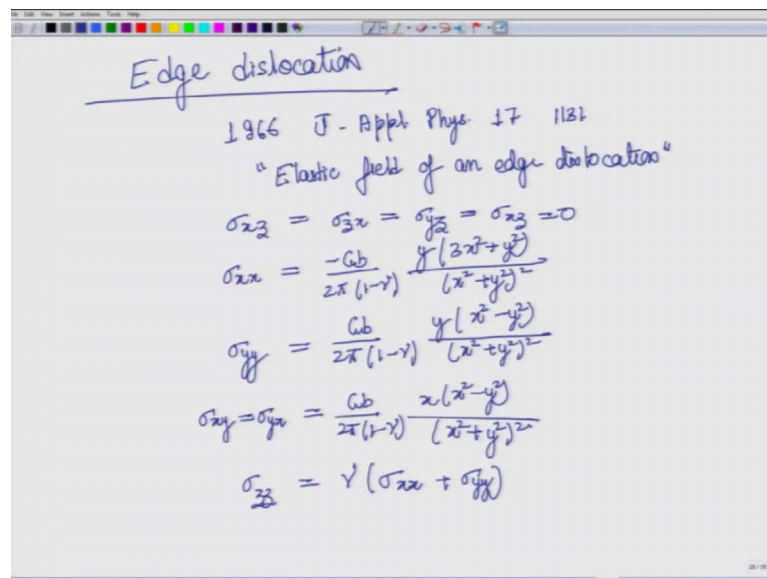


Defects in Crystalline Solids (Part-I)
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Lecture – 22
Stress State around Edge Dislocations+ Elastic Energy of Dislocations

So, these are the stress fields around edge dislocation.

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Edge dislocation

1966 J. Appl. Phys. 47 1121
"Elastic field of an edge dislocation"

$$\sigma_{xz} = \sigma_{zx} = \sigma_{yz} = \sigma_{zy} = \sigma_{zz} = 0$$
$$\sigma_{xx} = \frac{-Gb}{2\pi(1-\nu)} \frac{y(3x^2 + y^2)}{(x^2 + y^2)^3}$$
$$\sigma_{yy} = \frac{Gb}{2\pi(1-\nu)} \frac{y(x^2 - y^2)}{(x^2 + y^2)^3}$$
$$\sigma_{xy} = \sigma_{yx} = \frac{Gb}{2\pi(1-\nu)} \frac{x(x^2 - y^2)}{(x^2 + y^2)^3}$$
$$\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$

And as I mentioned in the last lecture, we are not deriving it, and the derivation is not very difficult. You can go and take a look at this particular paper and you will be able to find this derivation with we are just looking at the final solution.

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

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

$$e_{xy} = e_{yx} = \frac{b}{4\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}$$

$$\underline{\underline{\sigma}} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{yx} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{bmatrix}$$

$$\underline{\underline{\epsilon}} = \begin{bmatrix} e_{xx} & e_{xy} & 0 \\ e_{yx} & e_{yy} & 0 \\ 0 & 0 & e_{zz} \end{bmatrix}$$

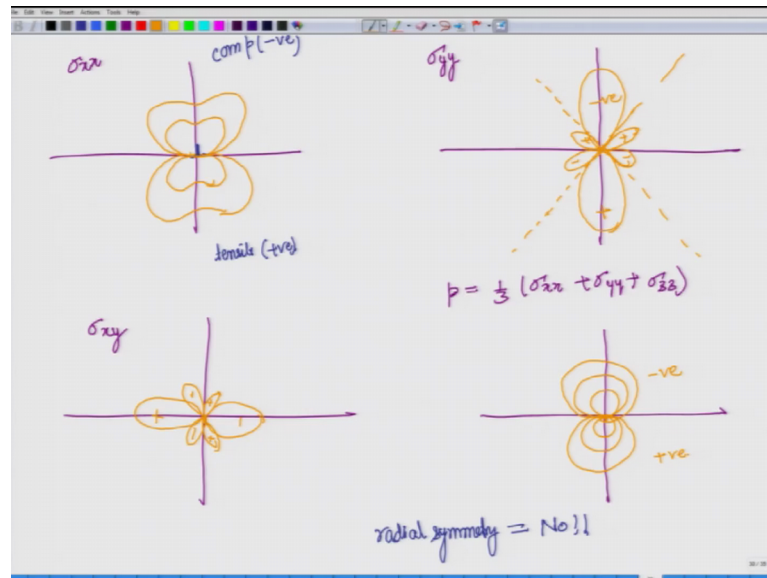
So, these are the stress fields, how would the strain fields look like and you will see that strain should look like this using the linear relations for elasticity.

