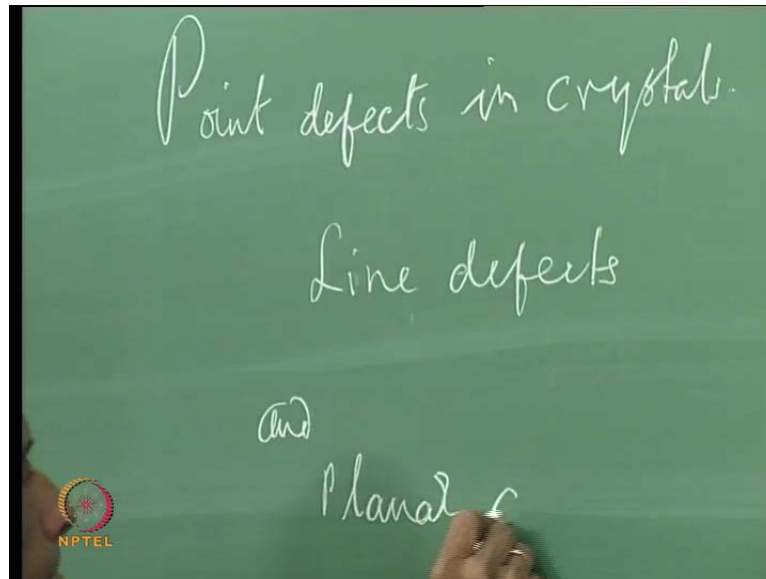


Condensed Matter Physics
Prof. G.Rangarajan
Department of Physics
Indian Institute of Technology, Madras

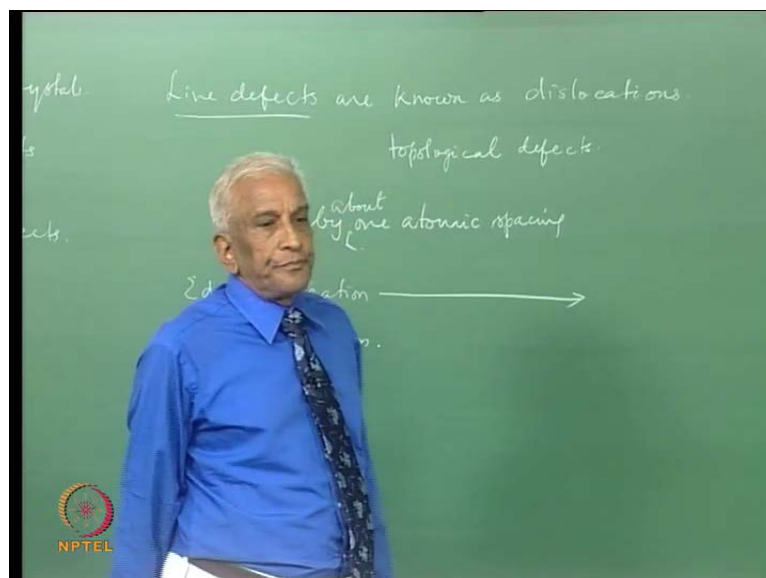
Lecture - 39
Defects in Solids –Line and Surface Defects

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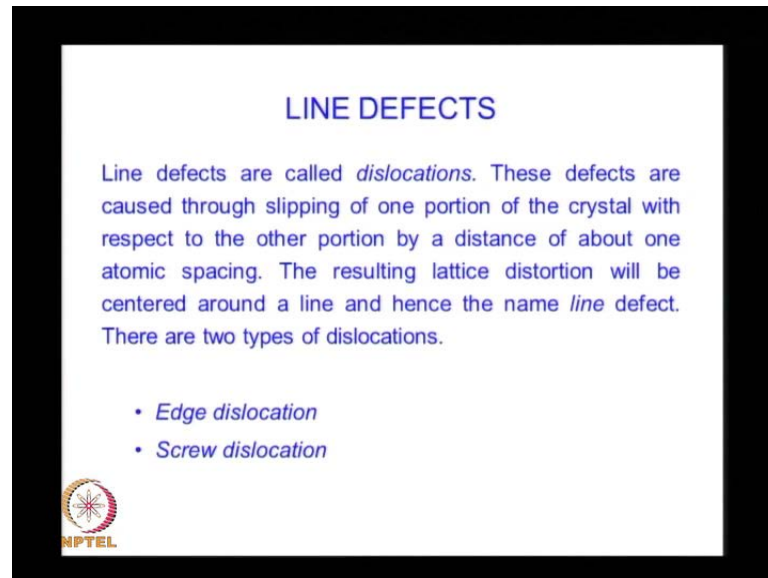
In the last lecture, we talked about point defects in crystals. Today we will talk about line defects and planar defects.

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Now, line defects are known as dislocations; you may remember that we already mentioned dislocations and their relevance to face transitions as topological defects in the first very first lecture of this course .


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LINE DEFECTS

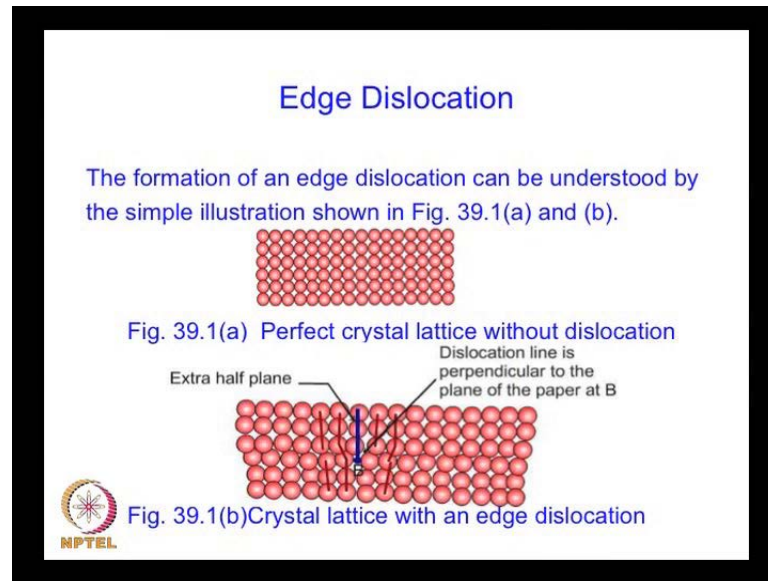
Line defects are called *dislocations*. These defects are caused through slipping of one portion of the crystal with respect to the other portion by a distance of about one atomic spacing. The resulting lattice distortion will be centered around a line and hence the name *line* defect. There are two types of dislocations.

- *Edge dislocation*
- *Screw dislocation*



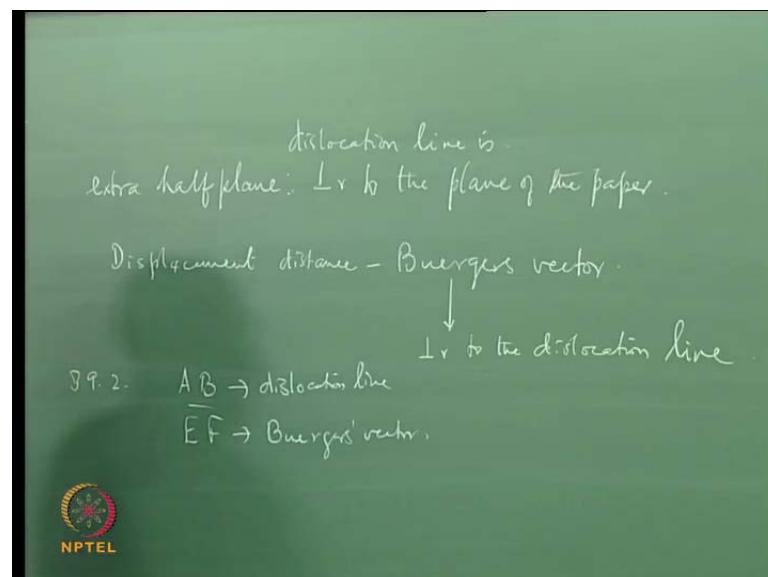
Today, we will see a little more about dislocations; dislocations are caused by the slipping of one portion of the crystal with respect to the other by a distance of about one atomic spacing. So, one portion of the crystal slips with respect to the other by a distance of the order of one atomic spacing. Therefore, the lattice will be distorted and this distortion will be centered around a line, and that is the reason why we call it a line defect. We can have two types of dislocations; one is edge dislocation, while the other is called screw dislocation.

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We will now consider edge dislocation, which is shown in figure 39. 1 (a) and (b), the figure 39. 1 (a) shows a perfect crystal without a dislocation, while this figure (b) of the same figure shows the crystal lattice, in which there is an edge dislocation. So, you can see that in the perfect crystal lattice, the atoms are regularly arranged, while the lattice with an edge dislocation you have an extra half plain.

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So, you have an extra half plane, because of the relative slip. So, this extra half plane is shown by the blue line, thick line in the upper half of the crystal lattice, well the bottom the line is perpendicular to the plane of the paper.

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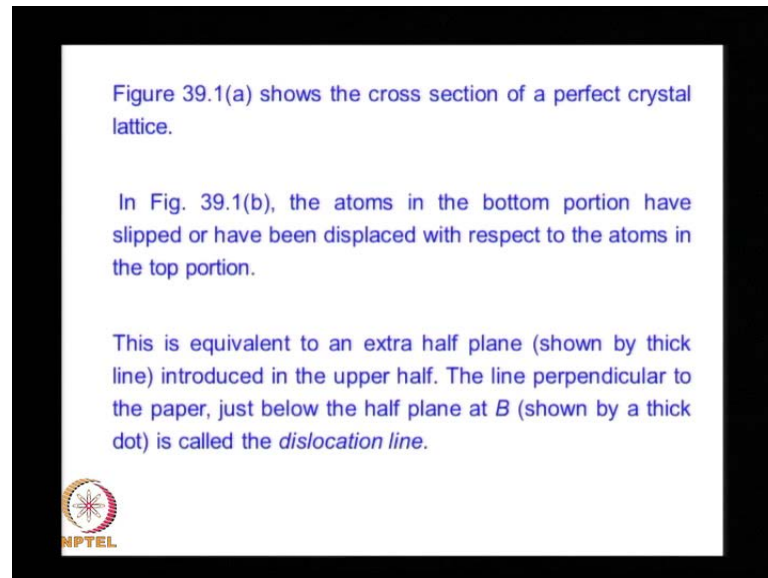



Figure 39.1(a) shows the cross section of a perfect crystal lattice.

