Materials Science
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Lecture 14
Crystal Imperfections

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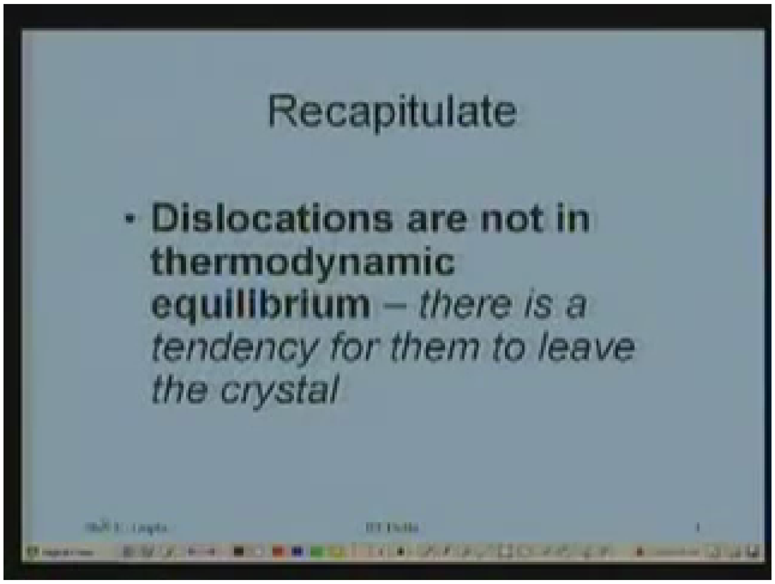

Now we had been discussing crystal imperfections and we were talking about dislocations. Just to remind us to what we were doing in the last class, I, in the class before we did discuss point defects which were in thermodynamic equilibrium and by their presence they lower the free energy of the crystalline solid. But dislocations like other imperfections as well are not in thermodynamic equilibrium. Thereby they have a tendency to go out of the crystal whenever they get the opportunity. In this course we shall also learn as to how these dislocations come about in a crystal. And once they come, it may not be easy for them to get out. So they are there not in equilibrium.

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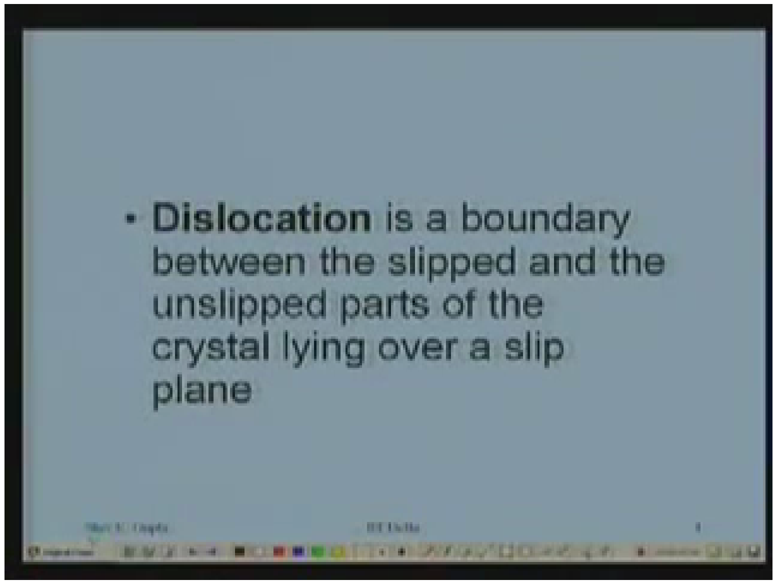

And we saw yesterday that dislocation is a boundary between the slipped part and the unslippped part of the crystal lying over the slip plane. And also we saw the slip plane is the plane which contains the two vectors, the Burgers vector, the dislocation line and the dislocation line vector itself.

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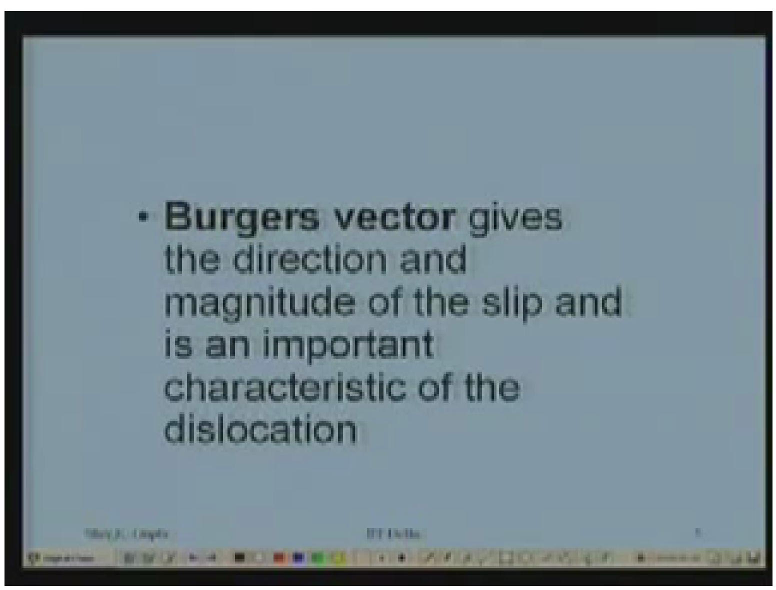

And we also described that Burgers vector of a dislocation gives a direction and the magnitude of the slip which is actually a relative slip between the slipped part and the unslippped parts and it is an important characteristic of a dislocation, besides the relationship in the edge dislocation with the screw dislocation and the mixed dislocation.

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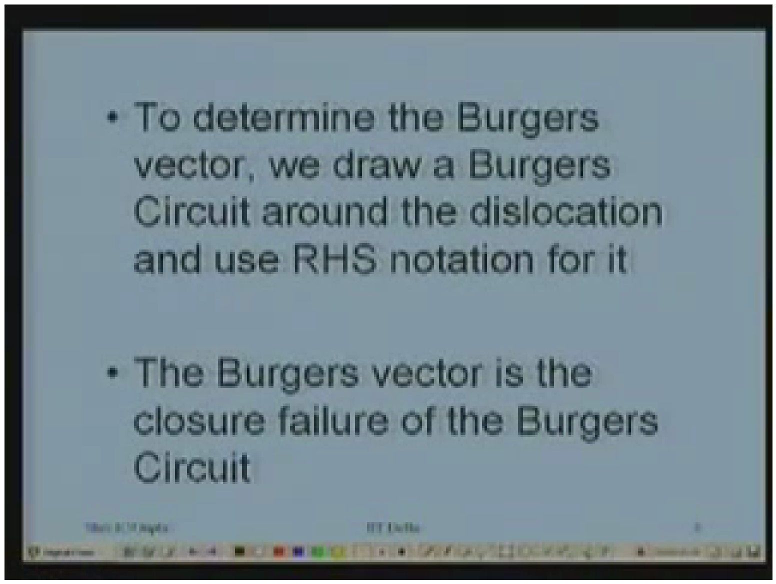

And also we saw that to determine the Burgers vector of a given dislocation, we draw a Burgers circuit which is a circuitous path drawn through the perfect parts of the crystal such that the net displacement along the path is 0. So we counted those steps and we saw that in the last class. However to avoid any kind of ambiguity in getting the b vector after we have arbitrarily chosen the t vector, we use the right hand screw notation in drawing the Burgers circuit. And then the Burgers vector is a closure failure of the Burgers circuit.

