

Introduction to crystal elasticity and crystal plasticity
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Week-05
Lecture-10

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Good Morning everybody, uhh let us start with the other part of the crystal plus plasticity. So far we have discussed imperfection and the slip system. In crystal imperfection specifically we explain that the different type of defects exists in the within the crystal lattices, that imperfections of defects can be classified like point defect, line defects, and surfedge defects. So several point defects we have explained and then line defects we have tried to explain in terms of uhh dislocation and how dislocation is characterize in terms of the Burger's Vector and finally we have described the surfedge defects for example the grain boundary can be considered as a surfedge defect exist in the crystal lattices.

So with the basic concepts of the defects we have started to analyze the plasticity in the crystal structure and further we have analyzed the slip system that actually associated with the deformation of the crystals and we have looked into the different slip planes and the slip directions for the very basic crystal structure for example FCC, BCC and HCP structures. And we have observed that the basic types of dislocation for example, (())(2:14) Dislocation and Screw Dislocations and accordingly we have define the different crystal planes where actually there is a deformation of the lattices happens with application of the extra load and this deformation we have experienced in sums of the shear stresses and for a specific type of

crystal structure there is some specified slip plane over which and specified direction over which basically slip occurs.

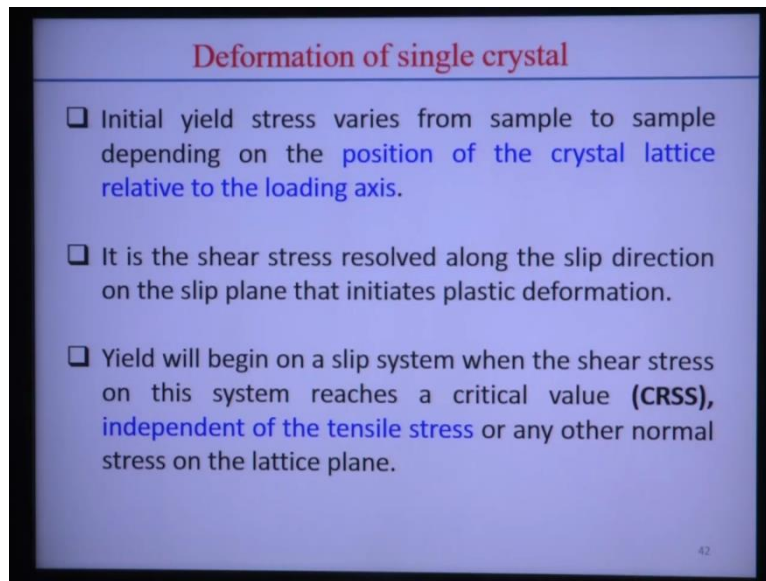
And we have seen there is a several combination of different type of slip system in BCC, FCC and HCP crystal structure.

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So in continuation with that slip system now we shift to the next topic that is dislocation geometry and energy stress field due to dislocation, dissociation of the dislocations dislocation mechanics will be explained as a part of the crystal plasticity with a last class we have simply explained the very basic types of the different crystals and their defects and now we will stick with a very basic terms generally used to explain the dislocation geometry and energy uhh corresponding to the stress field generated to the uhh existence of the dislocation.

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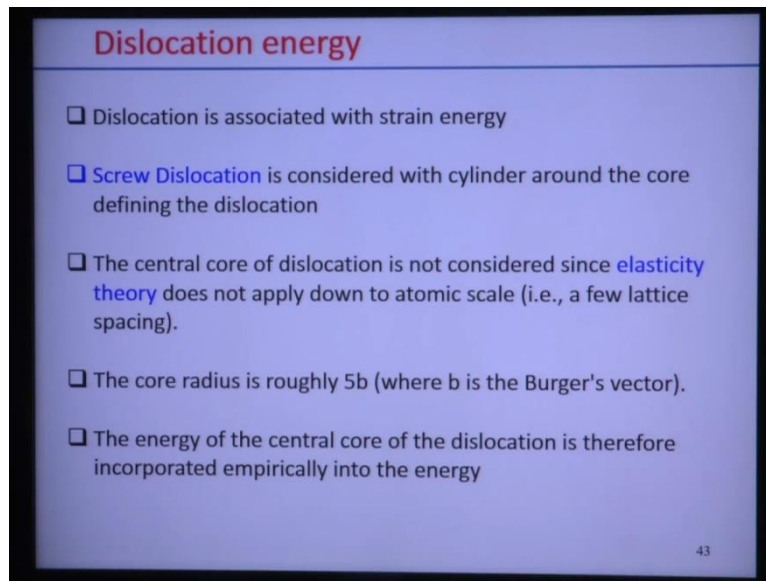


Now let us look into this first very two topics, first we just try to start with the dislocation geometry energy, by looking into that main key points of the deformation of single crystals. So first significant point is that initial yield stress actually varies from sample to sample depending upon the position of the crystal lattice related to the loading axis. This is the one key point for the deformation of single crystal.

And second point is that we have observed that the shear stress actually resolved along the slip direction on the specified slip plane and that actually initiates the plastic deformation in a single crystal structure. And next important point is that yield will actually begin on a slip system when the shear stress exist some critical value that is called critically resolved shear stress and that critical value actually independent of the tensile stresses or any other normal stresses that actually acting on the lattice plane.

That is the most significant point to analyze the slip system or deformation of the single crystal structure so, point here is that we simply separating the critically shear stress region shear stress value and with respect to the application of the other normal stresses in a single crystal structure.

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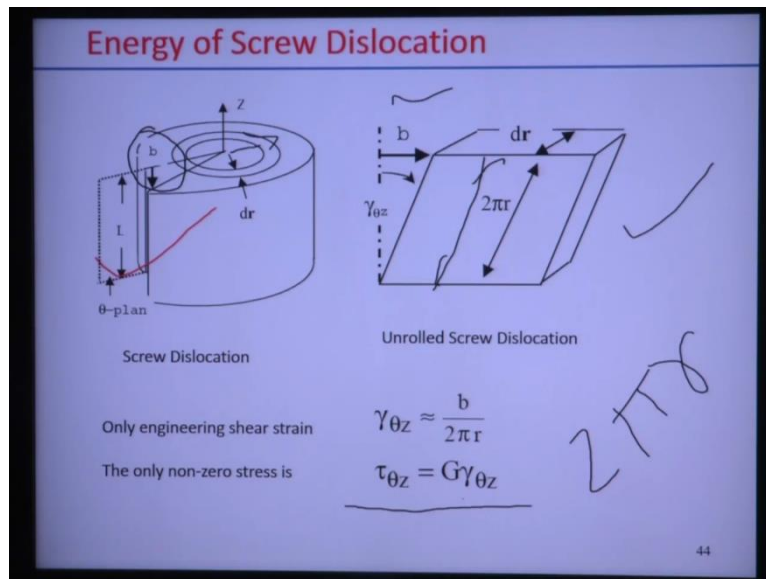


Now if we look into the term the dislocation energy. Definitely when there is the existence of the dislocation in a single crystal structure it is associated with some amount of strain energy and then we will try to explain the, or we will try to roughly estimate the amount of the strain energy associated with the Screw Dislocation and Edge Dislocation. Basically the Screw Dislocation and Edge Dislocation is the basic two elements of maybe ideal cases of the dislocation and that we can further complicated calculation start with this two types of basic crystal dislocation.

First when we try to explain the energy associated with the Screw Dislocation simply we can consider a $(\)$ (6:46) around the dislocation and we actually divide it into the two different zones one is the core of the dislocation and other is the elastic deformation zone. So the central core of dislocation actually is not considered in this elasticity, in this calculation using the elasticity theory because that core actually the existence of the core lies within the few lattice spacing or maybe just down to the atomic scale so continuum elasticity theory may not be applicable to estimate the energy associated with the core.

So then core radius is roughly most of the materials is around 5 times of the Burger's Vector for a specific material and the energy of the core is actually estimated empirically or we try to correlate the amount of the energy assisted with the core with respect to the other part of the energy estimation, for example outside of the core. Now how to estimate the energy associated with the Screw Dislocation.

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So if we look into the representation of the Screw Dislocation, we can see that this dislocation exist along z axis and the Burger's Vector which is parallel to the z axis is acting here, if you look into this, Burger's Vector. Now we can simply explain this thing if it is caught along the θ -plane, this is the total the height or this length actually represents that twice pi R and v here is the Burger's Vector and we have considered one element with respect to z axis at a distance R and then uhh elemental radius or elemental radius is dr.