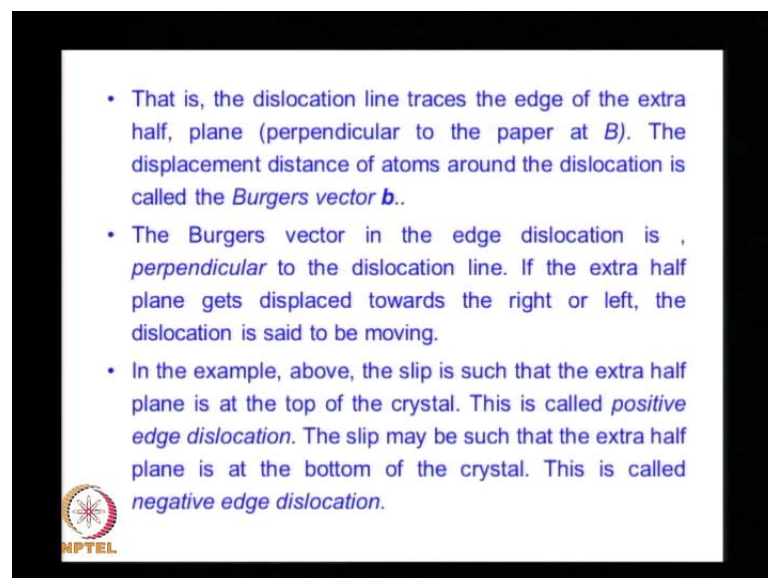
In Fig. 39.1(b), the atoms in the bottom portion have slipped or have been displaced with respect to the atoms in the top portion.

This is equivalent to an extra half plane (shown by thick line) introduced in the upper half. The line perpendicular to the paper, just below the half plane at *B* (shown by a thick dot) is called the *dislocation line*.




So, the dislocation line is perpendicular to the plane of the paper. So, this is shown in the figure by a thick dot at the bottom between the lower and upper parts of this.

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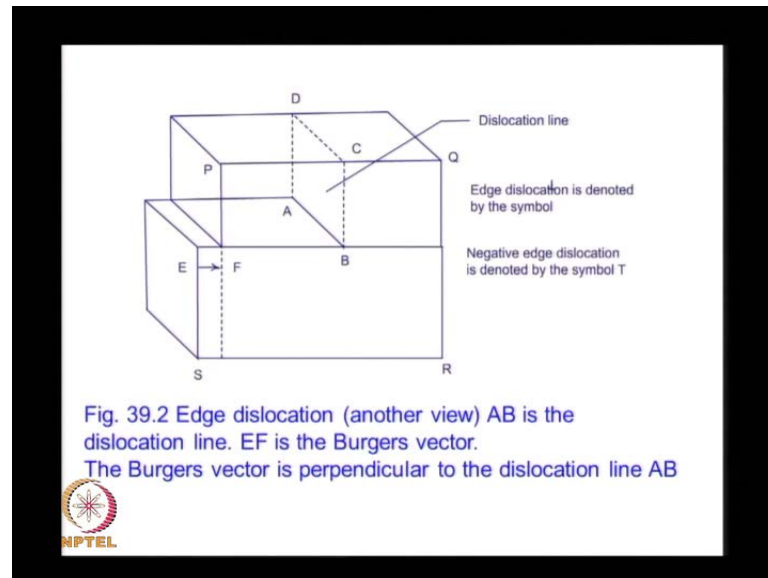


- That is, the dislocation line traces the edge of the extra half, plane (perpendicular to the paper at *B*). The displacement distance of atoms around the dislocation is called the *Burgers vector b* .
- The Burgers vector in the edge dislocation is , *perpendicular* to the dislocation line. If the extra half plane gets displaced towards the right or left, the dislocation is said to be moving.
- In the example, above, the slip is such that the extra half plane is at the top of the crystal. This is called *positive edge dislocation*. The slip may be such that the extra half plane is at the bottom of the crystal. This is called *negative edge dislocation*.



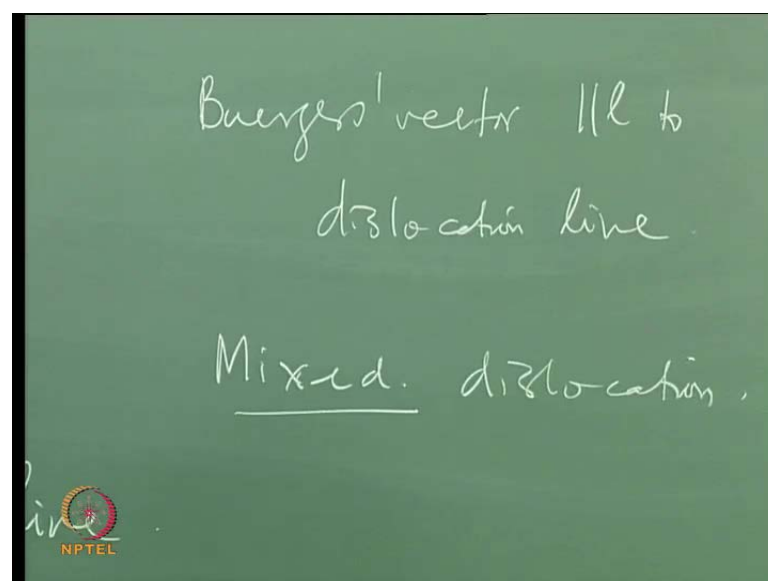
So, you have a displacement. This displacement distance is represented by what is known as the burgers vector. Now this burgers vector in the case of a edge dislocation is perpendicular to the dislocation line.

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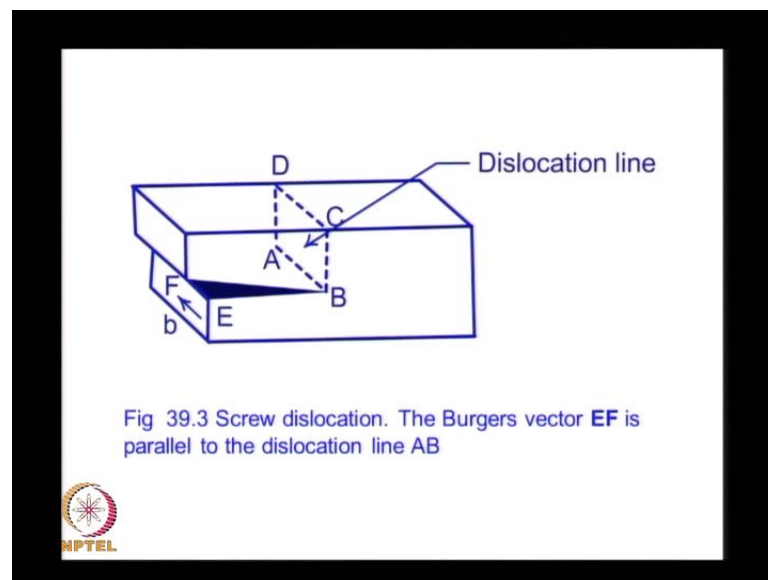
So, this is shown in the figure 39. 2, where AB figure 39.2 AB is the dislocation line, while EF is the burgers vector. So, the burgers vector EF is in this figure is obviously, perpendicular to the dislocation line AB.

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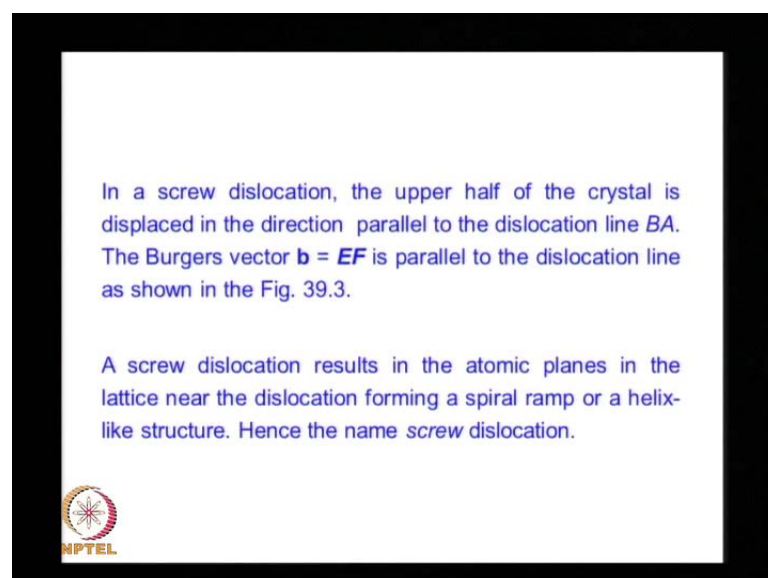
Now, this is the case, with an edge dislocation, you can also have a screw dislocation. If the screw dislocation the burgers vector is not perpendicular, but parallel to the dislocation line, such a situation is used usually created by a shear stress acting on the 2 parts of the crystal.

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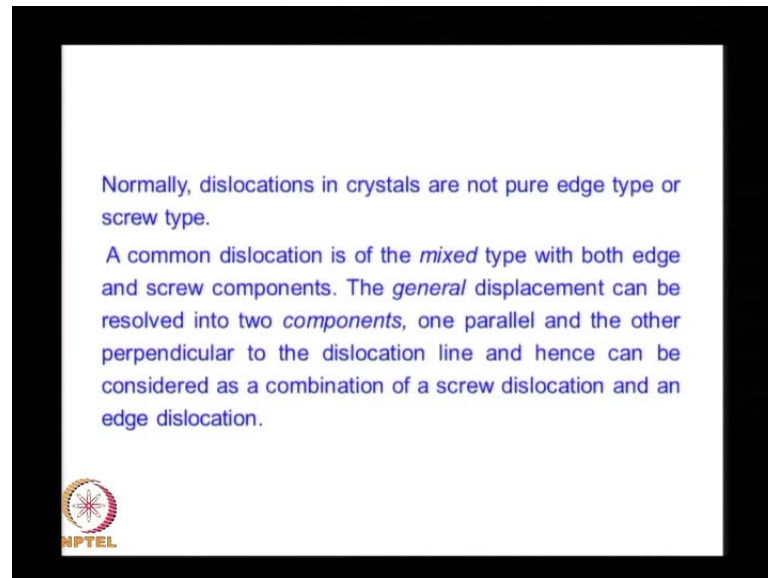
So, this is shown in the figure 39.3. So, you have the dislocation line and the burgers vector EF is actually parallel to the dislocation line AB .

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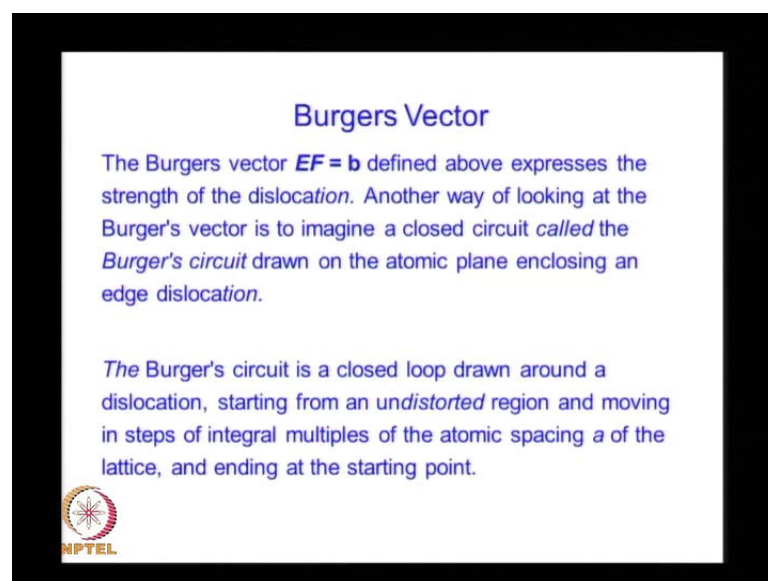
So, there is this results in a kind of spiral dislocation forming a spiral ramp, and therefore this is known as screw dislocation. Now in general, you can have a mixed kind of situation, where the dislocation is neither an edge dislocation nor a screw dislocation.