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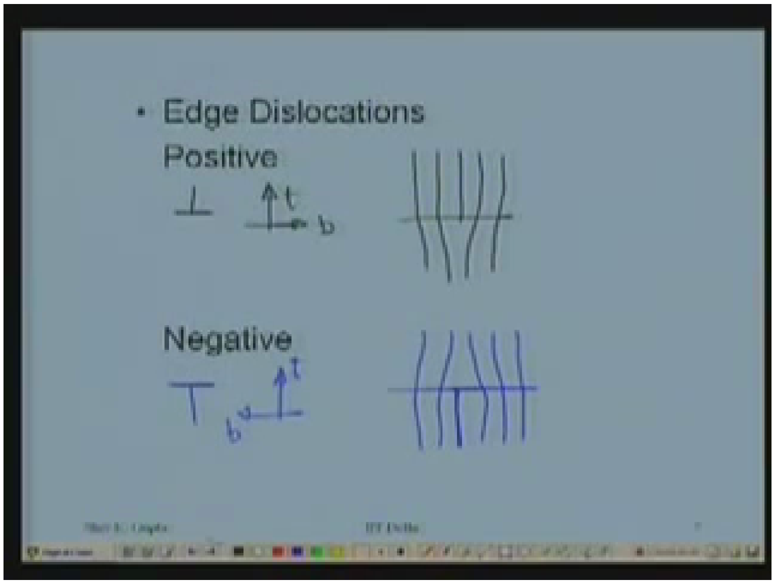

In the case of positive edge dislocation, symbol is and the relationship between t and b is this. And if you look at the arrangement, part plane comes and stops in the crystal at the slip plane. This is where your slip plane is. Similarly the negative dislocation, in here t and b are related like this and the arrangement here, in here is the slip plane and part plane is coming from the bottom. So that is the configuration for edge dislocation positive and negative.

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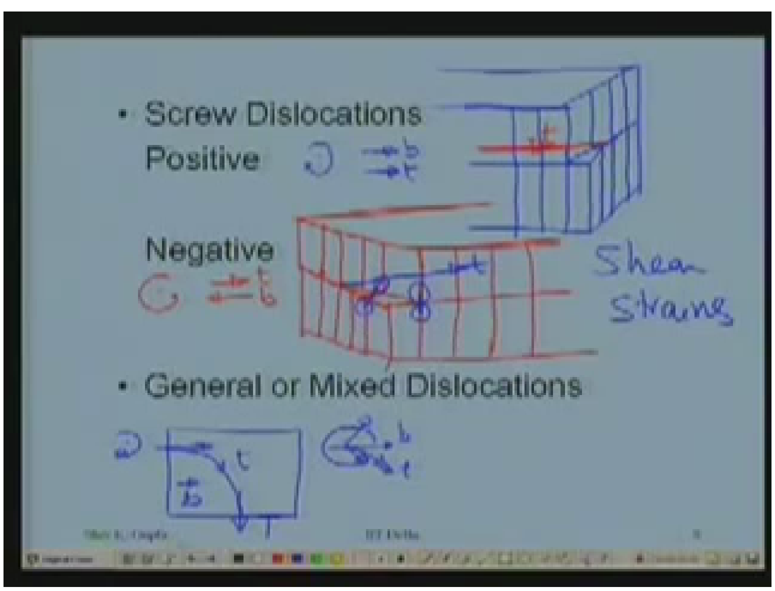

Then similarly we have seen the screw dislocation, the positive screw dislocation we represent like this. And here the b vector and the t vector are parallel. I will just show you the arrangement.

And there will be vertical planes in the front like this. That is the configuration for, and the dislocation line is right here. This is where the dislocation line is. And take the t vector going out or t vector coming in whichever way you want to take.

Well, similarly the negative dislocation I said we represent like this. And the t vector and b vector are related in this fashion which is antiparallel. And this configuration I showed you yesterday. And so on and so it go. That is the negative screw arrangement and that is the positive screw arrangement. And the relationship, well of course the we said earlier, dislocation line is here. You can take the t vector going in and then draw the Burgers circuit to get this.

However the mixed dislocation line is not a straight line, it is a curved line, right. In here let us say this is my slip plane and I said slip plane is the one which contains both the b vector and the t vector. All right, is a curved line, this is my t vector. Let us say my t vector goes in this direction. So here the t vector is going in this manner. Here the t vector is going out in this manner. And the b vector or the dislocation line is this. It remains same everywhere. So it becomes here a positive screw.

“Professor-student conversation starts.”

Professor: In here the t is like this, b is like that. This would be what? Negative or positive?

Student: Negative.

Professor: Yeah, it would be negative edge dislocation. Okay. And in here the b and t are, see let us put a tangent t like this but b is still there like this. Angle between b and t is going to be this, that is b and this is t. It is partly, it is an edge dislocation. Partly it is a screw dislocation. Okay. Because b can be resolved along t, the component of b along t is here. That shall give me a screw component. And the one which is here along, this shall give me the edge component. That b vector can be resolved.

“Professor-student conversation ends.”

So it is partially an edge dislocation, partially a screw dislocation elsewhere. That is what is mixed dislocation. While in the case of screw dislocations we had the shear stresses or shear strains around the dislocation. See, dislocation your bonds are stained because one atom is here, another one is there which were actually bonded like this earlier. They were bonded like this, now the bond is sheared. Instead of vertical bond, it has become slightly tilted, right.