So unrolled Screw Dislocation is represented the right hand side figure and here if you their existence only of the engineering shear strain on that theta z plane and we can estimate that from the very basic definition how to define the shear strain here is that Burger's Vector divided by the perpendicular length, so here perpendicular length is Y. It comes from the simply opening the elemental segment and that segmental length is twice pi into r, and then b by twice pi r is actually represents the shear strain in this case.

So this is a very ideal case and then only non-zero shear stress exists in this case, that is Tau theta z on this plane, so that can be estimated in terms of the shear modulus and shear strain. So this is the simply estimation of the non-zero shear stress in case of the Screw Dislocation, but what is the associated energy. So once we consider, if we look into that along the radial distance r we basically consider one elemental segment of radial distance dr.

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Energy of Screw Dislocation

For this infinitesimal region, the strain energy per volume is

$$\frac{dE_{\text{screw}}}{dV} = \int \tau \, d\gamma = \int (G\gamma) \, d\gamma = \frac{1}{2}G\gamma^2 = \frac{1}{2}G\left(\frac{b}{2\pi r}\right)^2 = \frac{Gb^2}{8\pi^2 r^2}$$

With cylinder volume $dV = 2\pi r L \, dr$,

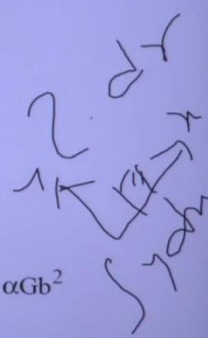
Incremental elastic strain energy

$$dE_{\text{screw}} = (2\pi r L \, dr) \left(\frac{Gb^2}{8\pi^2 r^2} \right) = \frac{Gb^2}{4\pi} \frac{dr}{r} L$$

The energy per unit length of a screw dislocation is

$$E_{\text{screw}} = \frac{E_{\text{screw}}}{L} = \int_{r_0}^r \frac{dE}{L} = \frac{Gb^2}{4\pi} \ln\left(\frac{r}{r_0}\right) = \alpha Gb^2$$

$\alpha = 0.5 - 1$ and $r_0 \approx 5b$



And looking into that elemental area we can find out the strain energy associated with the small element, radial element dr is simply intrication of the stress and strain. So this is the actually the elemental uhh with a small element the amount of the strain energy which is multiplied by the strain into element of the shear strain here. It can be like that we have, I think we have already explained that if this is the y axis and x axis and area of the specified curve can be represented or small element area can be represented like that, intrication of ydx , so that ydx actually represents the elemental area and if we intricate over the (\int) (12:20) then we can estimate the total area occupied this specified curve.

So similar things we can represents here in terms of the strain and stress axis and then over the strain and stress axis the elemental area actually represents here τ into $d\gamma$ that is the representation of the amount of strain energy per unit volume. Now once we intricate over, so this actually represents the amount of the strain energy per unit volume. So if we look into the further calculation we can find out that we put in the shear strain value and we can find out the amount of the strain energy associated with the in terms of the Burger's Vector and the radial distance R over which the elements is consider.

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Energy of Screw Dislocation

For this infinitesimal region, the strain energy per volume is

$$\frac{dE_{screw}}{dV} = \int \tau \, d\gamma = \int (G\gamma) \, d\gamma = \frac{1}{2}G\gamma^2 = \frac{1}{2}G\left(\frac{b}{2\pi r}\right)^2 = \frac{Gb^2}{8\pi^2 r^2}$$

With cylinder volume $dV = 2\pi r L \, dr$.

Incremental elastic strain energy

$$dE_{screw} = (2\pi r L \, dr) \left(\frac{Gb^2}{8\pi^2 r^2} \right) = \frac{Gb^2}{4\pi} \frac{dr}{r} L$$


The energy per unit length of a screw dislocation is

$$E_{screw} = \frac{E_{screw}}{L} = \int_{r_0}^r \frac{dE}{L} = \frac{Gb^2}{4\pi} \ln\left(\frac{r}{r_0}\right) = \alpha Gb^2$$

$\alpha = 0.5-1$ and $r_0 \approx 5b$

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Now this elemental volume can be calculated like that twice pi r is the periphery and L is extended the length of the dislocation or here we can say the length of the axis, length of the cylinder and if you multiply by dr that actually represents the elemental volume and so elemental total energy, if we multiply by the elemental volume then we can find out the total elemental energy is like, expression is represented like this.

Now the energy per unit length of the Screw Dislocation can be represented like this and where the radial distance actually varies from r_0 to r . So r_0 can be considered as a radius of the core and r up to what extent of the dislocation exists. So some finite value of r actually exist here and if we integrate over r_0 to r we can find out this is the expression of the dislocation energy associated with the Screw Dislocation. So this can be further represented by approximately alpha into Gb square or normally the alpha varies from 0.5 to 1 and normally r_0 that means co-radius can be considered as the 5 times of the Burger's Vector, or very simplified way we can assume the theory of elasticity, we can estimate the amount of energy associated with the Screw Dislocation, how we can further estimate on the limit of this core or R by looking into a very typical example.

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Energy of Screw Dislocation

Total strain energy (per unit length) for a screw dislocation

$$E_{\text{total}} = E_{\text{core}} + E_{\text{elastic strain}}$$

Roughly, due to r dependence

$$\frac{1}{4\pi} \ln\left(\frac{r}{r_0}\right) \approx \frac{1}{2}$$

$$E_{\text{screw}} = \frac{Gb^2}{4\pi} \ln\left(\frac{r}{r_0}\right) \approx \frac{Gb^2}{2}$$

Estimate the lower limit of r_0 and upper limit of 'r'

If $r_0 = 0$ and $r = \infty$ both would cause $\frac{U}{L} \rightarrow \infty$
 $\gamma \rightarrow \infty$ if $r_0 = 0$ i.e infinite shear strain

This is not reasonable – energy can not be higher than heat of vaporization

$$dU \text{ (or } dW) = \frac{L G b^2}{4\pi} \frac{dr}{r}$$

$$\therefore \frac{dU}{dr} = \frac{1}{r} * \text{constant}$$

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So since the estimation of the elastic energy didn't consider the energy associated with the core so total amount of the energy in practically Screw Dislocation consist of the two part, one is the energy associated with the core another is the energy associated with the elastic strain. So total energy is decomposed into two parts, core energy and elastic strain energy. So far we have calculated the elastic strain energy, now how to estimate the energy of the core. Just look into that, but before that the energy dislocation energy is generally estimation is that we have only show this is the estimation and we consider some term alpha and this alpha is normally consider as a hub.

Until and unless the information available for estimation of this alpha we can consider alpha as a 0.5 or half here. This is rough estimation, now how to estimate the lower limit of r_0 and upper limit of r , physically reasoning for that, if we look into that estimation of the elastic for Screw Dislocation and if the r_0 equal to 0 or if r tends to infinite in both the cases the strain energy per unit length actually tends to infinity. Even also if strain total strain is tends to infinity when r_0 equal to 0 that means when r_0 is equal to 0 at this point the amount of the strain is infinity but practically it is not reasonable so energy cannot be higher than that of the heat of vaporization, so with this typical analogy we can further represent the amount of the energy du or dw and with respect to the radial distance r so du by dr are here, so here du or dw both are equivalent. We have used other symbol here. So that ratio du by dr is basically some other parameter constant and it is proportional to the 1 by r .

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Energy of Screw Dislocation

Lower limit such that neglected energy of the core in the region $0 < r < r_o$ is equal to the over estimation of the integral for $r > r_o$.

$r_o = \frac{b}{4}$ can be suggested

The upper limit of R is half of the distance between dislocations.

If we assume $R \approx 10^5 b$ corresponds to $\rho = 10^{10} \text{ (1/m}^2\text{)}$

Since, $\ln\left(\frac{R}{r_o}\right) = \ln\left(\frac{10^5 b}{0.25b}\right) = 12.9 \approx 4\pi$

Therefore, $\frac{U}{L} \approx Gb^2$

However, most general estimation is $\frac{U}{L} \approx \frac{1}{2} Gb^2$

So if proportional to the $1/r$ then this right hand side actually represents the typical variation if we look into that du by dr , $1/r$ into some constant term because shear modulus Burger's Vector for specific material can be consider as a constant term here. So at r tends to 0, it becomes infinite. But actually there is a finite value of the amount of the strain so actually figure du by dr can be consider as here. So with respect to the actual du by dr and to compensate the amount of the that energy with respect to the $(1/r)$ calculation, we can simply compensate the amount of the over estimation and amount of the, actual amount of the core energy looking into this balance this energy.