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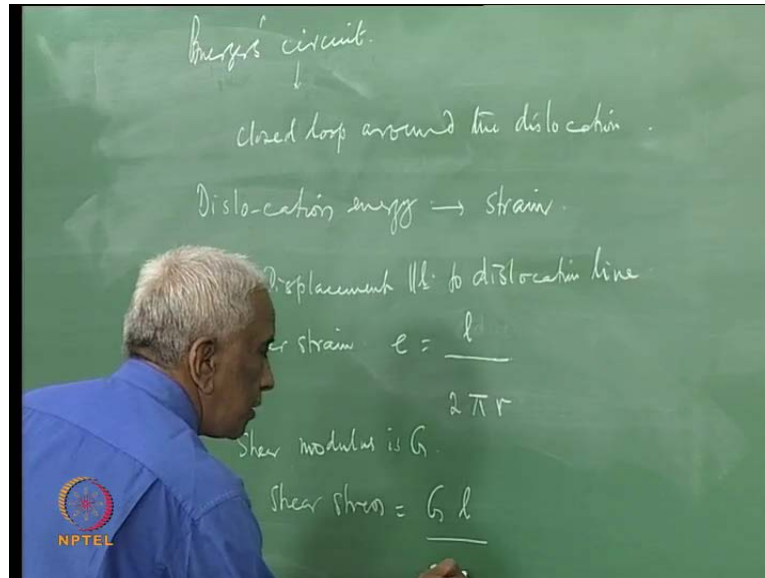
But a combination of these two that is the usual situation, and you can break it up into a component, which is parallel, and another component which is perpendicular to the dislocation. Therefore it is a combination of a screw and an edged dislocation.

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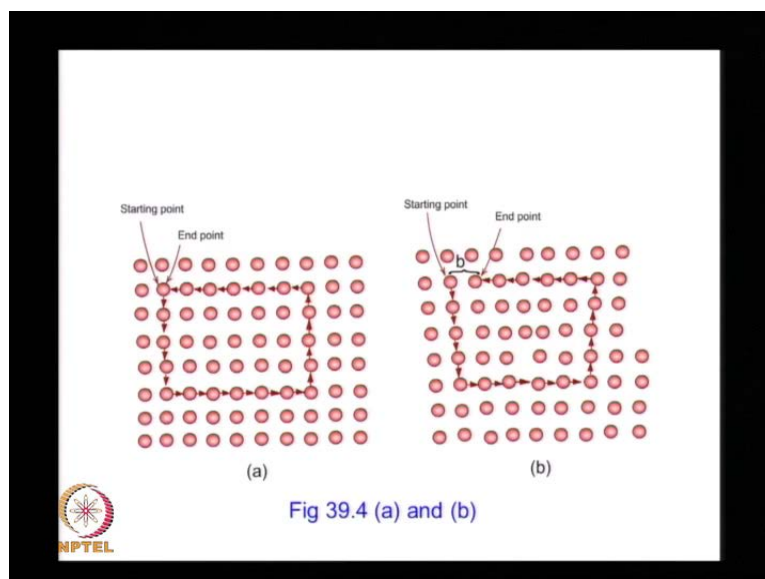
Now, this burgers vector, this gives a measure of the strength of the dislocation. In order to see this, it would be nice to consider, what is known as the burger circuit, which is shown in the next figure.

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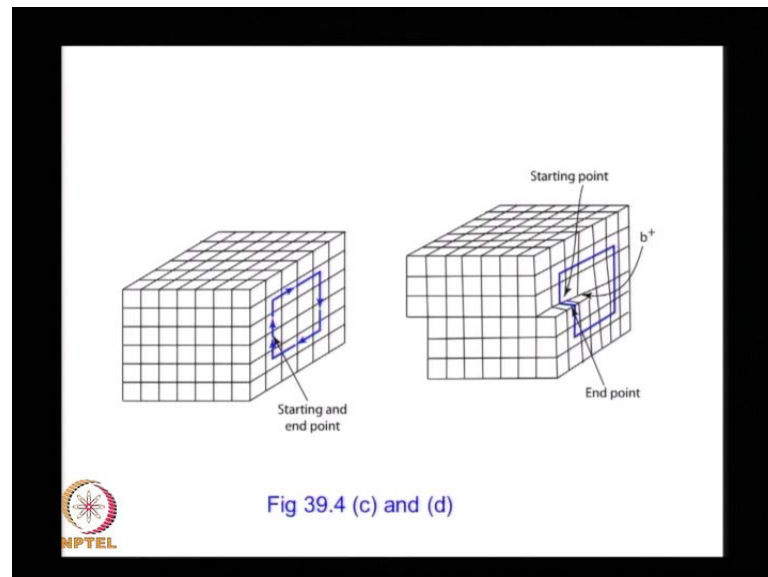
So, it is a close loop drawn around the dislocation, it starts from the undistorted region, and moves in steps of integral multiples of the atomic spacing, and ends back in distorting point.

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The next figure 39. 4 shows this burger circuit; and in the figure 39. 4 (a) you sees a perfect lattice without a dislocation, where the burger circuit is comes back and closes; whereas, in the figure (b) of the same you have a dislocation. So, there is a slip, which has occurred and therefore, the burgers circuit is not closed.

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And this is in connection with a screw dislocation, and the same situation is shown in a for an edge dislocation in 39. 4 (c) and (d). So, you can see that the circuits closest in a perfect lattice whereas, in a lattice with dislocation, the circuit does not close an additional step of (b) equal to the burgers vector has to be traversed in order that the circuit is closed.

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Dislocation Energy

- The formation of dislocation involves displacement of atoms and so certain strain energy is associated with a dislocation. The strain energy may be expressed in terms of the Burger's vector.
- Consider a cylindrical element (a shell) of radius r and wall thickness dr surrounding a screw dislocation as shown in Fig. 39.5.



We said that the burgers vector is a measure the strength of the dislocation. So, we will consider dislocation energy in order to see this, what is the energy involved in creating a dislocation. So, the formation of a dislocation involves displacement of atoms. So, there is a certain strain energy associated with the formation of a dislocation. So, this strain energy so the presence of a dislocation causes a strain in the lattice, and we are talking about the energy associated with this train.

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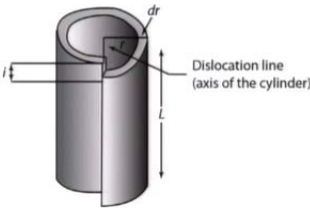



Fig. 39.5 Cylindrical shell around a screw dislocation

A displacement l parallel to the dislocation line produces a shear strain. The shear strain is given by

$$e = \frac{1}{2\pi r}$$


So, let us consider a cylindrical element, a shell of radius r or an wall thickness dr around the screw dislocation. So, suppose we talk about a displacement parallel to the dislocation line. So, that produces a shear strain. So, if the displacement is l , then the shear strain e is l by $2\pi r$, where r is the radius of the cylinder.

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If the shear modulus of the crystal is G , the shear stress is given by

$$\sigma = G \frac{l}{2\pi r}$$

An infinitesimal displacement dl involves work given by

$$dW = \sigma \times \text{area} \times dl = \frac{Gl}{2\pi r} \times \text{area} \times dl$$

the area on which the shear stress acts is $L \times dr$, where L is the length of the cylinder, so that

$$dW = \frac{GL}{2\pi} \frac{dl}{r}$$


So, if the shear modulus is G , then a shear stress is just stress by strain in the modulus. So, we know the strain, so strain times so $G L$ by $2\pi r$ that is the shear stress. Now this displacement involves work.

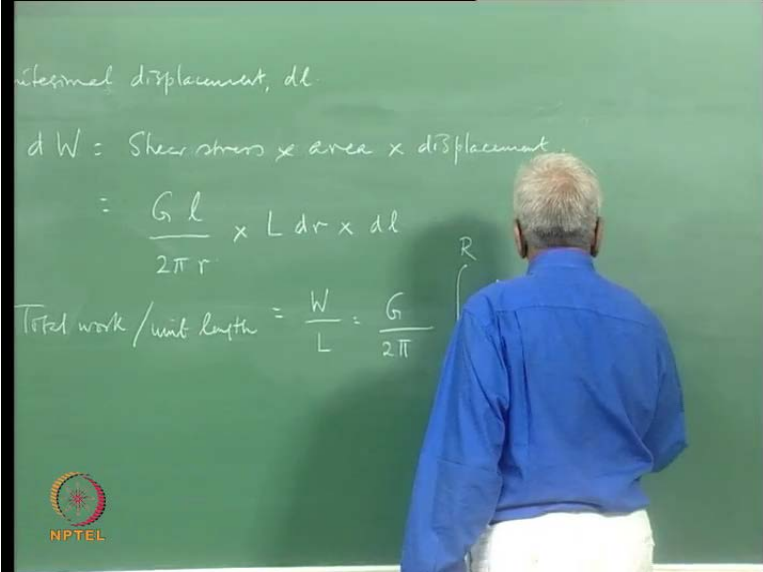

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infinitesimal displacement, dl

$$dW = \text{Shear stress} \times \text{area} \times \text{displacement}$$

$$= \frac{Gl}{2\pi r} \times L dr \times dl$$

Total work / unit length = $\frac{W}{L} = \frac{G}{2\pi}$


Suppose I have a displacement an infinitesimal displacement $d l$. Now that means that the work associated with this is the stress times times the area; so that gives the force into displacement. So, the shear stress is $G L$ by $2 \pi r$ times the area this is if the length of the cylinder is l , then it is $L d r$ that is the area and then you have $d l$ as a displacement. So, that would be the work.

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The total work done per unit length or energy per unit length is

$$\frac{W}{L} = \frac{G}{2\pi} \int_{r_0}^R \frac{dr}{r} \int_0^b |dl| = \frac{Gb^2}{4\pi} \ln \frac{R}{r_0} \quad (39.1)$$


Here r_0 is the radius of the dislocation core and R is an upper limit to the range of the strain field determined by the dislocation density.



So, if I want the total work per unit length of the cylinder is W by capital L which is G by 2π integral $d r$ by r from r nought to r integral $d l$ $d l$ is $2 b$.