So, there is a strain in the x x direction which is expected, then there is also strain in the y y direction, and then there is strain in the shear strain in the x y direction. So, e_{xy} is equal to e_{yx} is equal to $\frac{b}{4\pi(1-\nu)}$.

How does the stress and strain matrix look like for this edge dislocation? It would look like σ_{xx} σ_{yy} . So, we have all the normal stress components. You also have one shear stress components σ_{xy} σ_{yx} , all other elements are 0. So, these four elements are 0. So, this is the σ that is the stress tensor. Similarly we have the strain tensor which would look similar to this. We will have e_{xx} e_{yy} e_{zz} and a shear strain component e_{xy} and its counter plots e_{yx} all the other elements are 0.

So, this is how the matrix stress and strain matrix look like. Now let us look at how the real stress and strain fields look like.

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So, first let us draw for sigma x x again we will draw the contour plots. So, if you remember that for edge dislocation, there is actually a reference frame meaning in let us say we have this extra half plane. So, this is the extra half plane that I am trying to draw. So, extra half mean lies in this direction and there is extra half plane or there is a missing plane on the bottom side which means that on one side, there will be compressive stresses. So, there will be compressive stresses over here. And the on the other half side, there will be tensile. So, based on this what can you say about the radial symmetry should there be radial symmetry or should there be no radial symmetry.

Now, because there is one particular reference direction, there we cannot expect any radial symmetry. So, we should not be when looking at where is the radial symmetry ok. So, coming back to our counter plots for sigma x x, how does it look like? So, there on one side we have compressive. So, let us say that the compressive and negative. So, once and if you use the relation to plot ISO stress plot, this is how it would look like. So, this is the positive value and this is the same amount negative value sorry, this will be the negative value. If we say compressive as negative and tensile as positive sorry, the values would keep decreasing, but the form would remain same.

So, it will have mirror symmetry along y y direction. Although it may not look like from this drawing, but you must realize that it is just a hand drawing, but in reality there will

be mirror symmetry along y direction. So, this is how x would look like. Now how would the y look like?

Now, y is not so straightforward to predict, but if you plot it using the relation that has been given to you, you would see that it shows a form like this. So, that two main loops and then there are four small loops. And if we this is negative, then this also terms out to be negative, this also terms out to be negative and use this is positive, this is also positive. This is also position meaning this is compressive this is least two smaller loops are also compressive; this is tensile and these two are also tensile.

So, we are talking about the normal y direction. So, here you have the tensile even in the y direction and in these two small loops and on the positive y decide, we have negative meaning compressive. They are the atoms are being pushed together. So, this is the negative. And so, is the negative over here; the smaller two loops. And this is approximately not approximately. This is exactly here forty five degrees. So, you can draw line here like this which is at 45 degrees. And we will be able to predict or not predict, but draw the different stresses in different quadrants of these of the x y axis. We will come to that, but first let us look at other stress fields.

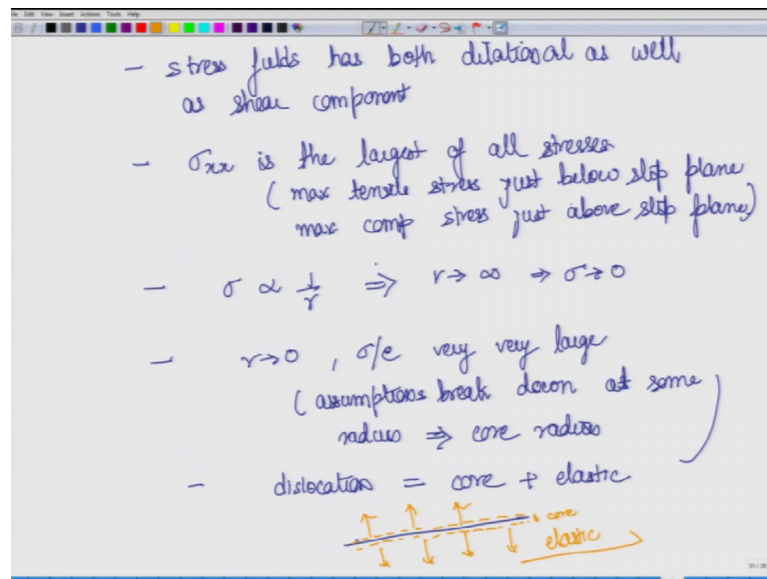
So, we have drawn x we have drawn y . Now let us get to the other one which is x y . Now x y again not easy to predict based on simple geometry, but using the relation that is given to you, you would see that it comes out similar to y y only that. And even if looking at the relation of y y and x y you would see that the relation is same except x and y get interchanged. And therefore, it is our just looking at the relation, you would be able to say that y y and x y would be rotated by 90 degrees. And therefore, you will have a plot like this.