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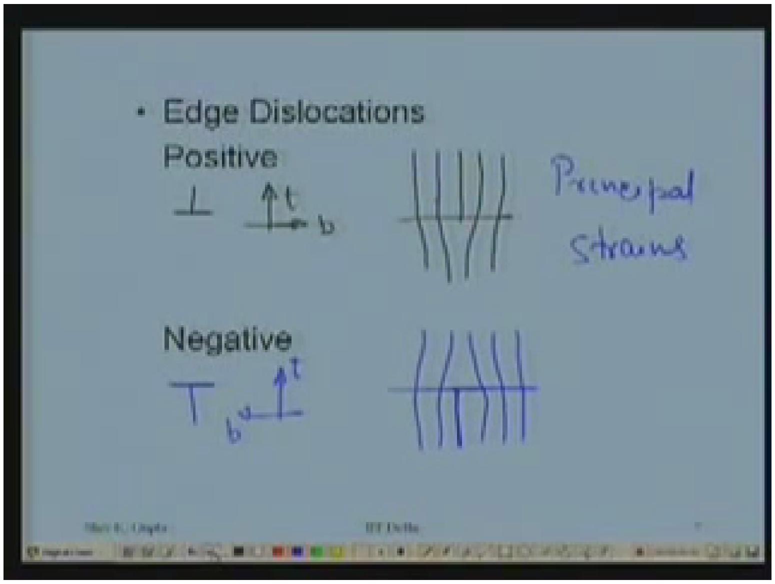

So in the case of edge dislocation of course, in the case of edge dislocation, there are compressions here and tensions there. Similarly there are tension here and compression there, are principal strains.

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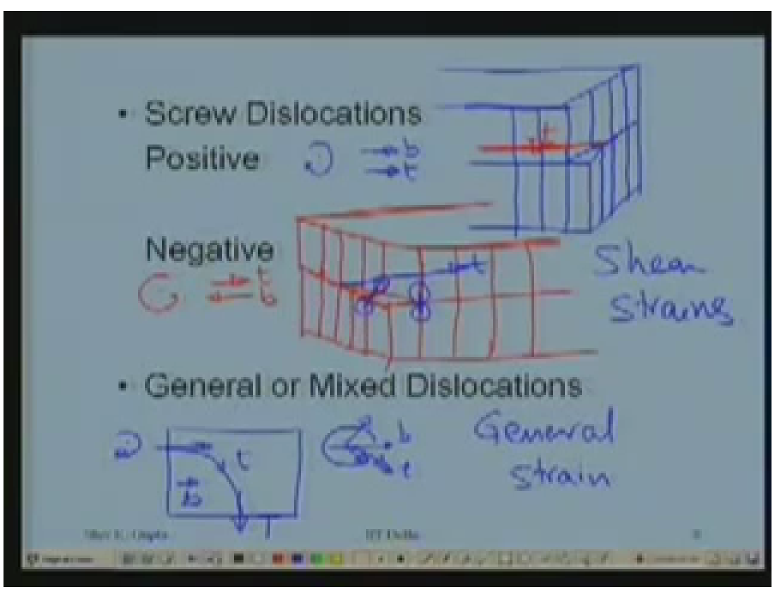

However in the case of mixed dislocation, I shall have the mixed state of strain, I shall have both or general state of strain. I could have shear component, I could have principal component. Okay. All right. So next we shall like to see some more characteristics of this dislocation line.

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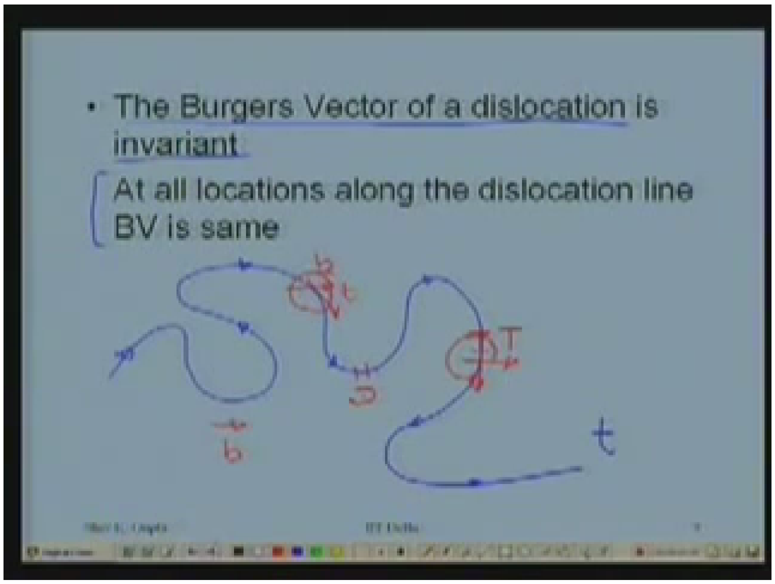

We have also seen this the, with the mixed dislocation we tried to work out the Burgers vector or the mixed dislocation line at two places and we found that to be same. So Burgers vector of a dislocation line is invariant. It does not change with the location of the dislocation. Whether it is mixed dislocation or edge dislocation, screw dislocation, it does not change. At all locations along this it is the same. So let us say I have dislocation line going like this. Let us define the t vector in this manner, it will be going like this, the t vector. Let us say the b vector of the dislocation line is this. Right.

"Professor-student conversation starts."

Professor: At this location can you tell me what is the this segment of the dislocation line which I marked, what is the characteristic of the dislocation line there?

Student: Sir, it is b into…..

Professor: It is a screw. b and t, both are parallel and it would be positive screw.

Student: Positive screw.

Professor: All right. Similarly let us ask me about this component here.

Student: It is negative in edge dislocations.

Professor: Yes, it is going to be negative edge dislocation, very good. Because t is going down here and b is this way. From b to t, the angle is 90 degree. It would 70 degrees, so it is a negative. Like this you can find out the character of the dislocation line which is varying from place to place. But the Burgers vector is not changing. All right.

Student: In some cases it would have, it will not be 270, not 90 and not 0, then?

Professor: The mixed dislocation. It is mixed dislocation, right? What you are asking is, and this is state, this is t vector and this is b vector, is the mixed state of dislocation, general dislocation. It has shear strains, it has compressive and tensile strains. The principal strain and shear strains, both are there. Therefore it is a mixed state of strain, it is a mixed dislocation right here. This segment is a mixed dislocation. Right? Or mixed dislocation you can also the general dislocation.

“Professor-student conversation ends.”