We can find out that over the region 0 to r_o is equal to the over estimation of the intrical r greater than r_o and then in this case if we consider r_o equal to $b/4$, but this is the typical calculation not necessary always r_o should be $b/4$, here the objective is to show how we can estimate this calculation. Now the upper the limit of r is normally consider the half of the distance between the two consecutive dislocations so that assume that between the two consecutive dislocation the effect of the energy associated with this things exactly meet points between the two dislocations and when it is just cross the meet point that amount of the energy associated to the next dislocation.

So it is quite reasonable to assume that the extend of the upper limit of the dislocation is meet way between the two dislocations, now if we assume that r equal to 10^5 into b corresponds to the dislocation density for a specific sample is 10^{10} $1/m^2$, in this case we can simply find out r by r_o . So here r_o is specified and from that stress

state value we can find out that logarithm of r by r0 is roughly 4 pi. So this estimation shows that you by L equal to Gb square.

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The upper limit of R is half of the distance between dislocations.

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So this estimation actually if we look into that previous calculation that alpha Gb square and we have already mention that alpha is lying between the 0.5 to 1 so this calculation actually following the limit. So this is the typical estimation of the energy per unit length in case of the Screw Dislocation but in general we use the energy per unit length of dislocation is half of Gb square.

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Energy of Edge Dislocation

For idealized edge component, one entire plane has been pushed into the other planes above the glide plane but not below

Poisson Effect along length of line, which yields a $(1 - \nu)$ in denominator for strain.

$$E_{edge} = \frac{Gb^2}{4\pi(1-\nu)} \ln\left(\frac{r}{r_o}\right) \approx \frac{Gb^2}{2(1-\nu)}$$

For many materials $\nu = 1/3$, so the energy of an edge dislocation is larger than a screw dislocation $E_{edge} = \frac{3}{2} E_{screw}$

Now we will come to that point of the estimation of the energy for the edge dislocation, first we will try to represent the idealized edge dislocation component, if we look into this figure, here one entire plane has been exactly pushed into the other planes above which the sliding of gliding plane but not below that. So over this plane if we look into their existence of the compression here and the dislocation line actually represents along the x_3 axis and the Burger's Vector b represents here which is basically following that perpendicular to the dislocation line here.

But in this case it is necessary to consider the Poisson Effect which yield $1/(1-\mu)$ term in the denominator. So μ is basically here the Poisson ratio and looking into that Poisson effect we can estimate the similar way, the energy associated with the Edge dislocation. Now the point is that why the Poisson effect comes into estimation when you try to estimate the dislocation energy associated with the edge dislocation. If we look into the stress field associated with the edge dislocation which is different from the Screw Dislocation.

We will discuss further in further slide, but point is that we considered the effect of the Poisson effect here to estimate the associated energy in case of the edge dislocation. And in case edge dislocation that we simply multiplying by the denominator $1/(1-\mu)$ term that is due to the effect of the Poisson ration. Now approximate estimation $Gb^2/(4\pi(1-\mu)) \ln(r_0/r_c)$ but here basically approximation estimation this logarithm term we generally that roughly we can estimated the 2π so that it is if you exclude the $1/(1-\mu)$ terms it is actually equal to the associated strain energy in case of the Screw Dislocation.

Now if we consider the μ equal to $1/3$ that means Poisson ratio is $1/3$ that actually in case of the most of the materials then we can find out that energy associated with the edge dislocation is more than that of the Screw Dislocation. Normally it is 1.5 times of the Screw Dislocation.

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Energy of Edge Dislocation

$$\frac{W}{L} = \frac{W^E}{L} = \frac{G b^2}{1-\mu}, \quad \mu = \text{Poisson's ratio}$$

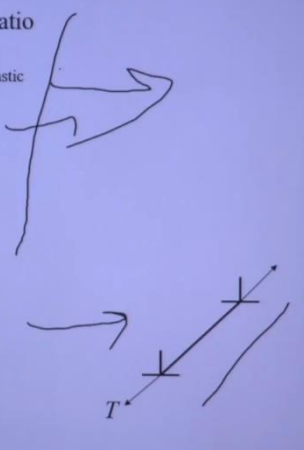
Now, $\frac{W}{L}$ i.e. $W^{\text{total}} = W^{\text{core}} + W^{\text{elastic}}$

$$W^{\text{core}} = 10\% \text{ of } W^{\text{total}} \approx \frac{G b^2}{10}$$

$$W_{L \text{ edge}} = \frac{G b^2}{1-\mu} \text{ if } \mu = 1/3$$

$$W_{L \text{ edge}} = 3/2 G b^2 = E_{\text{edge}} = \frac{3}{2} E_{\text{screw}}$$

Line tension = strain energy per unit length

$$T \approx \frac{1}{2} G b^2$$


The diagram shows a dislocation line with a half-plane of atoms above it. A force T is applied perpendicular to the dislocation line, representing line tension.

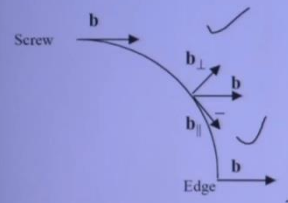
Now this is also further typical calculation to make the understanding of the how to estimate the energy associated to the dislocation, here if you see that total energy in case of edge dislocation again it is consist of the core plus elastic energy and normally the core energy can be consider as the 10 percent of the total energy. So estimation of the $G b^2$ by 10 and this is true for the Screw Dislocation and edge dislocation $G b^2$ square by 1 minus mu if mu equal to 1 by 3. So this at the typical estimation of the different parameter core, that means associated with the core energy, amount of the core energy and associated with the Screw Dislocation and associated with the edge dislocation.

So finally here also we can see that edge dislocation is the 1.5 times of the Screw Dislocation. But if we represent this is as the right side figure as a dislocation and there is a line tension t acting on this thing which is equivalent to the amount of the strain energy per unit length, if we look into this thing the unit consistency in this case also you can find out the energy, the strain energy per unit length is basically line tension in case of the or can be represented as a line tension in case of the dislocation.

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Energy of Mixed Dislocations

Estimation of the energy of a mixed dislocation
Assumption: ignoring interaction between the edge and screw components



At any general place along the dislocation loop
 $\mathbf{b} = \mathbf{b}_{\perp} + \mathbf{b}_{\parallel}$,
 with
 $b_{\parallel} = b \cos \theta$
 $b_{\perp} = b \sin \theta$

Approximately, $E_{\text{mixed}} = \frac{Gb_{\perp}^2}{4\pi(1-\nu)} \ln\left(\frac{r}{r_0}\right) + \frac{Gb_{\parallel}^2}{4\pi} \ln\left(\frac{r}{r_0}\right)$
 $= \frac{Gb^2}{4\pi(1-\nu)} \ln\left(\frac{r}{r_0}\right) [\sin^2 \theta + (1-\nu)\cos^2 \theta]$
 or $E_{\text{mixed}} = \frac{Gb^2}{4\pi(1-\nu)} \ln\left(\frac{r}{r_0}\right) [1 - \nu \cos^2 \theta]$

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Now we shift to the how to estimate the energy of the mixed dislocation. Because this is the most practical cases and if you look into any sample, because we can find out in case of mixed dislocation can be represented to the consist of the ideal case of edge and Screw Dislocation. So actually when you try to estimate the mixed dislocation and here we can assume the interaction between the edge and screw dislocation are neglected. To looking into or to consider this assumption we can find out that there is a one dislocation b within the dislocation loop, is the consist of the two parts, one is the edge dislocation another is the screw dislocation.

And of course this screw dislocation, this is the part, screw dislocation this one $b \cos \theta$ and the edge dislocation is $b \sin \theta$ here and approximately we can find out the dislocation energy for the mixed dislocation is the consist of the this is the energy associated with the edge dislocation and this is energy associated with the screw dislocation and we can find out the mixed dislocation is the to some extent in terms of the (θ) angle θ here but here you need to define the angle θ .

So this is the typical way we can estimate the or most simplified way we can estimate the dislocation energy associated with the mixed dislocations. Now with this theory of the estimation of the dislocation energy we will try to make understand how we can use this theoretical knowledge to estimate the energy associated with the one specific, so let us look into that very physical problem here.