So, again there are two main loops and then there are 4 smaller loops. And here also when this turns out to be positive, these two smaller ones are also positive. And this is negative that these two these two the smaller loops on the other side also turn out to be negative. And this is how it would look like. Now we have drawn x x , we have drawn y y , we have drawn x y . We can also draw on still another one which is hydrostatic stress which is p equal to 1 by 3.

σ_{zz} is some quantity dependent on x x and y y . So, we are not drawing it p is also dependent. So, we have we can just directly draw p and we will get a full understanding

of the overall stresses acting on this. And this will have not really a radial symmetry, but you can say half radial symmetry. So, this is how the pressure the order pressure or the hydrostatic pressure looks like. And so, here one of them is the negative component. So, this is the negative, this is the positive component and even the hydrostatic stress does not show radial symmetry. In fact, we should not even expect any radial symmetry over here.

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So, now what are the important points that we can note down regarding the stress and strain field for around the edge dislocation? Even the first and foremost is that stress field has both dilatational as well as shear components; dilatational or normal you can say this is one important factor or one important take away message from the different relations that we have seen and the stress field that we are drawn.

Another important thing is that although we is I have drawn the field, but we have not look at the exact magnitude. But when you go to the exact magnitude and even if you look at the relation, you would realize that σ_{xx} is the largest of all; the stresses σ_{xx} is the largest of all stresses. And here you can see that maximum tensile stress is just below the slip plane.

And similarly, maximum compressive stress is just above the slip plane. So, we have looked at the stress field has to for the two known. Another factor which is similar to

what we described about the stress and strain field of dislocation is that stresses are proportional to $1/r$.

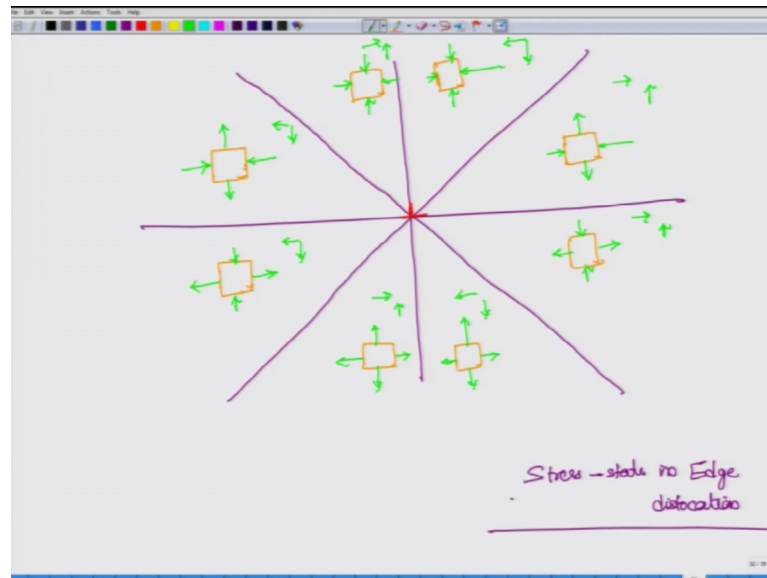
Now, what does that mean? Again it means that as r tends to infinity implies that σ tends to 0. Now this is something that we expected. On the other hand, when r tends to 0, stresses and strains become very very large. What does that mean that our assumptions breakdown at some critical radius which we call as core radius.

So, you can look at in terms of stress and strain fields and later on when we talk about energy, you can look at dislocations as two parts: one where you have the elastic component and one where you have the core component. So, there is a core component where whatever relations we have described is not valid and if you really want, you will have to use a non-linear elastic model. And on the outside whatever we have derived those relations will be valid and all our energy relations that we will go on to move on to next that those will also be valid.

So, this dislocation can be looked at core and elastic component. So, what we can say is that dislocation is equal to core plus elastic. So, this is the dislocation line. There is just small radius approximately 1 nanometer, there is the core and beyond this is the elastic field.

Now, this core as you can realize we have said is 1 nanometer in radius which means that when it comes to affecting or influencing other dislocations, they do not make much of a difference particularly when the distance is a little large. However, when the elastic field is the one that actually influences decides a lot of characteristics about the crystal because they have large range the effect of too much longer distance.