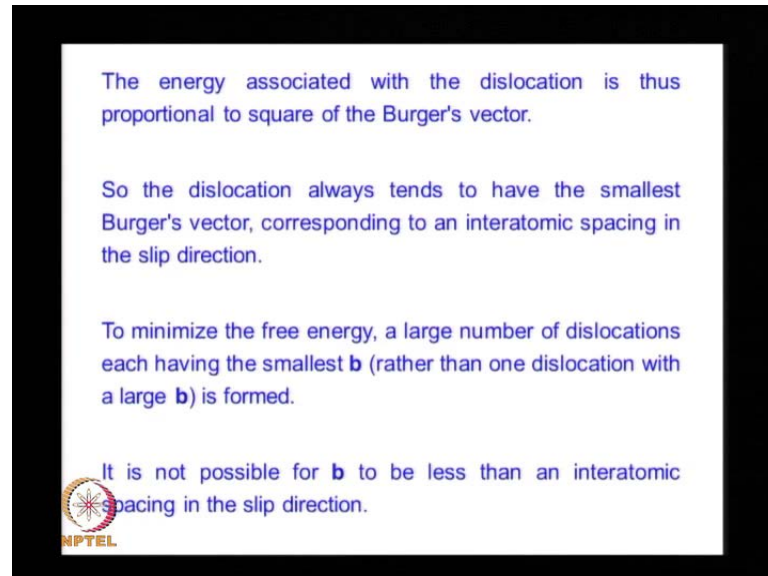
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$r_0 \rightarrow$ radius of dislocation core.
 $R \rightarrow$ distance upto which strain field exists.
 constant.
 Strain energy $\sim \underline{b^2}$.

$$\frac{d_1}{r} \int_0^b |dl| = \frac{G b^2}{4\pi} \ln \left(\frac{R}{r_0} \right)$$


Here r_0 is the radius of the dislocation core and r is the distance up to which strain field exist. So, evaluating this we get G I have left out $1Gb$ square by $4\pi r$ by r_0 .

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The energy associated with the dislocation is thus proportional to square of the Burger's vector.

So the dislocation always tends to have the smallest Burger's vector, corresponding to an interatomic spacing in the slip direction.

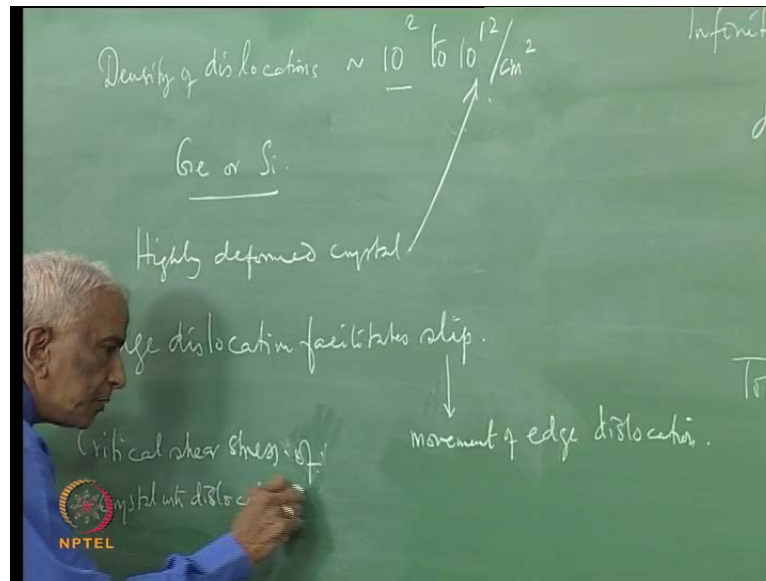
To minimize the free energy, a large number of dislocations each having the smallest \mathbf{b} (rather than one dislocation with a large \mathbf{b}) is formed.

It is not possible for \mathbf{b} to be less than an interatomic spacing in the slip direction.



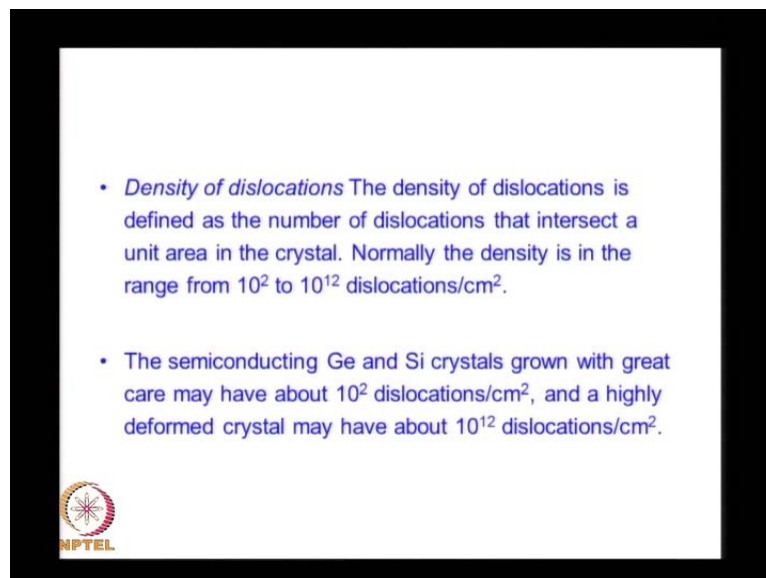
So, we see that the strain energy this total work which is the a measure of the strain energy goes as the square of the burgers vector. So, strain energy associated with this display dislocation goes as the square of the burgers vector. So, the dislocation always therefore, tends to have the smallest burgers vector in order to minimise the energy. So, the free energy is minimized by having a large number of dislocation with small burgers vector rather than a one dislocation with a large burgers vector of course, the burgers vector cannot be smaller than one interatomic spacing.

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Now, how many such dislocations are usually present in other words the density of the dislocations; obviously, in a perfect crystal the dislocation density is small.

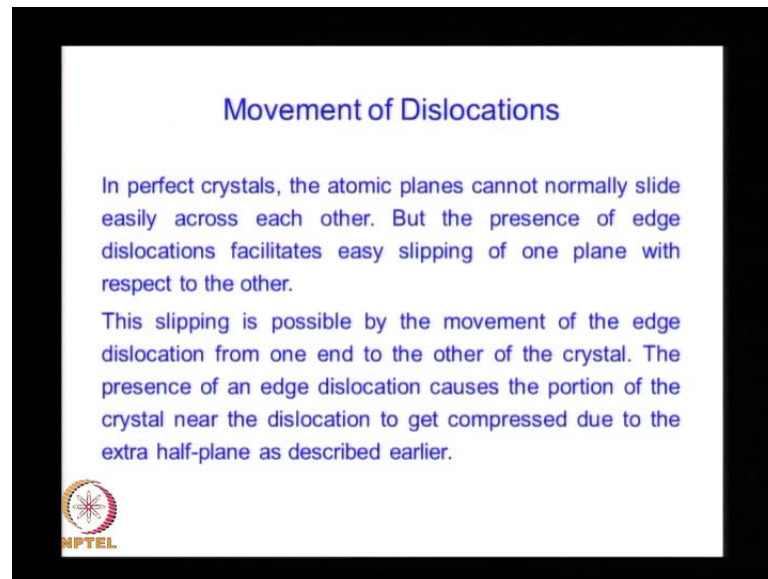
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So, the density is defined as the number of dislocations that intersect unit area in the crystal. So, normally it is in the range of 10^2 to 10^{12} per centimetre. So, if you consider semi-conductors like germanium or silicon which are grown in a very pure form the dislocation density is more in the order of 10^2 dislocations per centimetre square whereas, if you have a highly deformed crystal.

this is of the order of 10^{12} per centimetre square


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Movement of Dislocations

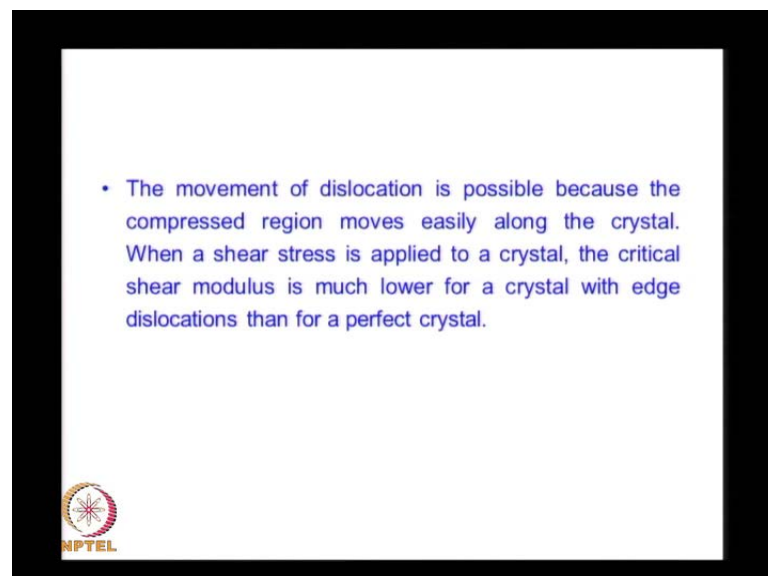
In perfect crystals, the atomic planes cannot normally slide easily across each other. But the presence of edge dislocations facilitates easy slipping of one plane with respect to the other.

This slipping is possible by the movement of the edge dislocation from one end to the other of the crystal. The presence of an edge dislocation causes the portion of the crystal near the dislocation to get compressed due to the extra half-plane as described earlier.




Now, in a perfect crystal the atomic planes cannot normally slide easily across each other, but if I have an edge dislocation it facilitates an edge dislocation facilitates the slip. So, a plane of the crystal can slip over another this slipping is possible by the movement of edge dislocation the slip is made possible by movement of edge dislocation, as we discussed even in the lecture one. So, the presence of an edge dislocation causes the one portion of the crystal near the dislocation to get compressed due to the half plane.

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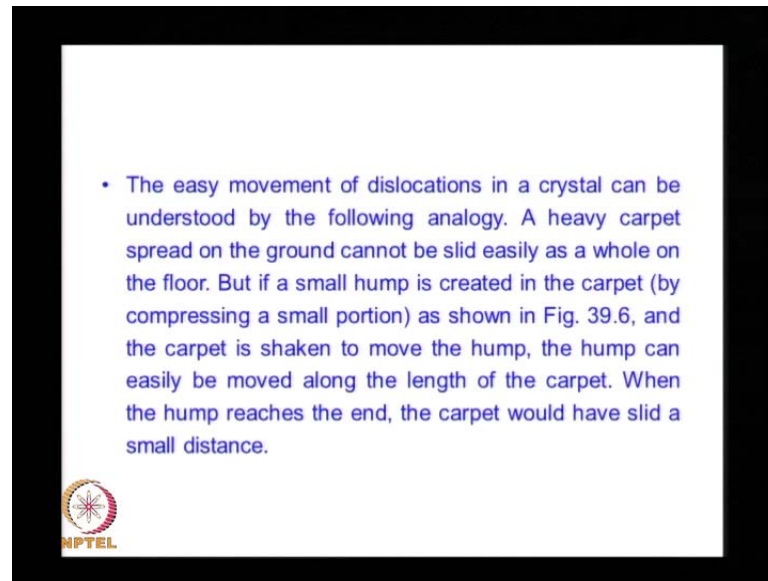


- The movement of dislocation is possible because the compressed region moves easily along the crystal. When a shear stress is applied to a crystal, the critical shear modulus is much lower for a crystal with edge dislocations than for a perfect crystal.