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Example

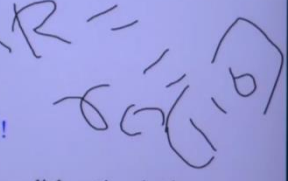
Calculate the elastic strain energy per unit dislocation length associated with screw dislocations in a metallic crystal of copper having a lattice parameter of $a = 0.361$ nm. Shear modulus of copper is 35 GPa. Assume that this energy is negligible beyond 4×10^{-6} m and that non-elastic core energy dominates at distances smaller than 1.6 nm.

In screw dislocation, strain energy per unit dislocation length

$$E = \frac{Gb^2}{4\pi} \ln(R/r)$$

Here, $G = 35 \times 10^9$ N/m²
 $R = 4 \times 10^{-6}$ m, $r = 1.6 \times 10^{-9}$ m
Copper follows FCC crystal structure.
Calculate the magnitude of Burgers vector!!

Elastic strain energy per unit length for screw dislocation is the numerical value of E (unit of force)



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Calculate the strain energy per unit dislocation length associated with the Screw Dislocation in a metallic crystal of copper having lattice parameter a equal to 0.361 nanometer. Shear modulus of copper is given but here the information like that this energy is negligible beyond the 4×10^{-6} meter and the non-elastic core energy dominate at distance smaller than 1.6 nanometer. So from this statement what we can estimate this things, from this statement we can find out that energy is negligible beyond certain length that means beyond certain length in the sense that energy associated with the beyond length maybe subjected to some other dislocation or maybe part of the dislocation associated with one specific sample.

So that statement actually defines the limit of the R , so R is define that term 4×10^{-6} meter, and second assumption that the non-elastic core energy dominates at distance smaller than 1.6 nanometer, this actually defines the size of the core, so here r_0 is basically 1.6 nanometer above which the we can apply the elastic theory to estimate the strain energy. So once from the statement we can find out the capital R or small r_0 then simply we can put the amount of the dislocation energy per unit length we can find out, but other information shear modulus is the material property that we can readily available and we can use that shear modulus value.

But here we need to find out the B , B means the magnitude of the Burger's vector so here the metal is copper and we know that the copper is having FCC crystal structure and once we know the crystal structure we can easily find out the full Burger's vector in this case. So for

FCC crystal structure how to estimate the full Burger's Vector to do that uhh we need to define what maybe the slip plane in case of FCC structure and that is 111 and that is the slip plane and what maybe the preferred slip direction that is 110.

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Example

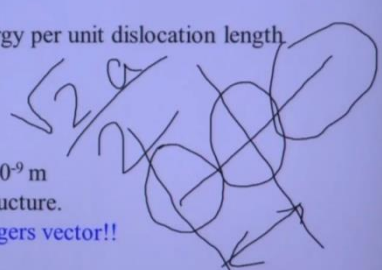
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 $R = 4 \times 10^{-6}$ m, $r = 1.6 \times 10^{-9}$ m
 Copper follows FCC crystal structure.
 Calculate the magnitude of Burgers vector!!

Elastic strain energy per unit length for screw dislocation is the numerical value of E (unit of force)

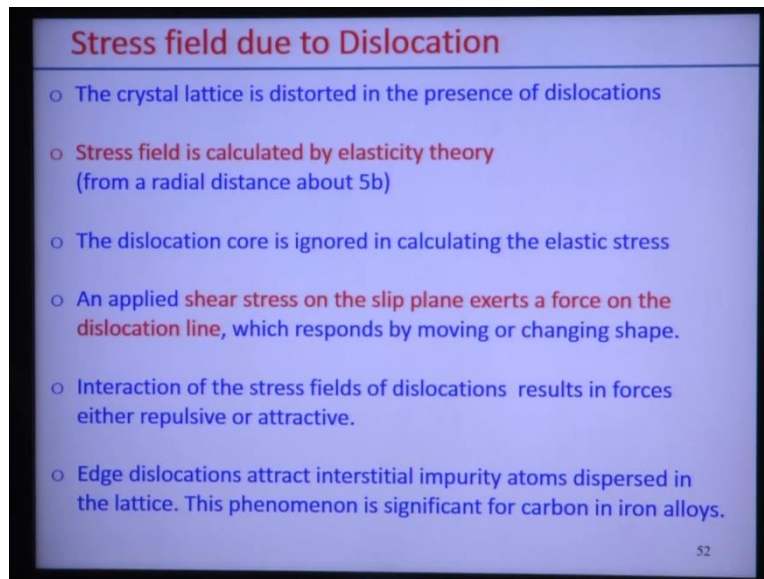


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So preferred slip direction equal to 110 is basically indicated the along the face diagonal, so along the phase diagonal the typical arrangement of the atom, so here the 1 layer of the atom displacement or half plane of the atom displacement is can be considered as this one. So 1 it is the shortage repeat distance along the phase diagonal so that shortest repeat distance along the phase diagonal represents the Burger's vector here.

So once we know the phase diagonal is basically the root to into lattice parameter or h plane and half of that Burger's vector so once the a is given, the lattice parameter is given and from there we can find out the Burger's vector so then the magnitude of the Burger's vector and if we put it here and we can find out the elastic energy associated with the Screw Dislocation in this case. So once we can estimate or typically estimate the amount of the strain energy associated with the edge and screw dislocation.

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Stress field due to Dislocation

- The crystal lattice is distorted in the presence of dislocations
- Stress field is calculated by elasticity theory (from a radial distance about $5b$)
- The dislocation core is ignored in calculating the elastic stress
- An applied shear stress on the slip plane exerts a force on the dislocation line, which responds by moving or changing shape.
- Interaction of the stress fields of dislocations results in forces either repulsive or attractive.
- Edge dislocations attract interstitial impurity atoms dispersed in the lattice. This phenomenon is significant for carbon in iron alloys.

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Now we will try to focus on the stress field associated with the dislocation, so since the dislocation is associated in some amount of the strain and associated with some amount of strain energy so of course it is important to analyze the stress field generated by the presence of dislocation and how we can represent this stress field in the different two idealized case that means in case of edge and screw dislocation. Now to estimate the stress field, the crystal lattice is distorted in the presence of the dislocation and of course here also stress field we can estimate simply by using the elasticity theory and we assuming that elasticity theory is applicable from a radial distance above $5b$ that means beyond the core in case of edge or screw dislocation.

And in this case definitely you are ignoring the effect of the elastic stress within the dislocation core and that one important point is here that applied stress on the slip plane actually exerts a force on the dislocation line which corresponds to the moving or changing the shape or maybe displacement of the layer of atoms, now interaction of the stress field of course here we will try to analyze this things due to the dislocation and that actually results in the either repulsive of the attractive forces during the interaction of the two different dislocation or maybe stress field of the dislocation.

Now significant findings from the interaction of the stress field you can explain that this thing edge dislocation attract basically interstitial impurity atoms disperse in the lattice and this maybe significant in case of the interstitial solution between the carbon and atoms. So

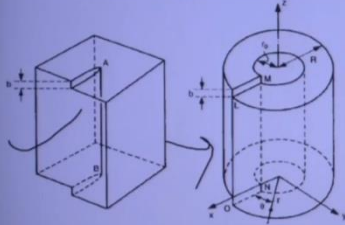
looking into the all the significant points let us look into the stress field associated with the screw dislocation.