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Now, to summarize the stress fields that we looked at for the edge dislocation, there is a very usual common diagram that you must have seen which describes the stress states for a screw dislocations. So, I will also draw it over here and like we said that now, here we can divided into 8 quadrants. So, this is your let us say this is your edge dislocation lies at the centre. So, this is the extra half plane this is the direction or this is where the plane is missing.

Now, we said that on the top side, we have all compressive stresses. So, if you were to draw, it would look like this. So, let us first draw a element to this want to which we will describe the different states of stress. So, even before that, let me write the caption what we are trying to define here is stress state in edge dislocation.

So, this is will be summary kind of map which describes the stress states including all the xx yy xy . So, these are the 8 sectors of quadrants into which we want to describe. Now we said that on the top side, we have only compressive stresses in the x x direction. So, we can draw it like this. So, it is all compressive in all the 8 quadrants.

And on the negative y side, what we have is the tensile. So, all the a 4 over here will have tense tensile. What about the yy ? We know that these two will be compressive and if you remember we had one big loop and two small loops. So, over here we have compressive and over here also we had compressive. So, it will come out in the y

direction like this and here this is tensile and these are the smaller part of the loops where it is again tensile. So, this will be like this.

Now, for the $x y$ we remember that if this is this, this and this they are in one side of one type and this is again the bigger loop and these are the two smaller loops where there will be of one type. So, if we described this by using this, then why we are drawing to because in shear stress to that is we must have we there must be two stresses acting. So, that there is a balancing between the two stresses. If we apply only one of them if we apply only one type of stress, then it will lead to rotation which we know is not really taking place.

So, it always occurs in pair like we saw a $\sigma_{x y}$ and $\sigma_{y x}$. So, if this is $\sigma_{x y}$ the other one is $\sigma_{y x}$. So, this is the direction of $\sigma_{x y}$ and to balance it in the other direction, we have $\sigma_{y x}$ and these are same for these two. Similarly for this is the bigger loop, this is the smaller loop; so this will again be like this. And how would it be for the other one? It will be opposite sign. So, it will become like this. So, this is the bigger loop and these are the smaller loops.

So, you can see that this picture summarizes all the three different stress fields that we saw earlier and it is easy to draw it, once you know how they will look like. And once you have this, you could you can see that you have various combinations some where you have x as positive and $y y$ has negative somewhere you have both of them positive somewhere you have or both of them negative.

So, all different combinations are actually take place when you are around edge dislocation. So, with this we come to end for different stress and strain fields inside edge dislocation. We have also seen the screw dislocation although we did not derive the relation for screw dislocation, but we look at the final solution of stress and strain field for the screw dislocation.

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Stress & Strain

Elastic energy

$$dE_{el} = \frac{1}{2} \sum_{i=1}^3 \sum_{j=1}^3 \sigma_{ij} e_{ij} \frac{dV}{l}$$

Screw dislocation

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

$$= 2 \cdot \frac{1}{2} 2\pi r dr \cdot \frac{Gb}{2\pi r} \cdot \frac{b}{4\pi r} = \frac{Gb^2}{4\pi} \frac{dr}{r}$$

Screw $E_{el} = \frac{Gb^2}{4\pi} \int_{r_0 \text{ (core)}}^R \frac{dr}{r} = \frac{Gb^2}{4\pi} \ln\left(\frac{R}{r_0}\right)$

Edge $E_{el} = \frac{Gb}{4\pi(1-\nu)} \ln\left(\frac{R}{r_0}\right)$

So, what is the next step? Once we have the stress and strain fields, what is what comes to your mind? What is it that we can gather or what extra information we can extract once you have the stress and strain field? And the answer is simple it is the elastic energy. The relation for elastic energy is very simple. If you look at it dE_{el} can be written as this is $\frac{1}{2} \sum_{i,j} \sigma_{ij} e_{ij} dV/l$.

So, σ_{ij} is the stress component, e_{ij} is also the stress components. So, the corresponding stress and strain components you multiply and into the volume into dV and since we are talking about energy per unit length. So, we will have to discuss divided it by l . So, this gives us the elastic energy per unit length for a dislocation line, once we have the stress field and the strain fields. And only with the only thing that we need to do is basically multiply the corresponding components.

So, now let us take it further and see how it comes out for a screw dislocation. So, when we take dV by l and integrate it over the region sorry we are not yet integrating. So, let us keep it in dr . So, we are talking about $2\pi r dr$ which is that volume per unit length and the two components, we have are $\sigma_{\theta z}$ and $\sigma_{z\theta}$.