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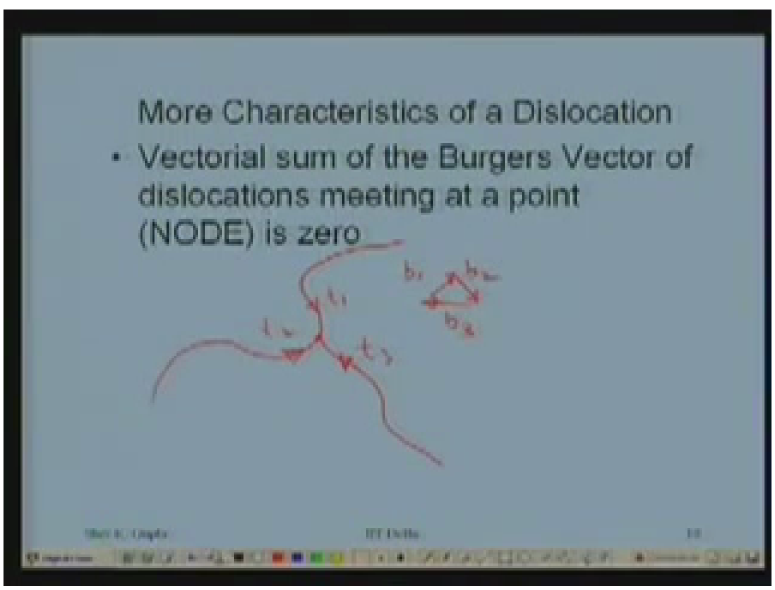

Now if there are dislocations meeting in a point in the crystal, say for example, there is a dislocation line here and there is another dislocation line like that and third dislocation line going like this, there are all meeting in a node here. So this dislocation is going toward the nodes, then the t vector is this going toward the node. t vector is this and going toward the node, t vector is this. So three vectors chosen like this.

Either I take them going toward the node or I take them going away from the node. Other case if I work out the Burgers vector and sum them up, some of the three Burgers vector would turn out to be 0. Right. That is let us say the Burgers vector of one is this, Burgers vector for two, okay, let us start from two for this here and we buckle to, this is b1, b2 and this will be b3. So the total sum of the three vectors would be 0. Okay.

We start from here, b1, add to it the b2, add to it the b3, the net would come back, the vectorial sum is 0, that is the meaning of it whenever there are dislocations meeting like this. Another important thing which we have, I talked about the dislocations meeting in a node inside a crystal because there could be curvilinear lines and they usually do form a jungle of dislocation in the crystal.

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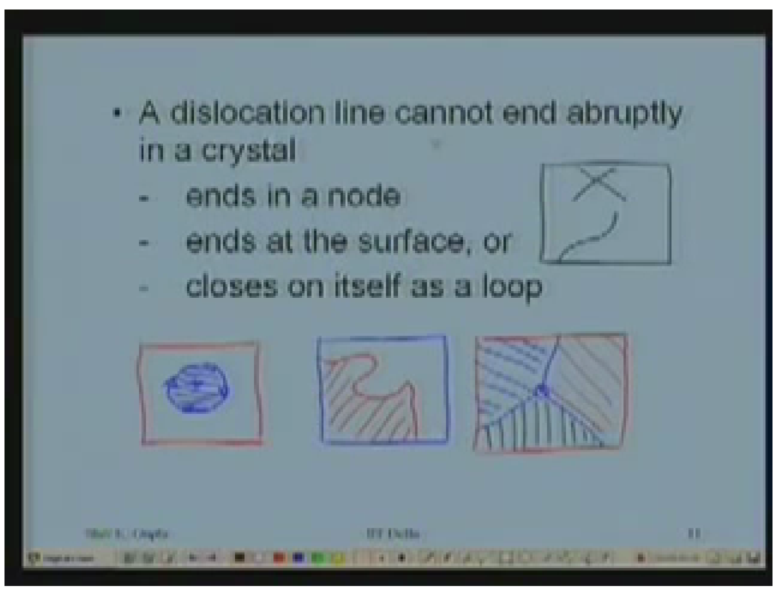

Dislocation line cannot end abruptly in a crystal. Either they end in a node inside the crystal like I showed you just now or they end on the surfaces which I showed you earlier pictures, edge dislocations, screw dislocation and the mixed dislocation. The ends of the dislocation line, straight line or the curved line, they are on the faces of the crystal. So they are coming out and ending on the surface of the crystal.

Or dislocation can close on itself as a loop. That is suppose this is the slip plane. In this slip plane I could have a dislocation line like this. We can choose the t vector whichever way we take, clockwise or anticlockwise, whatever you want to take. And then if I work out the b vector, you will see there are some places where we had some place screw, as to mixed dislocation. Loops can form like this. Then it is important to understand why it is happening.

It is happening because it is a boundary between the slipped part and the unslipped part of the crystal lying over the slip plane. That means what I am trying to say is that this inside is the slipped part inside the loop and outside the unslipped part. Two are distinct regions. It is possible to say that. Let say now when the dislocation ends on a surface like this, this let me say is the slipped part of the crystal. And that is the unslipped part. Clear-cut demarkation in the two parts of the crystal. All right.

And when it meets in a node like this, then there are three parts that three of them meeting. One is slip related to the other and this is slip related to this. Distinct regions are there and the continuity is provided by the node where there is not displacement. And therefore some of the three Burgers vector turns out to be 0. Otherwise the crystal would not have a continuity, there will be some kind of discontinuity there at the node which cannot happen.

So this is relatively slipped respect to that while this is relatively slipped respect to the other two. So slipped part and the unslipped regions of the crystal are very well defined. Then only I get the boundary and that is the dislocation line. So another words what I am trying to say is I cannot have a situation where I have a dislocation starting from here and it stops here in the crystal.

Which is the slipped part, which is the unslipped part? Can you define? You cannot. Right here when you come, you get into trouble where this is the slipped or this is unslipped, which one is this? This is the same region. So that is not allowed. That is not possible. No dislocation can end inside the crystal abruptly like this. Right.

We have seen there are strains associated with the dislocation line, whether it is edge, whether they are principal strains, screw dislocation where the shear strains and mixed dislocation or general dislocation, general state of strain. Whenever there is a strain, there would be some stress in the bonds. Bonds are strained means bonds are also stressed. There is a stress acting on it. There will be some strain in these two.