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Stress field of screw dislocation

Apply continuum mechanics: elastic distortion introduced by stress field of dislocations

Consider a dislocation in a crystal and built a hollow cylinder around it.



$$\sigma_{ij} = \begin{vmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{xy} & \sigma_{yy} & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & \sigma_{zz} \end{vmatrix}$$

Cartesian - cylindrical coordinate system

$$\begin{cases} x = r \cos \theta \\ y = r \sin \theta \\ z = z \end{cases}$$

Pure shear stress in Z direction

$$\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = 0 = \tau_{xy} \quad (\text{cartesian coordinates})$$

$$\sigma_{rr} = \sigma_{\theta\theta} = \sigma_{zz} = 0 = \tau_{r\theta} = \tau_{rz} \quad (\text{cylindric coordinates})$$

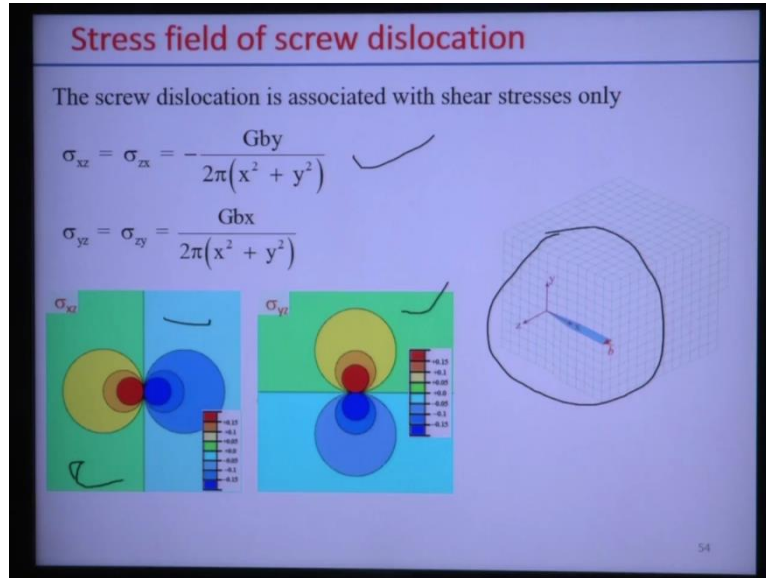
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If we look into that figure that this is the actual representation of the screw dislocations and where if you see the A B actually represents the dislocation line and the Burger's vector actually represent the parallel dislocation line. Now idealized case is like that it represent this things in this two dislocation, one cylindrical element and we define the core and out of the core zone, two different zone with respect to the z axis. So actually when you try to estimate the stress field due to the Screw Dislocation here also you use the elasticity theory and with the ideally representation of the Screw Dislocation in this case, we can find out the stress, this is the normal stress field here, that consist of the normal stress and the shear stress component and we can exchange or interchange between the cylindrical coordinate system to the Cartesian coordinate system by looking into the simple this transformation relation.

Now here if you see, if we represent the dislocation line along the z axis and Burger's vector also parallel to the z axis so in the Cartesian coordinate system we can find out the stress field is like that there are no normal stresses and there exist only the two shear stress component because of the pure shear along the z direction. If you look pure shear since there is a pure shear along the z direction so shear stress component associated with the xz or yz exist in this case but the shear stress associated with the xy plane is 0 here.

So this is the typical stress state in the Cartesian coordinate system in case of the (())(39:17) dislocation but if we look into that cylindrical coordinate system here also we see there is no normal stress compo and only the shear stress component on the theta z plane.

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Now if we look into that the Screw Dislocation or the representation of the stress field associated with the Screw Dislocation and over the Cartesian coordinate system so right hand side figure if you see this is the ideal representation of the Screw Dislocation from the Cartesian coordinate system and here if you see the two shear stress component is like that in terms of the coordinate xy and shear constant term, shear modulus G and the Burger's vector B and if we look into their distribution if you see that the figures, sigma x shape or maybe the shear stress of the xz plane, the rest color actually this side defines, the positive value that means tensile stress field and right hand side represents actually the compressive stress field that negative value indicates.

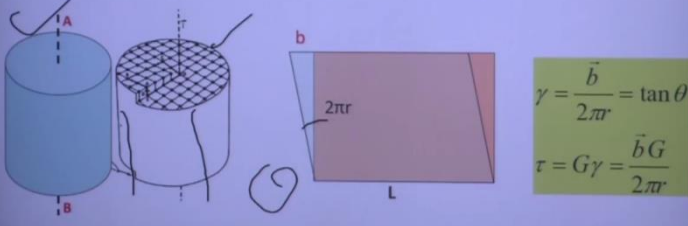
This is the schematically representation of the stress field associated with the Screw Dislocation and similarly stress field associated with the yz is like that also, red color represent the tension stress field and is the negative or compressive stress field, so like that.

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Stress field of Screw Dislocation

Assume: a perfect crystal of cylindrical shape (elastic body)
Introduce a screw dislocation along **AB**
The Burger's vector is parallel to the dislocation line.
Unwrap the surface of the cylinder into the plane of the paper

shear stress in a radial plane ($\tau = \text{const.}$) in z-direction
Obviously one obtains a pure shear in z-direction.


$$\gamma = \frac{\vec{b}}{2\pi r} = \tan \theta$$
$$\tau = G\gamma = \frac{\vec{b}G}{2\pi r}$$

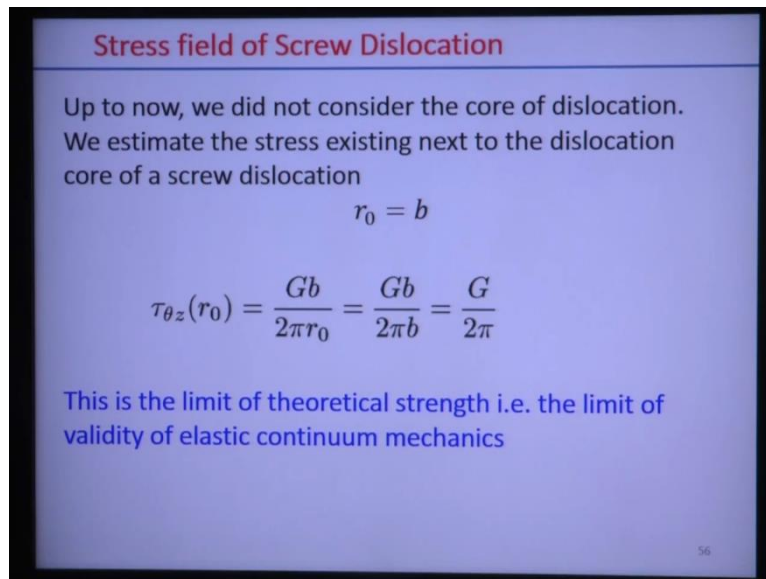
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Now if we try to estimate that the stress field associated with the Screw Dislocation by assuming that the cylindrical shape of the elastic body and here if you introduce screw dislocation along the AB and if we find out that this is the actual representation or maybe there is a area of the dislocation over which the stress field actually exist, this is the representation by the first cylinder and second is the actual representation of the dislocation line and the Burger's vector in case of the screw dislocation.

Now we observe that actually with this axis configuration the shear stress exist actually along the z directions, now nit will be more easy to understand the estimation of the shear stress specifically in case of other cylindrical coordinate system. Now simply if we look into that cylindrical element, if we simply open it up the cylinder element and representation of this thing and Burger's vector D, here L is the length of the dislocation along the axis and this actually represents, the height actually represents the periphery, perimeter, twice pi r.

So with the configuration of the, basic configuration of the estimate the shear stress or shear strain is like that shear strain is basically b by twice pi r which is equal to tan theta so this angle actually represents by theta and shear stress accordingly. So this is the simple way we can find out the shear stress associated with the screw dislocation.

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Stress field of Screw Dislocation

Up to now, we did not consider the core of dislocation. We estimate the stress existing next to the dislocation core of a screw dislocation

$$r_0 = b$$
$$\tau_{\theta z}(r_0) = \frac{Gb}{2\pi r_0} = \frac{Gb}{2\pi b} = \frac{G}{2\pi}$$

This is the limit of theoretical strength i.e. the limit of validity of elastic continuum mechanics

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Now so far in last slide maybe we have not consider the effect of the core to estimate the shear stress, now we estimate the shear stress existing next to the dislocation core of a screw dislocation. Here for example suppose r_0 equal to b if we assume that the elastic theory also exist within the core itself and assuming that r_0 equal to b . So size of the core is equal to b . So in this case we can simply estimate that shear stress associated with the screw dislocation with is G by twice π , actually this is the limit of the theoretical strain, either that means the limit of the validity of the plastic continuum mechanics.

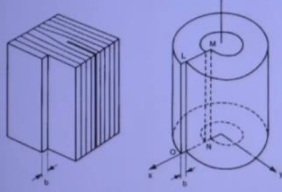
So that theoretical strain we have already estimated when you try to explain the slip system exist within the crystal structure, we have already estimated this thing, G by twice π is the theoretical limit of the strain. So with this analogy if we put r_0 equal to b then theoretical we can estimate the what is the strength of a theoretical limit of theoretical strength of the one specific lattice by analyzing the stress field associated with the screw dislocation.


