer Time: 33:02) 2θ in θ then θ equals small this would be this turns out to be $T d \theta$.

This you can see it in the transparency also this will be giving this to a force downwards, this $T \sin \theta$; the \sin if you look at it the component it is going to come down. If this dislocation has to be kept in that position, in equilibrium position; that means, there should be an opposite force which should act to keep that in that otherwise it will be continuously in bending correct that is like.

Student: (Refer Time: 33:45).

The other way we can look at it is that what will be this force which can keep it in equilibrium; that means, that if at dislocation is bent like this and this dislocation you assume that a small work is being done on this dislocation the dislocation line is trying to move in the opposite direction, what will be the force which we have to apply? That we can calculate it that is because if a dislocation moves from here a unit length of a dislocation by a small distance δS if it moves.

Then for that the stress which is applied this τ you consider, it is the stress into the area will give you the force that force moves a very atom by a distance when a dislocation most by a burgers vector correct. So, the total work done in that case will be equal τ into b into the length of the (Refer Time: 35:03) if a unit length which its being mod correct and this if we take it F will be equal to get the rate of change, correct, it will turn out to be T .

So, this is the sort of a force that we do not know what the τ is, but that force should be equal and opposite force should be applied in this direction. So, that this will be in equilibrium correct in that been conditioned. Then we can equate this when we equate all these terms this will be turning out to be T , what is T ? α into $G b^2$, we can write it your τ will be this is the energy this energy should be equal to T into $d\theta$ this is what the energy balance will be then what this will turn out to be $d\theta$ by $d l$ will turn out to be r the radius of curvature correct. So, this will turn out to be or it will turn out to be.

So, now we have got an expression which is essentially the τ equals $G b$ by R , this expression where do we use it? In the case of a Frank (Refer Time: 37:09) resource are in the case of an edge dislocation are in the case of a war 1 looping, where we have a critical radius where the loop will form they are also this expression which we use it to find out, what is going to be the stress and critical stress which is required for loop to form, correct.

So far we have considered both these cases, essentially the line tension and the self energy of a dislocation what are possible applications these cases we will consider later when we come to about the different types of sources for dislocation generation in the material and interaction of a dislocation with second phase particles. Then we will talk about how this expression is being used.

We will stop here, tomorrow what we will do it is we will be using where are the next class will talking about the forces which will be operating on and dislocation, what all the types of forces which. That is a very elegant wave method in which these forces could be calculated lets called as a peach (Refer Time: 38:36) force that aspect of it, we will discuss in the next class, we will stop here now.