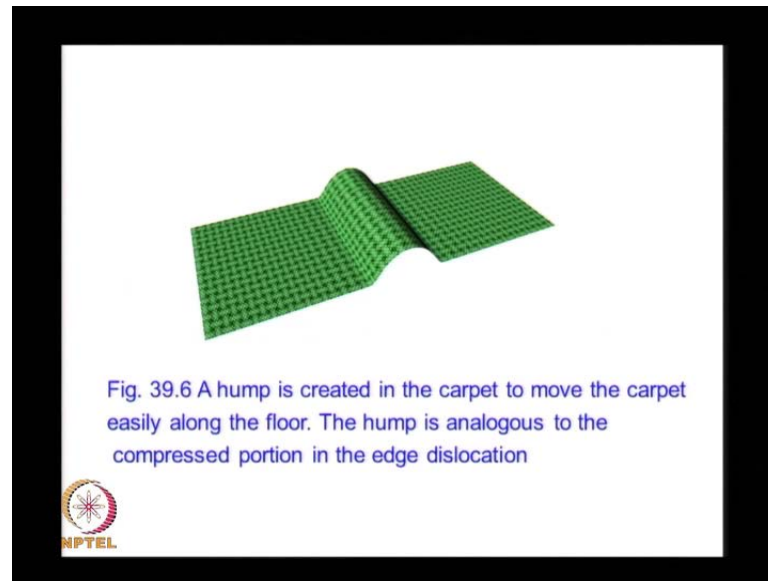
The movement of dislocation is possible because this compressed region moves easily along the crystal, when a shear stress is applied the critical shear stress is the stress that is required in order to facilitate such a movement. And this is much lower for a deformed crystal of a crystal with dislocation is much smaller than that of that for the perfect dislocation free crystal.

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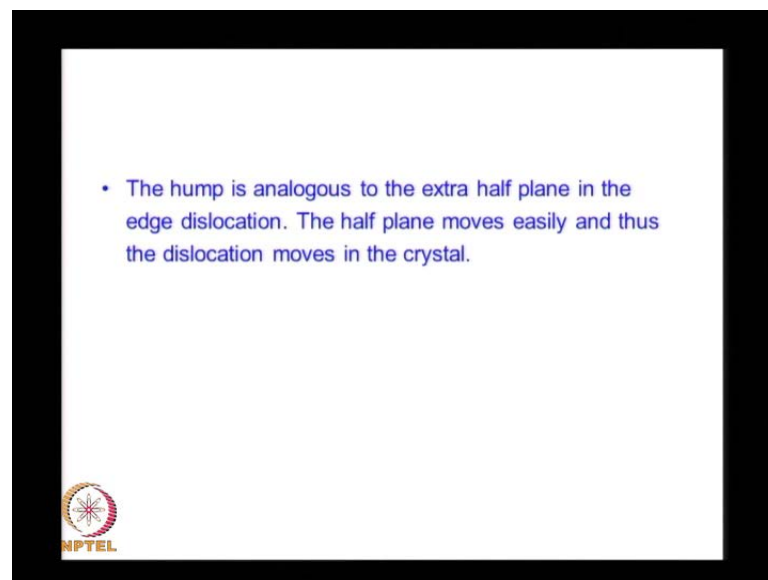
Now, this can be understood by a simple mechanical analogy like when you have a heavy carpet spread on the ground, it cannot be slid easily as a whole on the floor, but if there is a small hump in which is created in the carpet by compressing a portion as shown in the figure.

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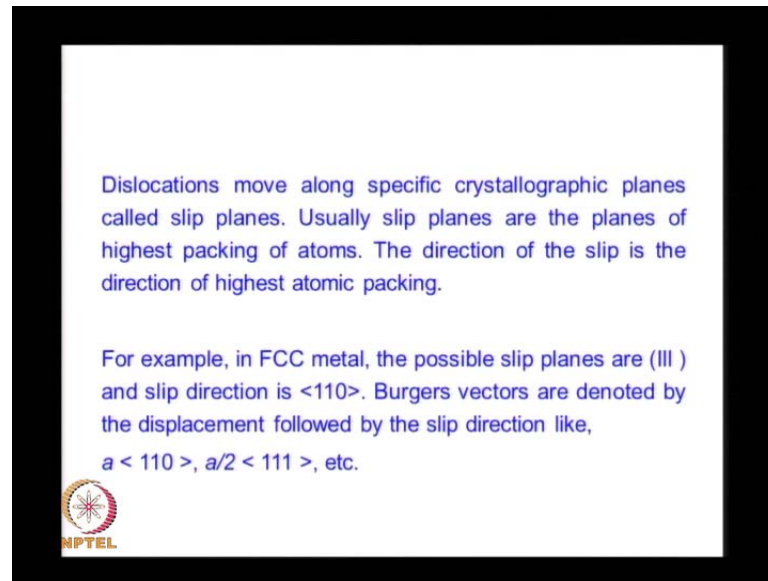
And then the carpet is shaken to move the hump then the hump can easily be moved along the length of the carpet, and the hump reaches the end the carpet would have slid a small distance, that is shown in the next figure.

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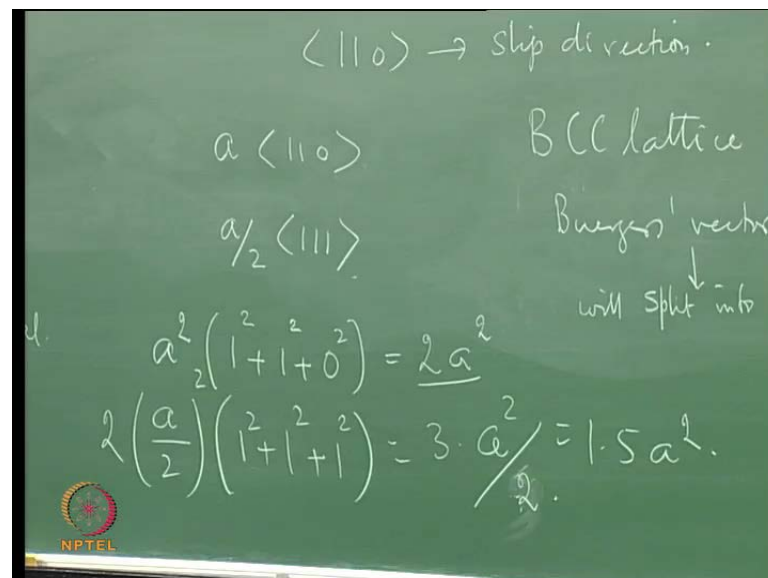
The hump is the analogue of the extra half plane in the edge dislocation. So, this half plane moves easily and thus the dislocation moves in the crystal.

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They move along crystallographic specific crystallographic planes, these crystallographic planes along which they move are known as the slip planes.

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So, the movement is not along any arbitrary direction usually these slip planes are planes of highest atomic packing. So, the atomic density is highest. So, the direction of the slip is the direction of the highest atomic packing. For example, if you have an FCC metal then the possible slip planes are 111, and the slip direction is 110. So, the burgers vectors corresponding to this are shown like a 110 are a by 2, 111, etcetera.

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Burgers vector is the shortest lattice translation vector in the slip direction. This is because the energy of formation of dislocation is proportional to b^2 : (see Eq. 39.1).

For example in BCC lattice if there is a Burgers vector equal to a with the slip direction $\langle 100 \rangle$, it will split into two dislocations each of Burgers vector $a/2$ with slip direction $\langle 111 \rangle$.




Now, the burgers vector is the shortest a lattice translation vector in the direction of the slip, this is because the energy as we discussed of formation of the dislocation is proportional to b square. So, if you have a BCC lattice if there is a burgers vector equal to a if that is. So, in the direction in the slip direction 100 , then it will split into 2 dislocations of each of burgers vector this will split into 2 burgers vectors of magnitude a by 2 in the direction 111 .

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This is because b^2 for a $\langle 110 \rangle$ is greater than twice b^2 for $a/2 \langle 111 \rangle$ as shown below:

$$b^2 \text{ [for } a \langle 110 \rangle] = a^2 [1^2 + 1^2 + 0] = 2a^2$$
$$2b^2 \left[\text{for } \frac{a}{2} \langle 111 \rangle \right] = 2 \frac{a^2}{4} [1^2 + 1^2 + 1^2] = \frac{3}{2} a^2$$

Table 39.1 gives the possible slip plane, slip directions the Burgers vector some simple crystal structures.




This is because b^2 for 110 is greater than $2a^2$ for 111 . For example, $a^2 + a^2 + 0^2 = 2a^2$. Whereas in the other case it will be $a^2 + a^2 + a^2 = 3a^2$. So, this is even though there are now there are 2 such. So, this will be $3a^2/2$ whereas, this is $2a^2$. So, this is $1.5a^2$. So, splitting of this burgers vector into 2 along 111 gives a lower energy than this.

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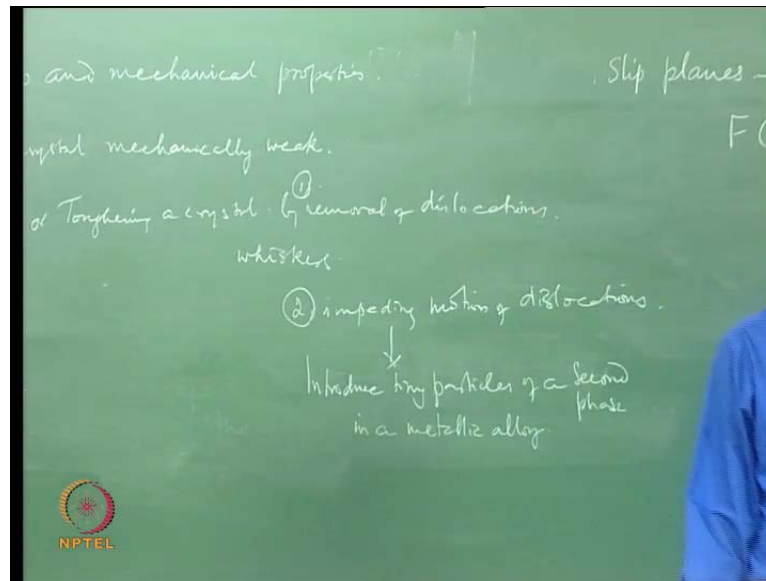
Crystal structure	Possible slip plane	Slip direction	Burgers vector
SC	$\{100\}$	$\langle 100 \rangle$	$a\langle 100 \rangle$
FCC	$\{111\}$	$\langle 110 \rangle$	$a/2\langle 110 \rangle$
BCC	$\{110\}$	$\langle 111 \rangle$	$a/2\langle 110 \rangle$
HCP	$\{001\}$	$\langle 110 \rangle$	$a\langle 110 \rangle$
	$\{101\}$	$\langle 110 \rangle$	$a\langle 110 \rangle$

Table 39.1 Possible slip planes, slip directions, the Burgers vector for some simple crystal structure



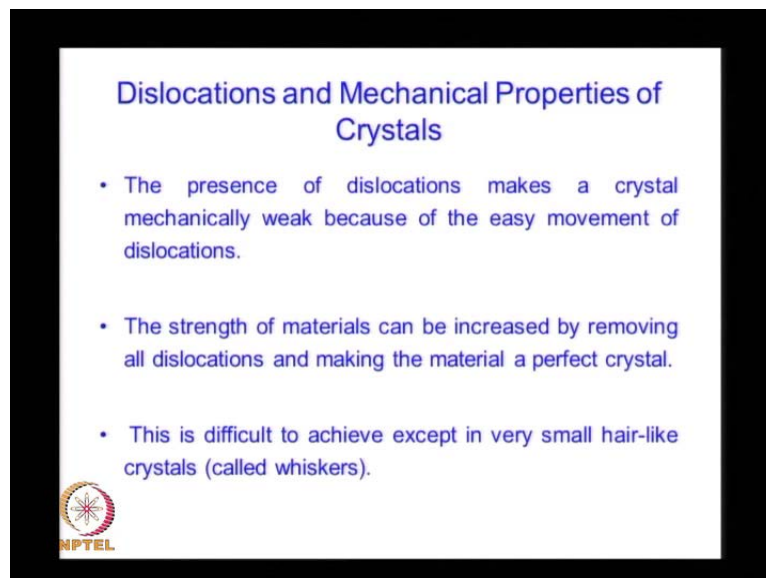
So, in the table 39 1, we are given the possible slip planes, and the slip direction along with the burgers vector for different crystal structures like the simple cubic face centred cubic body centred cubic and HCP hexagonal closed packing.