But practically this is theoretical strength is actually G by twice π is different from the in experimental measurement of the theoretical strength of the single crystal lattice so there maybe the due to the assumptions for this estimation but this is the very idealized case for this limitation.

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Stress field of Edge Dislocation

Consider a hollow cylinder around the dislocation and exclude the core due to plastic strain
 There is no shear in Z direction i.e. $\tau_{xz} = \tau_{yz} = 0$



$$\sigma^{xyz} = \begin{vmatrix} \sigma_{xx} & \tau_{xy} & 0 \\ \tau_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{vmatrix}$$


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Now if we look into that stress field associated with the edge dislocation similar way we can consider as the hollow cylinder around the dislocation and exclude the core due to the plastic core in this calculation or in this estimation but if we look into that the stress field associated to the edge dislocation their existence of the normal stress component and one shear stress component so that shear field is actually different from the screw dislocation, and if we look into that or if we try to estimate the stress field associated with the edge dislocation we can find out further that...

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Stress field of Edge Dislocation

- o dislocation - elastic stress fields in an infinite body
- o The core region is ignored in these equations (having singularity at $x = 0, y = 0$)
- o However, a real material cannot bear such 'singular' stresses

$$\sigma_{xx} = \frac{Gb}{2\pi(1-\nu)} \frac{y(3x^2 + y^2)}{(x^2 + y^2)^2} \quad \sigma_{yy} = \frac{-Gb}{2\pi(1-\nu)} \frac{y(x^2 - y^2)}{(x^2 + y^2)^2}$$

$$\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$

$$\sigma_{xy} = \tau_{xy} = \frac{-Gb}{2\pi(1-\nu)} \frac{x(x^2 - y^2)}{(x^2 + y^2)^2} \quad \varepsilon_{xy} = \frac{-b}{4\pi(1-\nu)} \frac{x(x^2 - y^2)}{(x^2 + y^2)^2}$$

$$\varepsilon_{xx} = \frac{b}{4\pi(1-\nu)} \frac{y[(3x^2 + y^2) - 2\nu(x^2 + y^2)]}{(x^2 + y^2)^2}$$

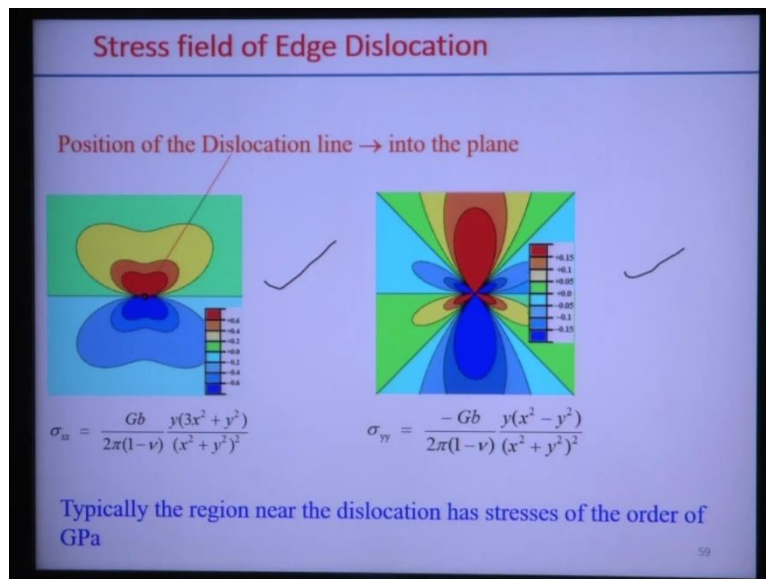
$$\varepsilon_{yy} = \frac{-b}{4\pi(1-\nu)} \frac{y[(x^2 - y^2) - 2\nu(x^2 + y^2)]}{(x^2 + y^2)^2}$$

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Typical expression of this thing, sigma xx sigma yy normal stress and sigma zz using considering the effect of the Poisson ration here but it is different from the Screw Dislocation and we can find out sigma xy that is shear stress variation and thus shear strain component, this is the typical estimation of the different components of the stresses that we can easily estimate. But to do that or specific observation here is that dislocation actually elastic stress field we assuming that exist in an infinite body and in this calculation the core region is ignore that already mentioned that, but this calculation indicate that having the singularity at x equal to 0 and y equal to 0.

But however the real material cannot bear such singular stresses, so in this case theoretically we can estimate or we can apply this theoretical estimation practically if we neglect the estimation had the core and of course we have already mentioned there is a finite size of the core exist varies the elasticity of theory cannot be applied. So that can be excluded assuming there the existence of the singularity at the core region.

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This is the typical distribution of the stresses in case of the edge dislocation if we look into that similar there is a with respect to the edge dislocation one sided there exist some positive values and another sided it the negative value that one sides is a compressive and another side is the negative tension. So similarly in case of sigma y1 this are the distribution of the stresses and all are represented schematically so but calculation shows that typically the region near the dislocation has stresses of the order of the GigaPascal, so we can maybe realize that this

theoretical estimate represents that near about the core is the stress exist in the order of GigaPascal.

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Hydrostatic stress in screw dislocation

Assume isotropic elasticity
 Dislocation is parallel to z-axis.

$$\therefore \tau_{z\theta} = -\frac{G}{2\pi r}$$

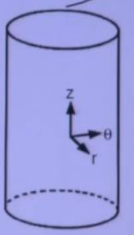
Now, $\tau_{rz} = \tau_{r\theta} = \sigma_r = \sigma_\theta = \sigma_z = 0$

The state of equation indicates the screw dislocation creates no hydrostatic tension or compression

$$\sigma_H = (\sigma_r + \sigma_\theta + \sigma_z)/3 = 0$$

There should not be any volumetric strain associated with screw dislocation

However, real crystal are elastically anisotropy and there may be small volumetric strain associated with screw dislocations



Now after looking into that stress field on the edge and screw dislocation we will try to estimate the hydrostatic in the screw dislocation and hydrostatic stresses in case of the edge dislocation. So to do that representation of the coordinate system, here the cylindrical coordinate system in terms of r theta z and we assume that the isotropic elasticity dislocation is represented parallel to the z axis and here you see the shear stress represents G by twice pi r that we have already shown how to estimate this thing and of course other component of the stresses not there, only there exist only dislocation along the z axis.

So this state of the equation indicates the screw dislocation actually creates no hydrostatic tension or compression. Simply if we look into the expression of the hydrostatic stress state, one third of the normal stress component, since all the normal stress components are 0 here so there doesn't exist any hydrostatic stress component in case of the screw dislocation. So since does not exist any hydrostatic stress component there should not be any volumetric strain associated with the screw dislocation. But however real crystal are elastically anisotropy so there may be small volumetric strain associated with the screw dislocation, so with this conclusion from the screw dislocation, hydrostatic stress in case of screw dislocation.

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Hydrostatic stress in edge dislocation

If Edge dislocation is parallel to z-axis and \vec{b} parallel to x-axis in edge dislocation

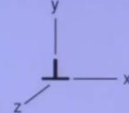
$$\tau_{xy} = \frac{G}{2\pi(1-\mu)} \cdot \frac{x(x^2 - y^2)}{(x^2 + y^2)^2}$$

$$\sigma_x = -\frac{G}{2\pi(1-\mu)} \cdot \frac{y(3x^2 + y^2)}{(x^2 + y^2)^2}$$

$$\sigma_y = \frac{G}{2\pi(1-\mu)} \cdot \frac{y(x^2 - y^2)}{(x^2 + y^2)^2}$$

$$\sigma_z = -\frac{2Gb\mu}{2\pi(1-\mu)} \cdot \frac{y}{(x^2 + y^2)}$$

$$\tau_{yz} = \tau_{zx} = 0$$



$$\sigma_z = \mu(\sigma_x + \sigma_y)$$

Maybe we can consider the hydrostatic stress in case of edge dislocation, so here edge dislocation is represented parallel to the z axis and Burger's vector is parallel to the x axis in this edge dislocation so with this configuration of the edge dislocation over the stress axis x, y and z. We can find out that the expression of the shear stress is this, expression of the normal stresses and other shear stress component are 0 here and sigma z can be normal stress represented in terms of the effect of the Poisson here.