So, corresponding strengths will multiplied with. So, these two are similar quantities x . So, we multiply it by 2 into $\frac{1}{2} 2\pi r dr G b$. So, dE_{el} is equal to Gb^2 by $4\pi dr$ by r . So, thankfully the terms are very simple and we can integrate it. So, your E_{el} would be Gb^2 by 4π integrating and remember we have two integrate from

what will be the smallest radius. We can integrate only from r core, we cannot go below r core.

So, we will go from r naught which is equal to core to some large radius R beyond which we will say that there is no elastic field $d r$ by r and this comes out to $\ln R$ by r naught. So, this is for a screw dislocation. And people have shown that if you go for the edge dislocation, the relation is exactly same except you will also have a factor of $1 - \nu$, because in the stress and strain you remember we had the factor $1 - \nu$ arising from the compression in the lateral direction compression or the dilation in the lateral direction. We still have this we retain this component $1 - \nu$ and rest of the relation is exactly same.

So, you can see that we have a relation for screw dislocation and edge dislocation, because we had the stress field and the strain field that we had obtained. Now that brings us to the next question on what should be the value.

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The image shows a whiteboard with handwritten mathematical derivations for the energy of a dislocation. The equations are as follows:

$$E_{el} = \frac{Gb^2}{4\pi} \ln\left(\frac{R}{r_0}\right)$$

Annotations for the above equation: "core radius (b to 4b) 1 nm" and "R ~ ? (grain size ~ D/2)".

$$E_{Total} = E_{el} + E_{core}$$

$$= \frac{Gb^2}{4\pi} \left[\ln\left(\frac{R}{r_0}\right) + B \right]$$

$$= \frac{Gb^2}{4\pi} \ln\left(\frac{eR}{b}\right)$$

Annotations for the above equations: "ln e", "R ~ 5 μm", "b ~ 4 Å", "ln e R / b ~ 8π", "α ~ 0.5 to 1.5".

$$E_{Total} = 2Gb^2$$

$$E_{Total} = \alpha Gb^2$$

$$E_{Total} = Gb^2$$

Annotation for the last equation: "E_core < 10% of E_Total".

So, let me first write it down in a simple fashion for screw dislocation which is we were when we integrated it. We simply put in r naught and r . So, r naught we it is very easy to realize it is equal to the core radius and core radius as we set, you can take b to $4b$ or if you are talking about value, you can take it equal to 1 nanometer.

So, that part is solved, but what about r ? What should be taken the value of the uppercase R which is the outer limit up to which we should calculate the elastic strain energy? Yes it is true that the elastic strain energy component becomes small and smaller as we keep increasing radius R , the uppercase R . But they should still be some way to say- what is this R . And a simple solution for that is to take R as the grain size basically d by 2. If the grain diameter is D , then r will be equal to D by 2. So, that also solves the problem. Now we know both the parameters over here R and r naught.

So, this is the elastic energy component. But if you want the total energy component, what would you need? So, would need E elastic plus E core right. But E core, how do we know E core? We do not know. So, what we can do is we can simply use some unknown parameter b . So, it will become something like.

So, now here b or basically $G b^2$ by 4π times B represents the energy of the core and this B itself if people have said that it is approximately of the order of $1/n$ e ok. So, although this is unknown quantity, but the people have said that this is of the same order as $1/n$ e and it means that we can replace B by $1/n$ e and this relation would become $G b^2$ by 4π $1/n$ e R by b

So, now we have a relation as which with certain assumptions where the assumption is that the core energy is represented by $G b^2$ by 4π times this constant B and then we said that B is equal to $1/n$ e. And therefore, the core energy relation comes out something like this. Now if you take the usual values something like R equal to 5 micrometer, b equal to 4 angstroms; then $1/n$ e R by b can be taken approximately as 8π . And if it is equal to 8π , then it means that E total becomes. So, this becomes 8π . So, 8π by 4π there is 2. So, it is equal to $2 G b^2$. So, you see with certain assumption, we are seeing that what will be the final form of the relation, what is the approximate relation with of this with respect to the elastic energy and it comes out to be E elastic is equal to $2 G b^2$.

Now, they are there are certain assumptions over already made over here. So, in order to make sure that those assumptions remain assumption, we can change these 2 to a unknown parameter α . So, E total becomes $\alpha G b^2$ where α is usually found to be of the order of 0.5 to 1.5. As a first order of approximation now we can say

that E_{total} first order of approximation E_{total} is equal to $G b^2$ and another thing that you would realize at E_{core} is less should be always less than 10 percent of E_{total} .

So, we will conclude at this point with these relations, and we will talk more about energy in the next lecture.