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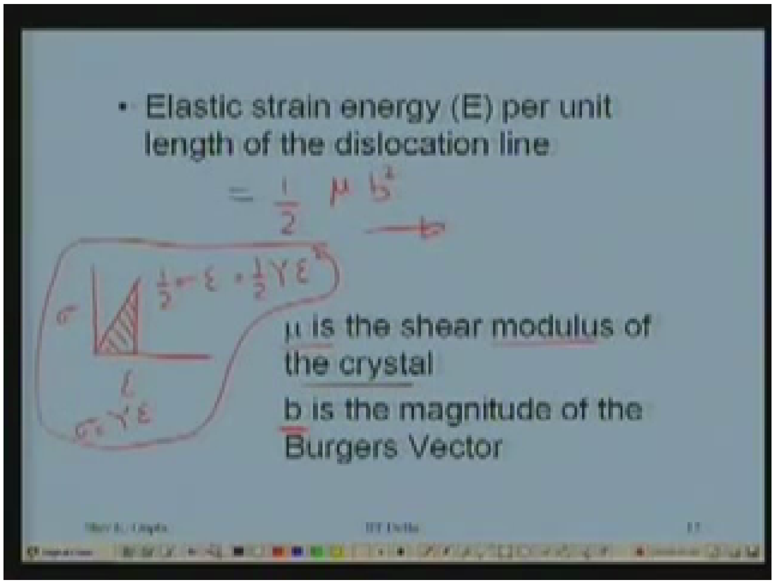

I consider elastic strain energy and work out the model. It is just simply said energy per unit length of the dislocation line is 1 by 2 mu times magnitude of the Burgers vector square, right. That is the energy of the dislocation line per unit length. Multiply it by the length, you will get total energy stored in the crystal.

“Professor-student conversation starts.”

Student: What is mu in there?

Professor: Mu is the shear modulus of the crystal. b is the magnitude of the Burgers vector. Right. This is you can see parallel of this when you would see the Hooke’s law. This is the stress, this is the strain. Energy per unit volume is here, it is 1 by 2 sigma times epsilon. And you know Hooke's law is obeyed, so sigma is equal to Young’s modulus into epsilon. If I substitute this sigma by Young's modulus into epsilon, this becomes 1 by 2 modulus times epsilon square.

“Professor-student conversation ends.”

You see that I do not write the above relationship but I am showing how it is got. b is the magnitude of the Burgers vector is the amount of displacement. This is the measure of the strain. Mu is the shear modulus, okay, which is because I am talking about the shear taking place. So that is instead of modulus I am using Young’s modulus, I am using the shear modulus. So that is the energy or elastic strain energy stored in a dislocation line whether we will take this as this model respect to our edge dislocation, screw dislocation and mixed dislocation. A small difference between them, the energy is for edge and screw but we shall keep using this formula. In this course we shall use only this one.

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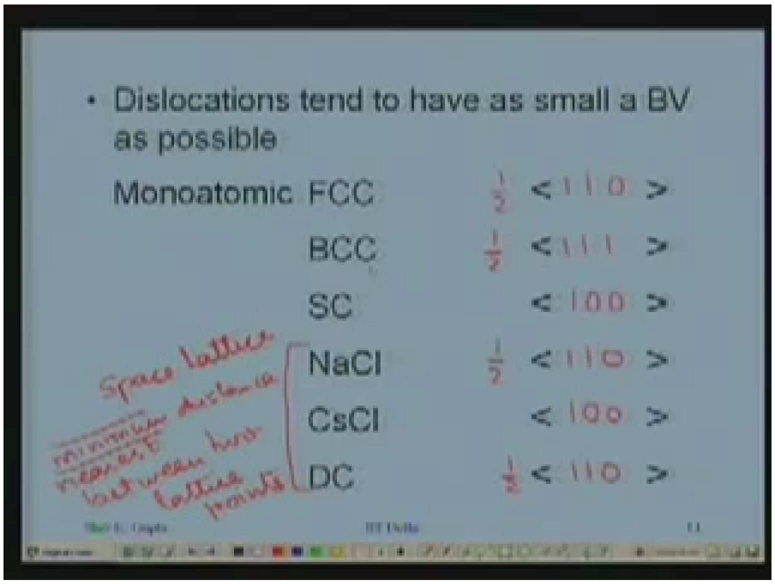

Now from this energy you can see that half mu b square and I already told you that dislocations are present and they are not in thermodynamic equilibrium. Meaning thereby by their presence they are increasing the free energy of the crystal. So tendency of the crystal would be to have as small an increase as possible for every dislocation. So dislocations would like to have as small an energy as possible.

Shear modulus is a characteristic of the material and I told you which is structure insensitive property. We shall see what decides this shear modulus or the elastic modulus. But Burgers vector, mu b square by 2, b square if you can minimize, that should be the minimum energy of a dislocation line. That will be little more stable dislocation, that kind of dislocation in the crystal. So I am considering the monatomic FCC crystal.

“Professor-student conversation starts.”

Professor: And the what is the smallest distance between a displacement which you can do from one location to another for an atom in FCC? Smallest displacement you can do is from corner to the face center.

Student: t by (())(26:33)

Professor: So which I can write as 1 by 2 of 110. Any face diagonal, 110 family when I write, it could be any face diagram. All right, Half 110. Similarly in BCC what is the minimum displacement?

Student: b by Q.

Professor: Kernel to the body center, let us say that. And this case is represented in terms of mirror indices, 111 and that is the magnitude. Right. Similarly in simple cubic?

Student: 100.

Professor: Magnitude is 1 here. And sodium chloride?

Student: a by 2.

Professor: It is the minimum distance between an cation to anion, right? What is he says a by 2 but that is not correct. If I do that, what would happen? Make a part plane, what would happen is below the part plane, ions of the same sign will come together and there will be very strong repulsion between them. When cations, cations come closer, there will be very strong repulsion and that is going to be an unstable configuration of the dislocation.

What provides the stable configuration is when I make the displacement so that an anion goes to the anion, cation goes to the cation. That displacement is again from corner to the face center because it belongs to the FCC space lattice. Now you shall see the other three which I am showing. It is the displacement from one lattice point to the next which gives me the stable displacement for a dislocation line or the Burgers vector of the dislocation line.

Sodium chloride would be again like in the FCC, half 110. In caesium chloride similarly which is caesium and the body center chlorine at the corners, displacement from corner to the body center would mean going from chlorine to caesium. That means two ions with same sign coming together again. So we will have to make the displacement, chlorine goes to the chlorine, that is from the edge one corner to the other corner. And that would be again 100. This is again the space lattice, is simple cubic.

Same is true about diamond cubic, it will be again half 110. So these three say the minimum distance between the lattice points. So you have to look at the space lattice. And this is the minimum distance between two lattice points or nearest distance between two lattice points. Instead of minimum if you want to call nearest, that would be I think more close. Nearest distance between two lattice points.

So that is what is happening here. And that if I continue this, this is holding valid for monatomic crystals also. This distance is from one lattice point to the next. Also from one lattice point to the next and one lattice point to the next. Here the situations are simpler, because all atoms are alike. Right. And again it turns out to be one lattice point to the next which is the nearest distance.