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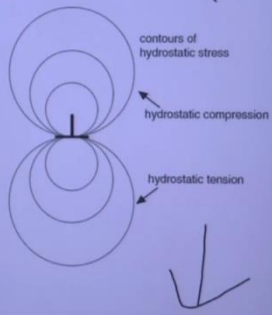
Hydrostatic stress in edge dislocation

$$\sigma_H = (\sigma_x + \sigma_y + \sigma_z)/3 \quad (\text{hydrostatic stress})$$

$$= -\frac{2}{3} \frac{G}{2\pi(1-\mu)} \frac{y(1+\mu)}{(x^2 + y^2)} = -A \cdot \frac{y}{(x^2 + y^2)}$$

$$A = \frac{Gb(1+\mu)}{3\pi(1-\mu)}$$

This volumetric strain causes interaction between edge dislocations of same sign and tend to form walls with one another.



So with this expression, specific configuration of different stresses in case of (())(52:08), we can estimate hydrostatic stress also here so simply the average of the three normal stress

component that actually represents the hydrostatic stress and here if we estimate the hydrostatic stress expression is like this, so while A is the constant term, the constant term is the material parameter, shear modulus and the Poisson's ratio, so if we represent the distribution of the hydrostatic stress component in case of edge dislocation, we can find out that some contour plot of the hydrostatic stress and upper side actually represent the compressive, lower side is the tensile field.

So this volumetric strain actually causes the interaction between the edge dislocation of the same sign and tend to form wall from one another. So several significant explanation can be derived over the estimate of the hydrostatic stress component in case of edge dislocation.


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Hydrostatic stress in edge dislocation

- Hydrostatic tension caused by one dislocation is partially annihilated by hydrostatic compression of its neighbor.
- Lowers the energy level and stable configuration forms a low-angle grain boundary.
- In substitutional solid solutions, solute atoms are attracted by edge dislocation just above the edge .
the solute atoms helps to relieve the hydrostatic stress.

→ $d_{\text{solute}} < d_{\text{solvent}}$
(above the edge dislocation)

→ $d_{\text{solute}} > d_{\text{solvent}}$
(below the edge dislocation)



Let us look into that what are the physical consequence of the hydrostatic stress component in case of the edge dislocation. If we look the first significant points is that hydrostatic tension caused by one direction is partially annihilated by hydrostatic compression of its neighbor. So lowers the energy level and stable configuration forms a low angle grain boundary. This is another significant conclusion from this stress hydrostatic stress state in case of edge dislocation but if substitution solid solution occurs here the solute atoms are attracted by the d just above the edge.

But whether the movement of the solute atoms whether upper, above or below the edge dislocation that depends on the size of the solute and solvent atoms. If you look into the small solute atoms is generally attracted on the above the edge dislocation and the large solute

atoms is generally attracted below the edge dislocation. So these are the typical conclusion can be made from the hydrostatic stress field in case of the edge dislocation.

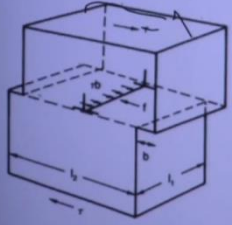
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Interaction of dislocations

Applied shear stress (τ) exerts a force on a dislocation
 Motion of dislocation is resisted by a frictional force
 Work done by the shear stress = Work done by the frictional force

$$W_\tau = (\tau l_1 l_2) \times b \quad W_f = (f l_1) \times l_2$$

f = frictional force per unit length



$W_\tau = W_f \Rightarrow f = \tau b$

M.F. Ashby and D.R.H. Jones, Engineering Materials 1, 2nd ed. (2002) 64

Now if we look into that the interaction of the dislocation, but to do that first you have to estimate the forces on the dislocation, how we can do that. So one thing is that, of course applied shear stress actually imparts on amount of the course the dislocation. So but if we try to estimate in such a way that motion of the dislocation is resisted by the frictional force then the amount of the work done balance between the by the shear stress and by the frictional force, then we can roughly estimate the amount of the force actually acts on the dislocation due to the application of the shear stress.

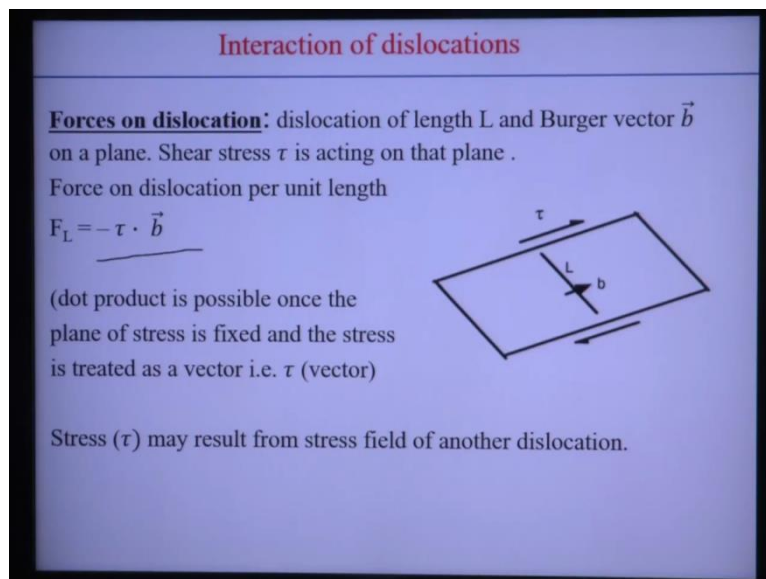
If we look into that figure here, shear stress is acting this direction it is shown and the length over which, the one is the length l_1 another is the length l_2 that constitute on the area over which the shear stress is acting and perpendicular to the length direction l_2 that actually represents the dislocation segment here. Now work done due to the applied shear stress τ is basically applied shear stress τ into l_1 into l_2 this is the total force due to the applied shear stress and when multiplied by the Burger's vector b , Burger's vector.

Actually here the Burger's vector will represent the uni-strain that means, when the actually atom travels when for the shortest repeat distance, that is the representation of the full Burger's vector here, so assuming that the atoms displaced over the full length of the Burger's vector b , so then w_τ is the amount of the work done with the applied shear stress and if we consider the consequence, what will be the frictional resistance here, so f assuming that

f is the frictional force for unit length and that frictional force per unit length which is acting over the length l , so that is the total frictional force f into l and the distance movement in this case equal to l here.

So if we equate this thing we can find out frictional force f equal to, f is equal to τ into b , the shear stress into Burger's vector that means force per unit length so this is the way we can find out back we represent the frictional force or resistance force per unit length with a applied shear stress.

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Now how we can do the further analyses, in a different way, let us look into that, dislocation length of l having Burger's vector b on a specified plane over with the shear stress τ is acting on that plane, now force on the dislocation per unit length can represents at the dot product between the shear stress between the Burger's vector. Since shear stress can be represented or can be treated as a vector here so then looking into that dot product we can find out the force on the dislocation per unit length so that is basically we can say equivalently is the frictional force per unit length.

Now this shear stress actually results from the stress field of the another dislocation, so point is that here we assuming the applied stress field, this is applied stress field τ here, but this τ may have the results from the other uhh stress field with the interaction of the other dislocations so it comes from the externally in the sense that we represents the τ here to estimate the force per unit length in case of the uhh when we try to interact with the another dislocation.

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Interaction of screw dislocations

Two screw dislocations exert an attractive force on each other of

$$F_L = -Gb_1 \cdot \frac{b_2}{2\pi r} \equiv \left(\frac{Gb_1}{2\pi r} \right) \cdot b_2$$

b_2 is the Burgers vector of the dislocation of concern

Negative sign indicates they repel each other if the dot product is positive.

Two dislocations repel each other if their combination would result in an energy increase (Frank's rule)

If the angle between b_1 and $b_2 > 90^\circ$
then

$$|\vec{b}_1 + \vec{b}_2| > |\vec{b}_1| + |\vec{b}_2|$$

So when two screw dislocation exerts an attractive force on each other now we will try to enter the interaction of the different dislocation so consider that case that the two screw dislocation they actually exerts an attractive force with each other then how we can estimate the force per unit length in this case. For ex the b_2 is the Burger's vector of the dislocation concern and other cases the shear stress is actually stress field or stress release due to the dislocations of Burger's vector b_1 that shear stress we can easily find out that estimation of the shear stress Gb_1 by twice πr , so that shear stress estimation from the Burger's vector or one dislocation is τ_1 .

And another is the directly consequence another dislocation which is represented by the Burger's vector b_2 and with this two interactions we can represent the force per unit length simply dot product between these two force or two vectors. Then if we look into that and we can make the conclusion, the negative sign actually indicates they repel each other if the dot product is positive and that sign configuration actually consider depending upon the, try to analyze this interaction of the dislocation.