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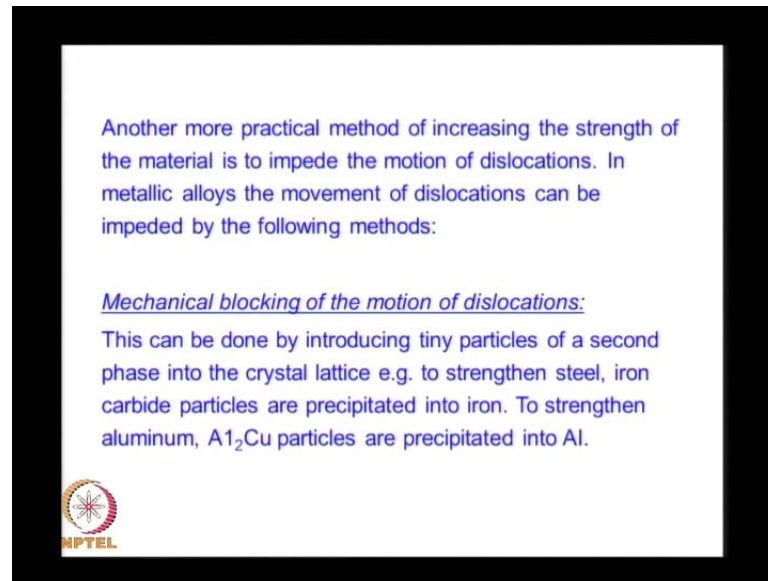
Now, dislocations have a very important bearing on the mechanical properties, if dislocations are present the crystal is mechanically weak.

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So, the strength of materials can be increased by removing all dislocations, and making the crystal nearly a perfect crystal usually, this is extremely difficult toughening make hardening or toughening a crystal by removing of dislocations is usually an extremely difficult thing to achieve and except in what are known as whiskers.


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Another more practical method of increasing the strength of the material is to impede the motion of dislocations. In metallic alloys the movement of dislocations can be impeded by the following methods:

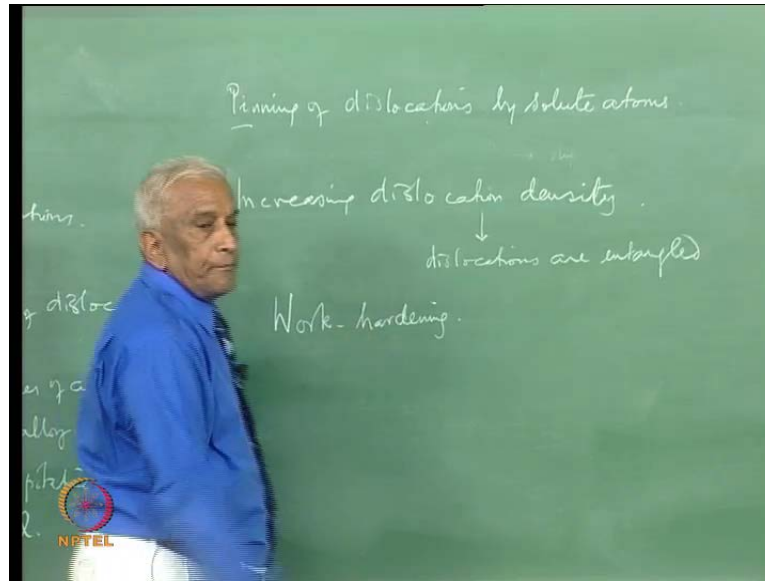
Mechanical blocking of the motion of dislocations:

This can be done by introducing tiny particles of a second phase into the crystal lattice e.g. to strengthen steel, iron carbide particles are precipitated into iron. To strengthen aluminum, Al_2Cu particles are precipitated into Al.



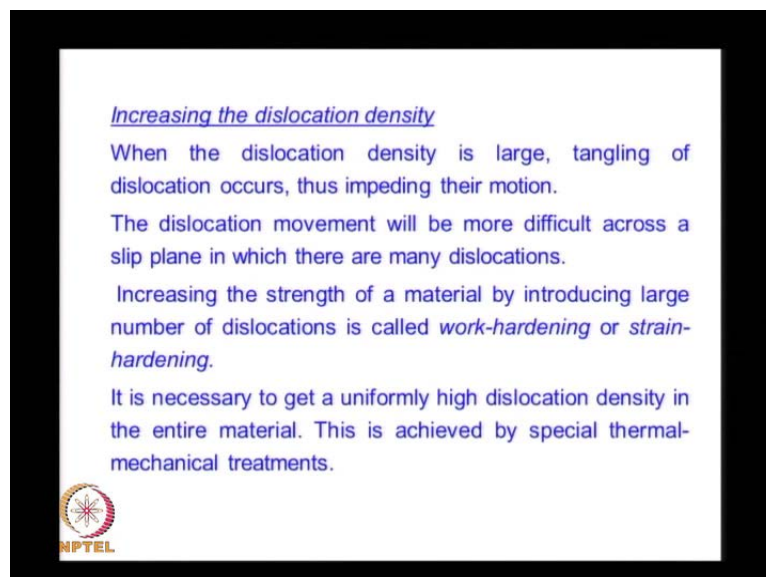
So, these are hair like crystals. So, another more practical method is to impede this is removal the second is impeding the motion of dislocations. For example, in metallic alloys the movement of dislocations is impeded, when you have a mechanical block by introducing tiny particles of a second phase introduce tiny particles of a second phase in a metallic alloy; that is a possible way of doing this. For example, iron carbide particles are precipitated into iron to make the iron tough to strengthen aluminium for example, you have Al to Cu, this is the phase, which is put into aluminium. So, these are some typical situations in which the motion of the dislocations is impeded by the introduction of the second phase.

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Yet another method is to pin the dislocations. So, this is another method by solute atoms the solubility of a foreign atom will be greater in the vicinity of a dislocation than elsewhere therefore, the solute atoms tend to get collected near each dislocation during cooling. So, this increases the energy required for moving the dislocation thus preventing their movement. So, that is called the pinning.

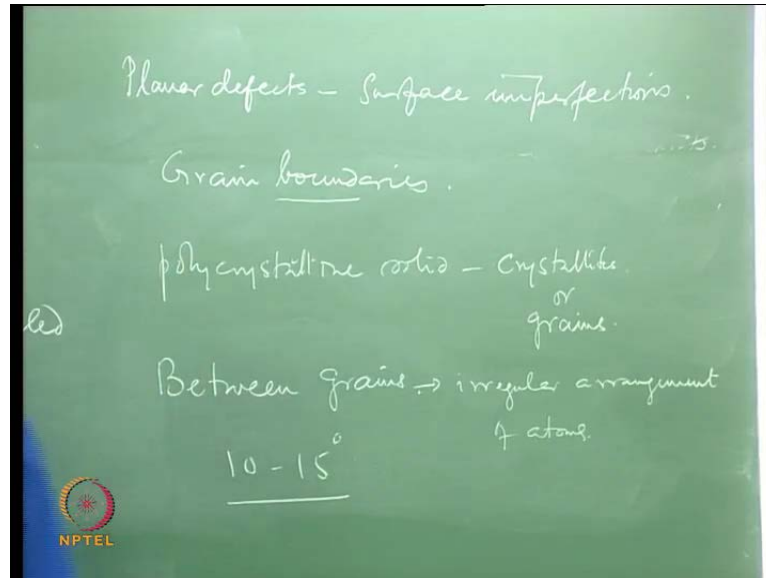
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So, this strengthens the alloy then you can also increase the dislocation density, you can introduce more dislocations, if the dislocation density is large then the dislocations get

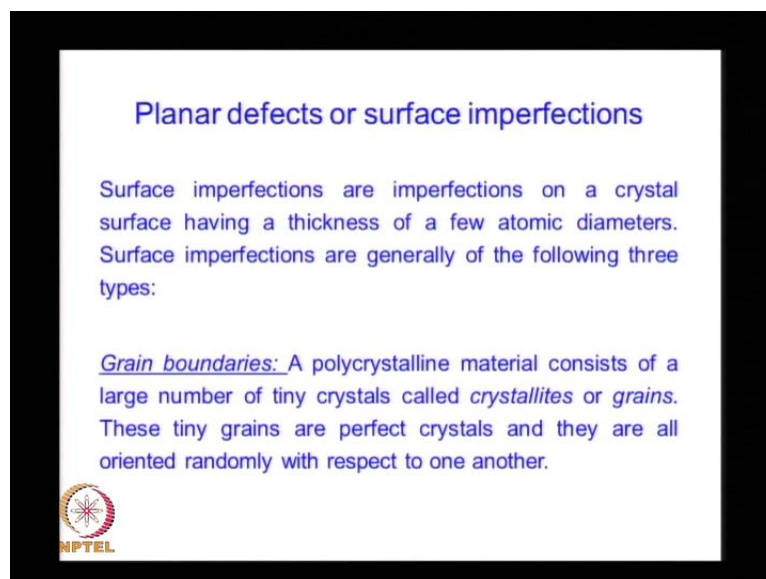
entangled. And thereby are prevented from moving. So, this will be the dislocation movement will be more difficult across a slip plane when there are many dislocations. So, in order to do this you do what is known as work-hardening.

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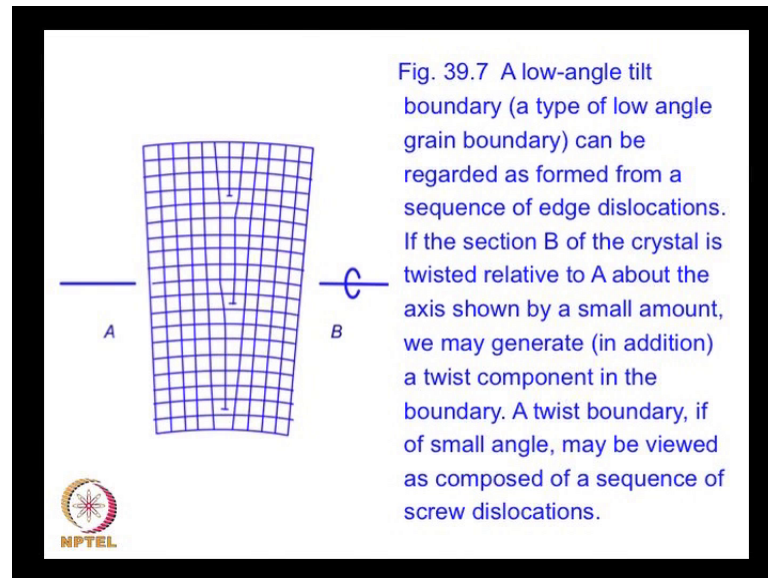
Next we go on to planar defects their planar are really surface imperfections they can be of different kinds. Now this again have thickness of a few atomic diameters. So, one of one typical class of these planar defects is known as grain boundaries.