Student: Sir, you can explain in the case of NaCl what happens if the a by 2 is removed?

Professor: I thought so, okay, if you want, I can do that. All right. I need a, all right, I think I do not have it here.

"Professor-student conversation ends."

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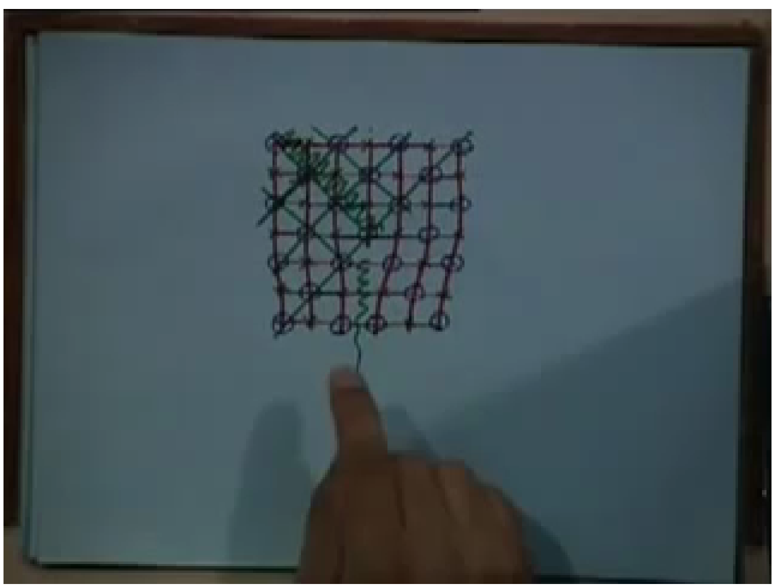

Okay, let us make sodium chloride. All right. And I place cations here. All right. Let us say this is my part plane. I make this displacement and this is my part plane up to here. What happens to the other planes just check that. This plane is continuing with anion, cation, anion, cation, anion, cation, anion, like that. But see now the situation just below the part plane somewhere here. This is far off because the bond is stretched. These are the two anions coming together, two cations coming together, two anions now coming really together.

That is what is making it unstable. But if you make the displacement like this, and use this as the part plane, you can draw a similar structure with starting this you have cube like this. You can make a cube. Make this as part plane. You will see that when you try to make this, there is always an opposite ion in between which is sitting here. So anions will not come close to anions, cations will not come to cations which is only the opposite charges will remain together.

You please make this picture yourself with this orientation and make this as the part plane and see what happens. Okay. And when you make this as part plane, either this set of cations or that set of cations will go along with the plane. Let us say take this one, only then it is electrically neutral, these anions and these cations because my displacement is from here to there. So whatever is in between, that is also displaced. Right.

So therefore this is the plane is going to be slightly thicker. It is not that and that is what shall make it stable configuration. Is this point clear? Okay, good. But please do sketch this yourself so that you understand what we are talking about.

“Professor-student conversation starts.”

Student: Sir…….?

Professor: Now changed. I changed, okay good. Let us go to the next.

“Professor-student conversation ends.”

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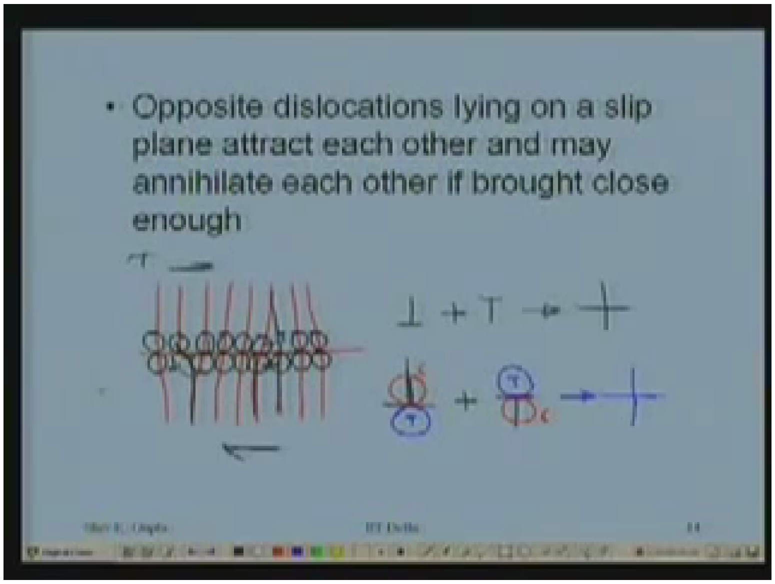

Next we find the characteristics. The opposite dislocations lying on a slip plane attract each other and may annihilate each other if brought close enough. I will just demonstrate this with the help of let us say this is my slip plane. On this slip plane let me add this as one dislocation line. Here I have one positive edge dislocation and here I have one negative edge dislocation. Both of them lie on the same slip plane. All right.

These are the atoms are placed. It is possible for us to make them (britan), make them come together. There is an, I said there is an attraction between them. They would like to come close to each other. Let us say I try to apply a small stress like this, a shear stress. This is pushing the top part of the crystal to the right, bottom to the left. It is possible that on doing so, the stress may be enough for this atom to bond with this one so that it comes slightly to the left and this one comes slightly to the right and form a bond. So part plane comes here.

Similarly on this side now when I am applying the force this way, this is going to slightly to the left and this one goes slightly to the right and they can form and this becomes a part plane. Like this the part plane can shift and they can come one over the other exactly and they will make a perfect crystal. Right. That is I have a dislocation like this, add onto this a dislocation like that and I get a perfect crystal. Right? And all the strains from the crystal would have gone. All the additional free energy which was there in the form of (mu) half mu b square, is gone.

No dislocation is there in the crystal, energy is lowered of the crystal. Right. So the opposite dislocations lying on the same slip plane have an attraction towards each other. Also it can be seen like this: when I have a dislocation like this, I have compressive strains here and I have tensile strains here. Similarly when I have added to it another dislocation like this, I have compressive strains here and I have tensile strains here.

When they come together, a negative strain and positive strain, they add because this is vectorial addition of this and therefore the net displacement can become 0. And ultimately I end up with a crystal without any strain whatsoever. There are no strains in it. It becomes strain free. Compressive strain cancels the tensile strain here and this tensile strain cancel the compressive strain here and this is now common slip plane, we get a perfect crystal.

"Professor-student conversation starts."

Student: Sir, but they should be very close enough. Is there any limit so…..?