But two dislocations with this sign convention two dislocation repel each other if their combination would results in the energy increase. Now we will try to enter the explanation of the interaction of this thing in terms of the associated energy that this whether there is a change of the level of the energy with the interaction or the dissociation of the two dislocation is better represented by the Frank's rule, that I will try to explain later on.

But with this configuration of the or sign convention of the present set of analysis between the interaction of two dislocation we can say if angle between this two Burger's vector b_1 and b_2 is greater than 90 degree then their result and magnitude is greater, should be greater than that of the individual component. This is the typical conclusion with the interaction of the screw dislocation. Now we will try to do further analysis with when there is an interaction of the two dislocations.

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Interaction of edge dislocations

Interaction of two parallel edge dislocations (more complex):
 Edge dislocation is parallel to z-axis and \vec{b} is parallel to x-axis,

$$\tau_{xy} = \frac{G}{2\pi(1-\mu)} \cdot \frac{x(x^2 - y^2)}{(x^2 + y^2)^2}$$

The mutual force on that plane is:

$$F_L = -Gb_1 \cdot \frac{\vec{b}_2}{2\pi r(1-\mu)} \cdot \frac{x(x^2 - y^2)}{(x^2 + y^2)^2}$$

For dislocation of like sign ($\vec{b}_1 \cdot \vec{b}_2 > 0$) there is mutual repulsion in the region, $x > y$ and attraction in the region $x < y$.

mutual repulsion → reaction cause an increase of energy
 mutual attraction → reaction cause a decrease of energy

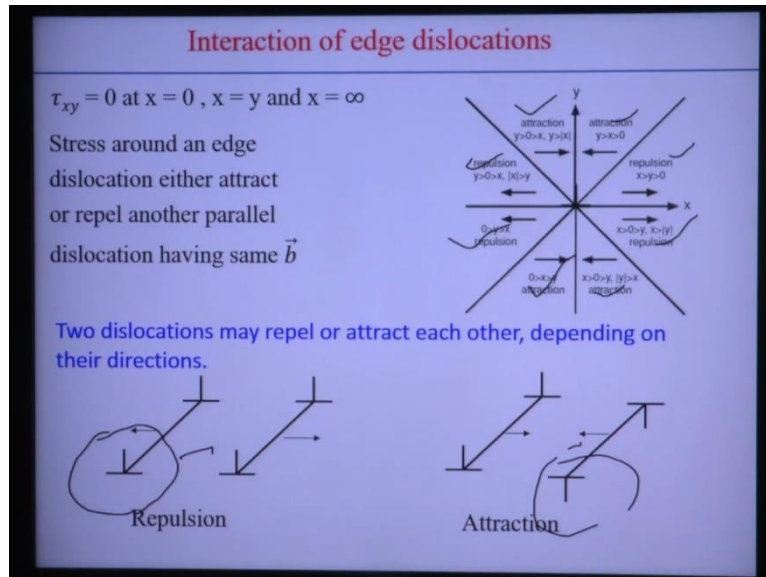
Prediction according to Frank's rule

Now interaction of the two parallel dislocation, parallel edge dislocation it becomes more complex but let us try to explain this thing, how interaction can be done, first we consider one edge dislocation which is parallel to the z axis and b Burger's vector is parallel to the x axis. So in this case the shear stress can be represented like this, G by twice pi 1 minus mu and x into, $x^2 - y^2$ by $x^2 + y^2$, that estimation is already explained, now the mutual force on that plane due to the interaction of this two edge dislocation can be represented like this, simply doing the dot product of this.

Now from this we can find out the for the like sign of dislocation if the Burger's vector dot product greater than 0 then we can conclude there is a mutual repulsion in the region when x greater than y and mutual attraction in the region x less than y . So looking into the sign convention we can several conclusion whether with the interaction of the two dislocation can create some attractive force field or repulsive force field in this case.

Now mutual repulsion actually when you try to link with the energy level mutual repulsion actually the reaction cause an increase of the energy level mutual attraction actually uhh there is a decrease of the energy level so that can be better explained by the Frank's rule.

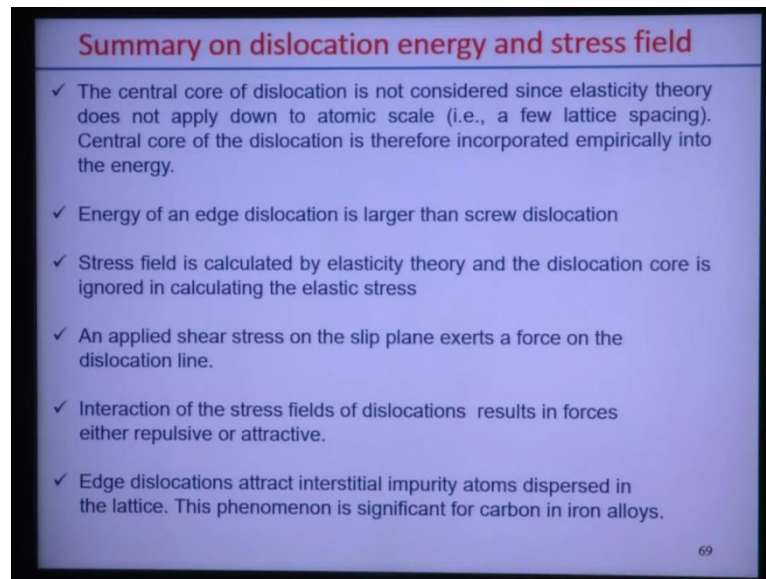
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Now within the interaction of the stress field if we look into this thing we can make the right hand side conclusion that there is a attraction on this two areas, her also repulsion and these two is the attract. So this area can be estimated by simply plotting on the xy coordinate this amounn of the force field here and we can define the different zones whether there is an attractive force field or repulsive force field looking into that interaction of the different edge dislocation.

Now as a simply representation of the dislocation that two like sign dislocations there exist some repulsion and opposite sign maybe if you can consider this as a positive edge dislocation and we can consider this is a negative edge dislocation. So two positive edge dislocation they actually exerts, repulse with this repulsive force exist between this two positive edge dislocation and there maybe the attraction between the two opposite side uhh or two different edge dislocation having opposite signs, positive or negative.

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Summary on dislocation energy and stress field

- ✓ The central core of dislocation is not considered since elasticity theory does not apply down to atomic scale (i.e., a few lattice spacing). Central core of the dislocation is therefore incorporated empirically into the energy.
- ✓ Energy of an edge dislocation is larger than screw dislocation
- ✓ Stress field is calculated by elasticity theory and the dislocation core is ignored in calculating the elastic stress
- ✓ An applied shear stress on the slip plane exerts a force on the dislocation line.
- ✓ Interaction of the stress fields of dislocations results in forces either repulsive or attractive.
- ✓ Edge dislocations attract interstitial impurity atoms dispersed in the lattice. This phenomenon is significant for carbon in iron alloys.

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So with this we can summarize the dislocation of the energy and the stress field associated with the dislocation first point is that when you try to analyze or when you try to estimate the dislocation energy we simply neglect the effect of the core because the elasticity is not applicable within the core region and because the size of the core exist within the few lattice spacing, but this core energy can be empirically correlated with respect to the elastic energy outside of the core region.

Second point is the we observe that the energy of an edge dislocation is larger than that of the screw dislocation. Third point is the stress field is calculated elastically by using the elastic theory and dislocation core is neglected in this calculation. Forth point we observed that the applied shear stress on the slip plane exerts, actually creates some force on the dislocation line and we have tried to estimate that force per unit length by analyzing the interaction of the two different dislocations.

Interaction of the stress field of the dislocations is a result of the force which maybe attractive, which maybe the repulsive depending upon the nature of the dislocation whether it is positive or negative or what it is just screw or left hand screw or right hand screw dislocation. And finally that from the estimate of the hydrostatic stress field or volumetric strain exist in the edge dislocation we make conclusion that the, that presence of the or theoretical estimation of the edge dislocation actually explain whether interstitial impurity in case of carbon, iron carbon solution whether which point it will be attracted depending upon the volumetric positive or negative hydrostatic stress field exist.

So with this I conclude this estimation of the dislocation energy and the stress field associated with this. Thank you very much for your kind attention.