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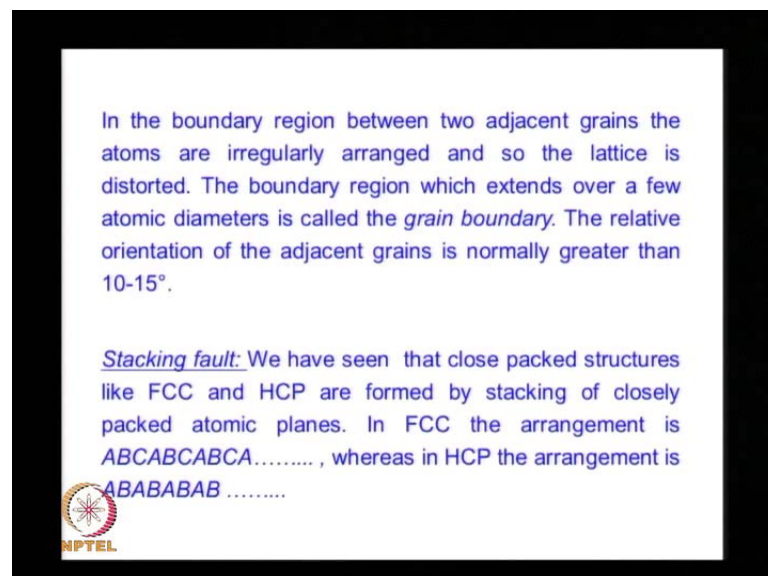
Any actual crystal will consist of poly crystalline material. So, it has many crystallites. So, these are also known as grains. So, inside the crystallite they are perfect crystals, and they are all the crystallites are oriented randomly with respect to one another.

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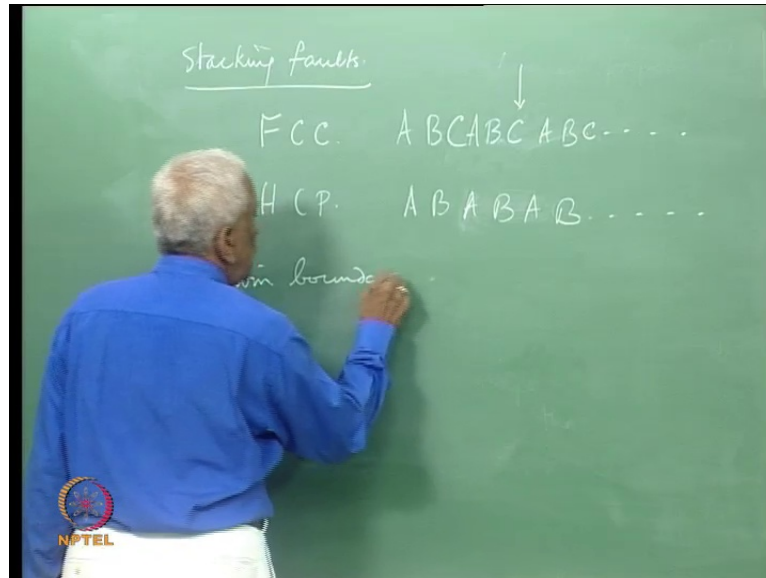
Then the next figure shows a low angle tilt boundary a tip type of low angle grain boundary, which can be regarded as formed from a sequence of edged dislocations. So, you have a large number of edged dislocations as well as screw dislocations and in the boundary region between 2 adjacent grains that is known as the grain boundary.

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So, the atoms are irregularly arranged as can be seen from this figure. So, this is the relative orientation of the different grains is usually of the order of 10 to 15 degrees the angle between the different grains

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Another class of planar defects is known as packing faults, this is because if you have hexagonal closed packing or cubic closed packing in FCC or HCP. If you take the different planes the stacking is has the sequence.

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In crystals with these close packed structures, if one of the planes slips or one of the planes is missing, then the arrangement has a fault. For example, in FCC crystal if the arrangement is

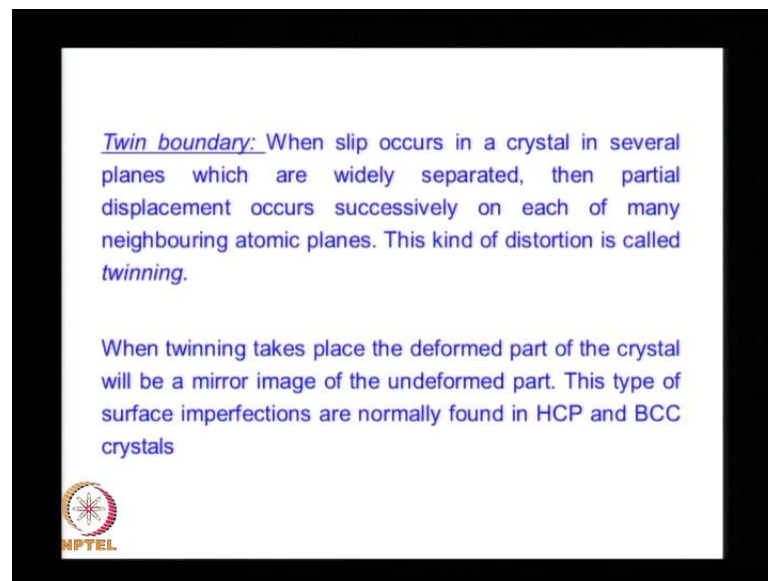
↓

ABCABCABABCABC

One of the planes in the sequence is missing (C plane is missing as indicated by the arrow). At this point, the stacking has become ABAB like HCP stacking. Such an imperfection is a *stacking fault*.

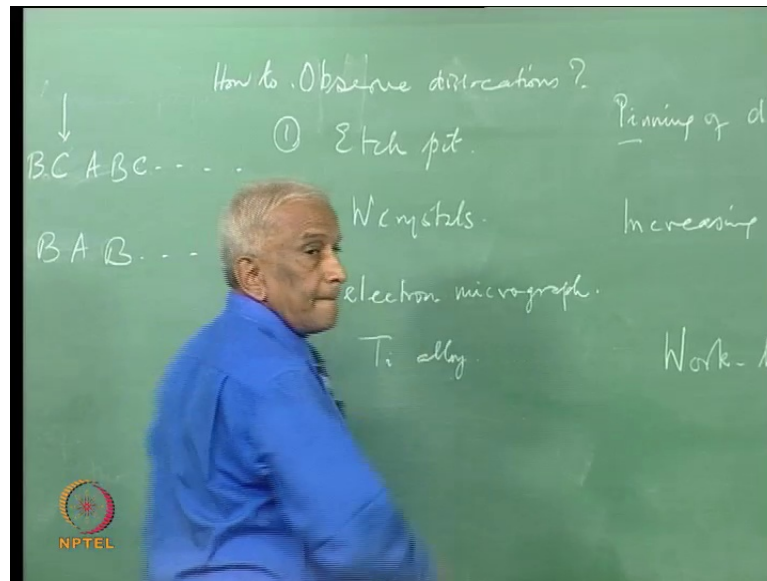
So, the stacking is different in the 2 cases and the if one of the plane slip or one of the planes is missing then there is a fault. So, suppose you have an FCC and then one of them is missing for example, one of the C is missing in this region this will become a HCP kind of packing because of the missing C. So, then you have a fault a stacking fault due to the difference in stacking, then you can have also a twin boundary which is a boundary between crystals which are twins.

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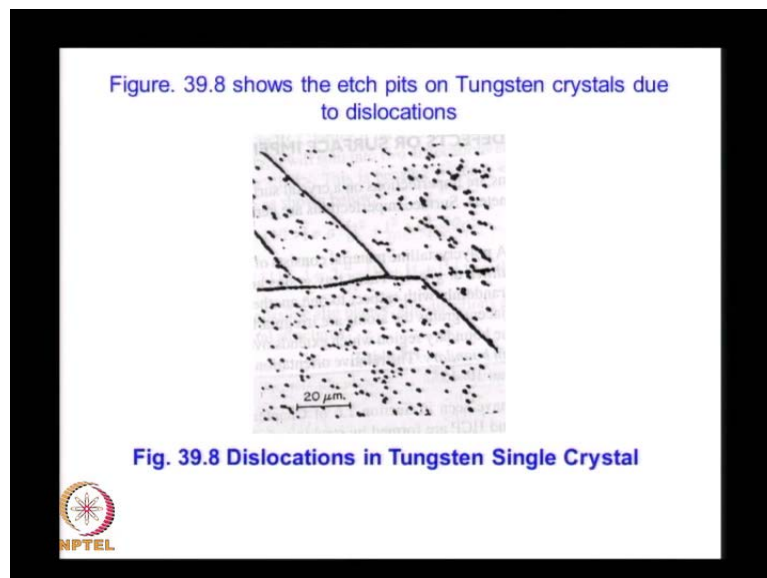
So, you have partial displacement occurring successively on each of many neighbouring atomic planes. So, this is known as twinning. So, this kind of the boundary between twinning's.

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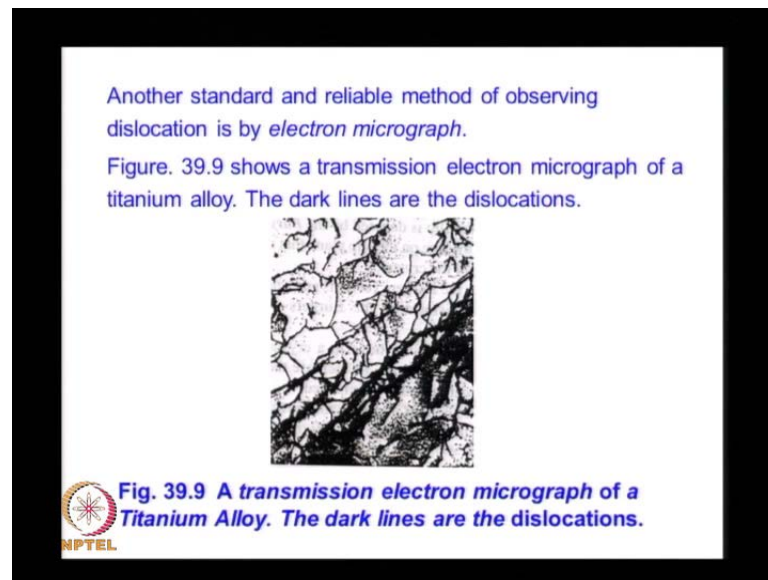
How do we observe dislocations one method is known as etch pit. So, you take the crystal for example, tungsten.