Professor: No, if there are opposite signs lying far off, there is a forced attraction between them, there is an attraction. But when they can come towards each other, I am not guaranteeing that. I said that let me apply this stress. By applying this stress I try to bring them together. If I do not apply any stress, would thermal energy bring them together? It depends how high the thermal energy is. And secondly usually thermal energy provides a random processes. Sometimes atoms are going this way. Sometimes they are jumping this way, sometimes jumping up.

So it is not making it go in a particular direction. Right. So it may, if they are very close and we are applying stress, possibly and the temperature is high, it may happen. I am not saying that it will always happen. Distance is more, definitely it is not easy for them to come towards each other.

Student: External help have to be used?

Professor: At times, yes. And sometimes if the temperature is very high and they are close by, it can happen. Okay. So both thermal energy and the external help, both are required.

"Professor-student conversation ends."

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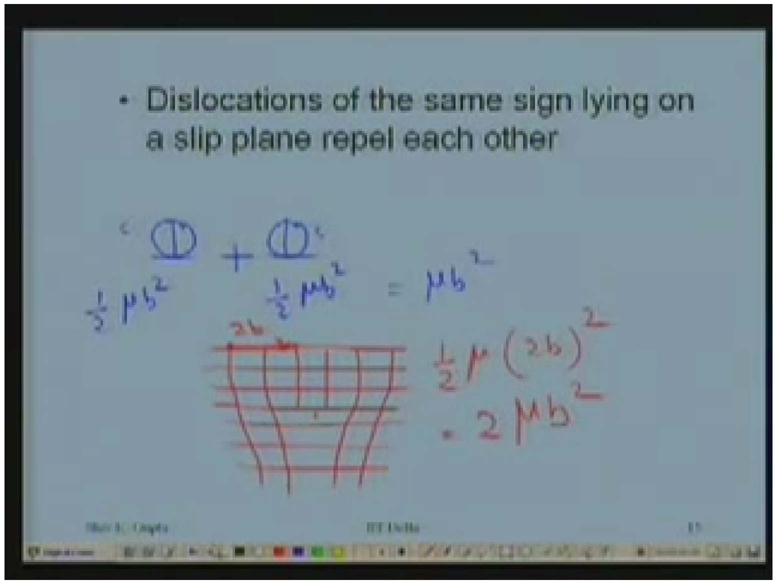

Dislocations of same sign lying on a slip plane repel each other. Obviously, if they are of the same sign, that means this compressive strain here and this compressive strain here when they are coming closer to each other, will add up. When the strains add up, they add up linearly. What happens to the strain energy? It goes to the square of the strain, I just now showed. So it will become very high. Say for example, what happens here? Right now the two dislocations on the same slip plane but far apart, its energy is 1 by 2 mu b square.

And this energy is also 1 by 2 mu b square. So total energy is mu b square. When I brought this, bring this dislocation together close to each other, what the configuration would be? Let us see that configuration. This part plane and this part plane, both have come together.

"Professor-student conversation starts."

Professor: What is Burgers vector of this dislocation line?

Student: It is 2b.

Professor: It is going to be from here to there which will be 2b. If I consider one single dislocation, what is the energy of this? 1 by 2 mu 2b whole square, that is the magnitude. So it becomes 2 mu b square which is double of this. Compare that. So why there is a repulsion? You can see now that because crystal is trying to have or system is trying to have as low free energy as possible. So by keeping them apart, energies are mu b square but bringing them closer, energy become 2 mu b square. There is an (extr) increase in energy by the amount mu b square. Right. Therefore there is a repulsion between them.

“Professor-student conversation ends.”

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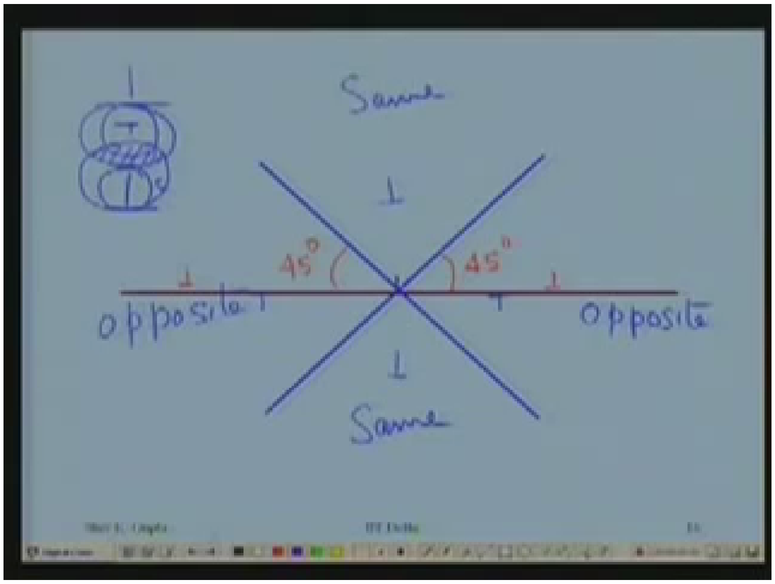

Other interactions, these are the interactions between the dislocations. Here I show you, this is a central dislocation and there is an region in the crystal around it. I talked about dislocations of the same sign lying on the same slip plane here, they repel. But dislocations of opposite sign are attractions I show let us say by blue. These will be attractive. This is what we have talked about. Right. However when I go in a region just above this, if I have a dislocation of this sign, there would be an attraction between this and this.

“Professor-student conversation starts.”

Student: Sir, what this cross represent? Means you know….

Professor: Pardon. Is the region around the dislocation line. And this is an angle of 45 degrees from the slip plane. Why this is going to attract? This we use the blue color for that usually. Here and here, these will attract each other. I will try to arrange one over the other. Can you see that when I have a dislocation like this, I have here tensile strains? When I have dislocation just below this, the same sign, I have compressive strains here. So I can make the bigger field of the strains.

"Professor-student conversation ends."

So there is a region here where there is a positive strain, negative strain meet each other and cancel. So is the volume of the crystal where strain energy is not throughout. So energy of the crystal is lowered by this. So same sign attract. Here opposite sign attract, here opposite sign attract, here is the same sign, here also the same sign. So the whole region in the crystal around a dislocations line which is straight line, I divided into four parts, four segments.

By slip plane making angle of 45 degrees, another plane here, another plane there. So between this region, same sign dislocations attract. In this region, same sign dislocations attract while in this region only opposite kind of dislocations attract each other. Right. So that is the interaction of dislocations with dislocations whether it is edge, screw or anything, right? As on the sign we are talking about, same or opposite.