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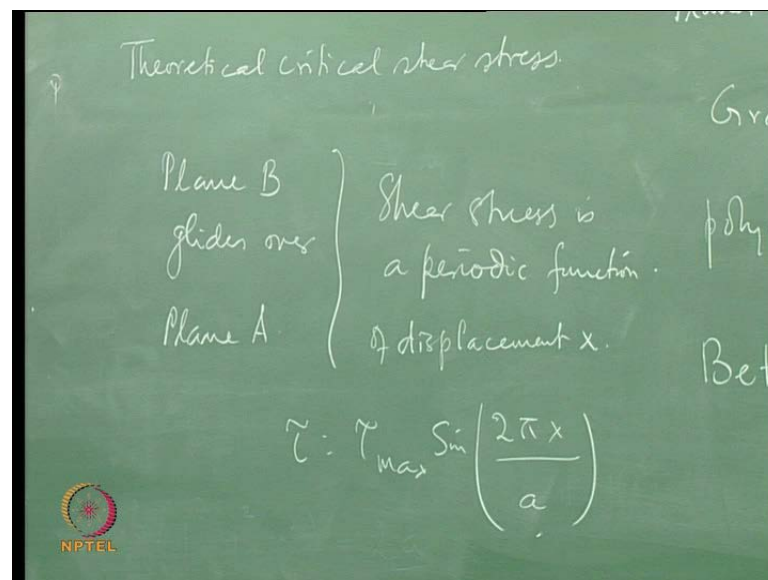
So, figure 39 8 shows tungsten crystals who's surface is etched with acid, and then you can see look at the dislocations.

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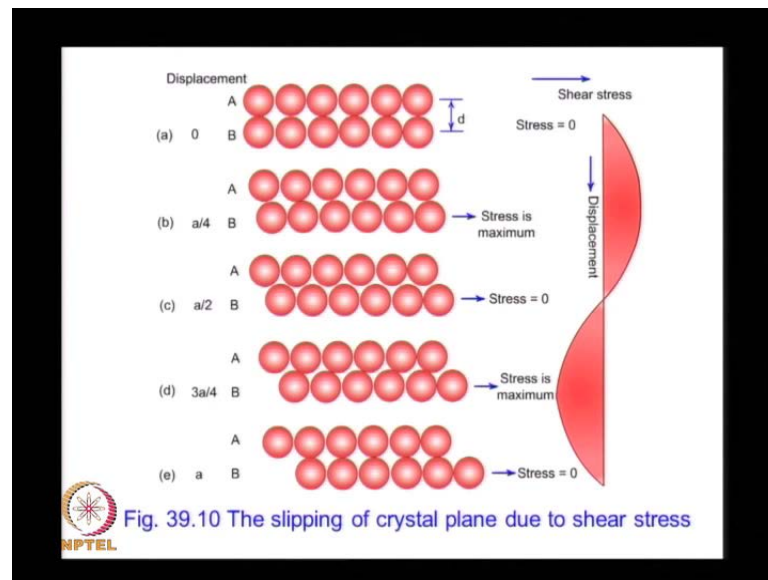
Another method is by electron micrograph. The next figure shows an transmission electron micrograph of a titanium alloy in which the dark lines show the dislocation lines. Now, before concluding we want to talk about the theoretical critical shear stress.

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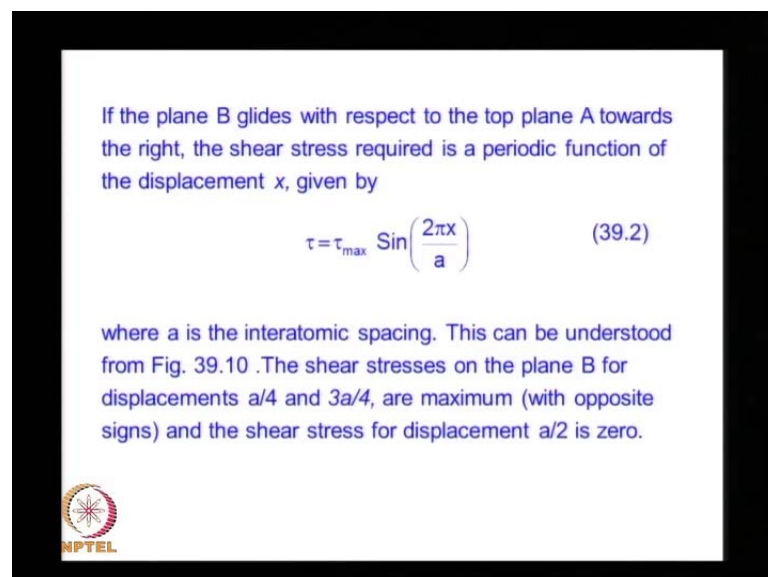
So, this is critical shear stress is the minimum stress in the slip direction, that is capable of producing a relative motion of the atomic planes.

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So, this can be calculated by considering 2 atomic planes A, and B as shown in the figure suppose I consider 2 planes glides over plane A.

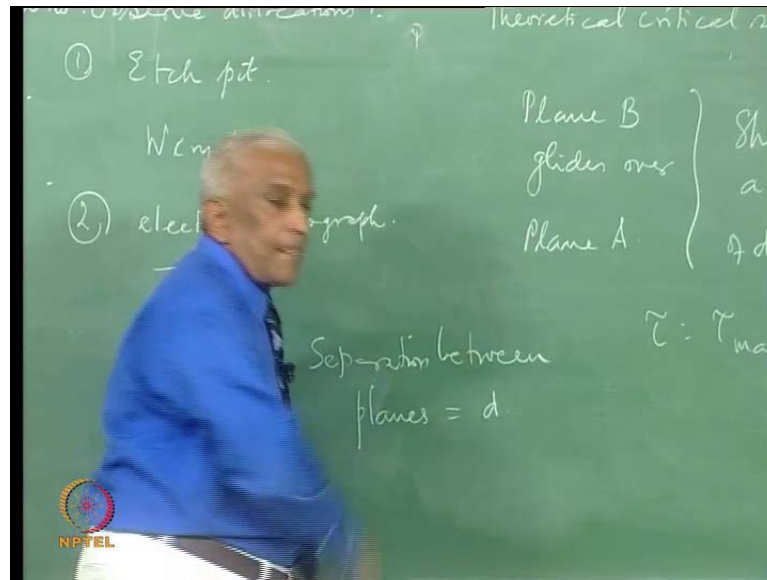
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So, the shear stress required for example, is a periodic function of the displacement x . So, we can write this as τ is some $\tau_{\max} \sin 2\pi x$ by a , where a is the interatomic spacing this can be seen in the figure 39 10, where the slip shows that the stress is zero in a the position a while the stress is a maximum. When there is a displacement of a by 4 as shown in b then the stress is again zero for c, where the displacement is a by 2 and again

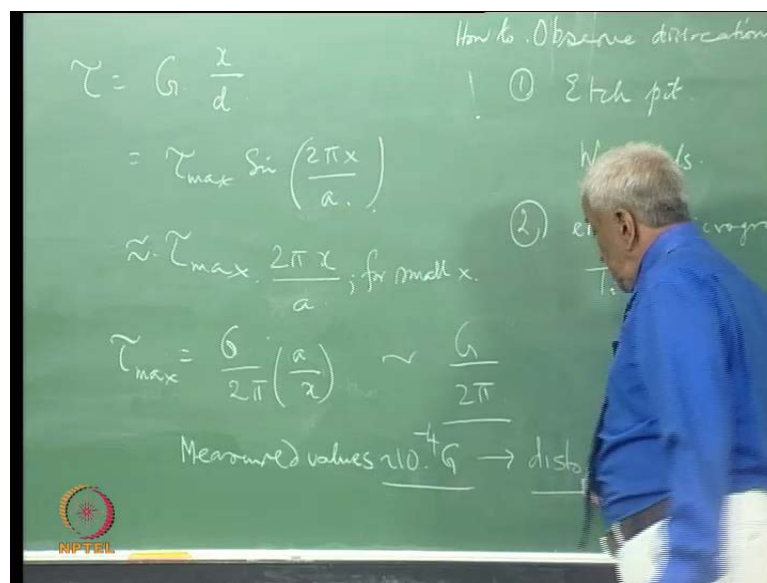
goes to a maximum in the section d which a has a , which corresponds to a displacement of three a by 4. Then again the stress becomes zero when it becomes a , so there is an oscillatory kind of variation of the shear stress.

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And if the separation between the 2 planes is d , then we can calculate shear stress using the shear modulus.

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So, this will be the shear stress τ in G the shear modulus times the strain x by d . So, therefore, this will be equal to $\tau_{\max} \sin$.

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From Eqs (39.2) and (39.3) ,

$$\tau = \tau_{\max} \sin\left(\frac{2\pi x}{a}\right) = G \frac{x}{d}$$

For displacements x , small relative to the interatomic spacing a

$$\tau = \tau_{\max} \left(\frac{2\pi x}{a}\right) = G \frac{x}{d}$$
$$\tau_{\max} = \frac{G}{2\pi} \frac{a}{d}$$


And for small displacements we can replace this sin by therefore, these 2 we can write tau max as is G by 2 pi into. So, G by 2 pi into...


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Since $d = a$,

$$\tau_{\max} = \frac{G}{2\pi} \quad (39.4)$$

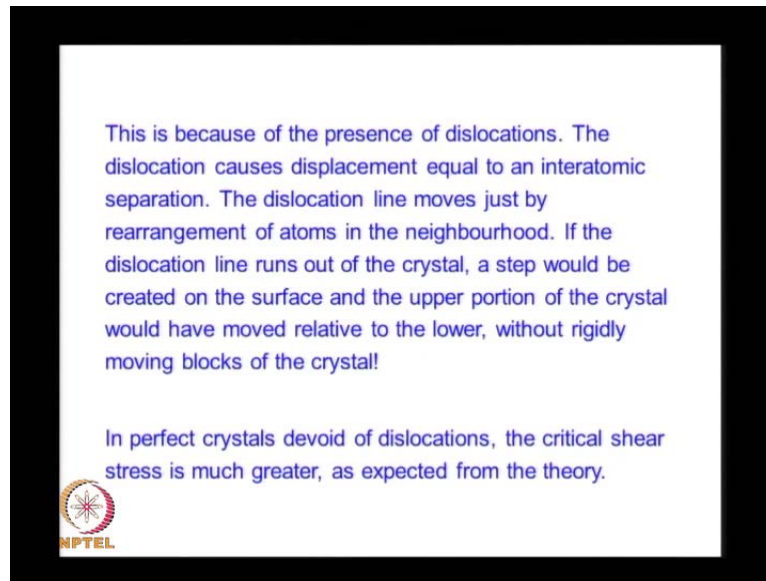
τ_{\max} is the *critical* resolved stress τ_c referred to in the last section.

The rigidity modulus of metals is of the order of 10^9 Pascals. So according to Eq. (39.4) the critical shear stress required for slipping of the crystal planes is about $G/6$, which is very large. But the observed critical shear stresses are $= 10^{-4} G$.



Since, these are comparable for therefore, we have this as G by 2π . So, the theoretical stress critical shear stress is just one sixth of the shear modulus, which is a very large quantity, but the actual measured critical shear stresses are of the order of 10 to power minus 4 measured values are only about 10 to power minus 4 G . So, there is a big difference by 4 orders a magnitude and this is because of dislocations.

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So, the presence of dislocation is able to explain the reason why measured critical sheared stress is 4 orders of magnitude lower than the calculated values. So, they dislocations cause a very spectacular change in the mechanical strength of a solid. So, the concept of a perfect solid fails, and dislocations is the really the accounts for the actual observed behaviour of solids.