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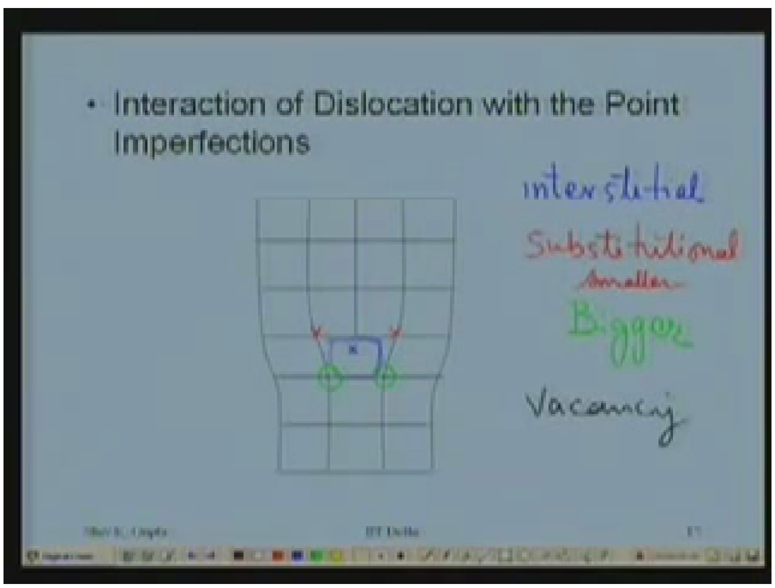

Now I would like to look at the interaction of the dislocations with the point defects. So far we talked about the point defects. So other than the dislocations, let us see how do they interact. I had just taken example of edge dislocation. In the edge dislocation, their bonds are shorter, compressive strains are there. Here the bond longer, there is tensile strains are there. So the point imperfections can be let us say an interstitial solute or interstitial atom.

If it is an interstitial atom, it would like to find an interstitial location where it can sit without straining the neighborhood and minimize the energy if possible. Usually we told you that the atoms which we have, thus bigger than the void spaces available in closed-pack structure like octaval voids in FCC, 0.414 is small enough for even small atoms to sit there. So when interstitial atoms sits, for example, carbon sitting anion, it strains the neighborhood.

"Professor-student conversation starts."

Professor: However if you can find the bigger void space, it will go and sit there, it will not strain the neighborhood so much. Where is the location where the void space which is bigger in volume?

Student: Below part plane.

Professor: Below the part plane. See, this is the much bigger region and it can sit here. That is the interstitial void which can sit there. Just below the edge of the part plane, it can sit. Right. Similarly I can have substitutional impurity atoms. Substitutional atoms could be smaller, could be bigger. If I have a smaller atom, if I have a smaller substitutional atom, it requires less space to sit. Where would it sit?

Student1: Edge of the part plane.

Student2: Above.

Professor: Towards the edge, towards the part plane, right. So this is where it would like to sit. So less space is there, it requires only less space to sit. But if I have a bigger substitutional atom, in this tensile region it would like to sit here. Right. So this is how the point imperfections interact. Now vacancy is also point imperfection. How would it interact, the vacancy? Around the vacancy, what are the kind of strains?

Student: Tensile.

Professor: Tensile strains. Where would it go?

Student: In compressed region.

Professor: In compressive region. If it goes in the compression, I can interact like this with it. Right. All right.

"Professor-student conversation ends."

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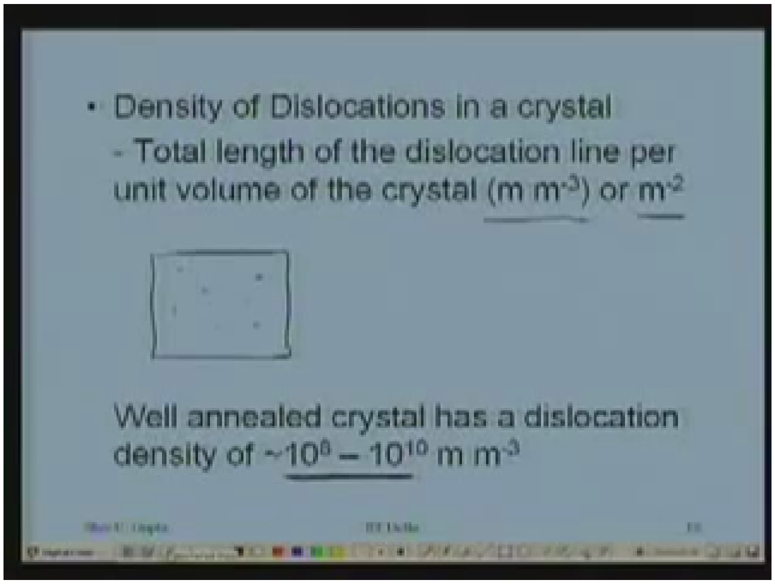

Now after this we will talk about a few more characteristics. The density of a dislocation in a crystal, means the length of the dislocation line we express per unit volume of the crystal and that is either expressed meter per cubic meter or per square meter. The way these are measured is a small difference. Meter per cubic meter, it is the total length of the dislocation line per unit volume of the crystal.

As we measure per square meter, let us say we take, usually crystals are opaque. We take a surface of the crystal, prepare the surface, properly polish it and find out the number of dislocations intersecting the surface. This number per unit area of the surface we have chosen is what it is. The way it is measured, there is a small difference between this and this. Statistically if I have 2, but that 2 factor we shall ignore when we talk about the out of the magnitude, 10 to the power 12 per cubic meter per cubic meter or 10 to the power 11 meter per cubic meter kind of dislocation length we talk about you can ignore the factor of 2.

Now well annealed crystals have a dislocation density in the range of 10 to the power 8 to 10 to the power 10 meter cubic meter. Well annealed, what I mean by this is that I have tried to keep it an elevated temperature. Annealing gives the connotation that the crystal has been kept at an elevated temperature where available thermal energy is high. That thermal energy tries to have the dislocations get out of the crystal. Either the same kind dislocations coming together, no, opposite kind dislocations coming together and annihilating or they go out of the surface and get out of the crystal. Right.

Those are the things but even after doing all that, I am left with length of the dislocation line of the order of 10 to the power 8 to 10 to the power 10 meter per cubic meter. If I have 10 to the power 8, which is usually more than 10 to the power 8, 10 to the power 8 meters means 10 to the power 5 kilometers. It is 0.1 million kilometers, is the length of the dislocation line in a cubic meter of the crystal. Right. It is not a small length but the total volume which is affecting I said is still very small. Despite this length total volume which is affecting of the crystal is very small. All right. Then we stop here and start from here in the next class.