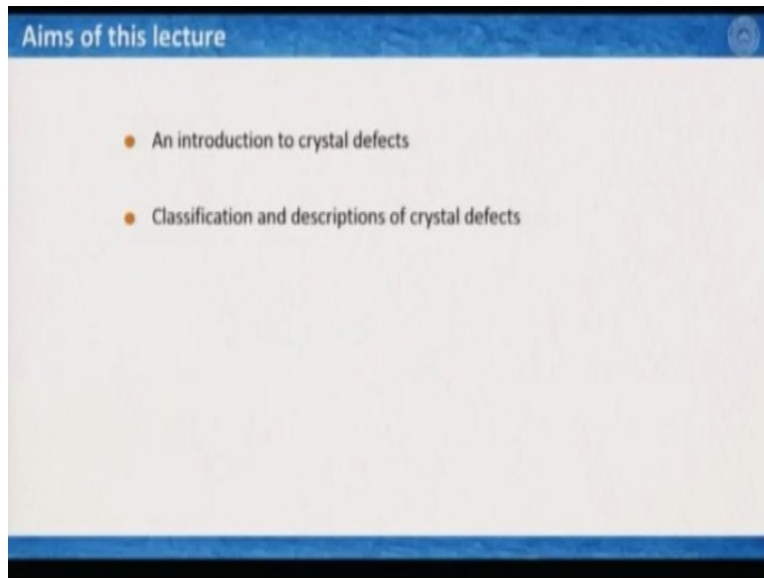


Structural Geology
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Lecture - 13
Deformation Mechanism
Part – I: Crystal defects and associated structures

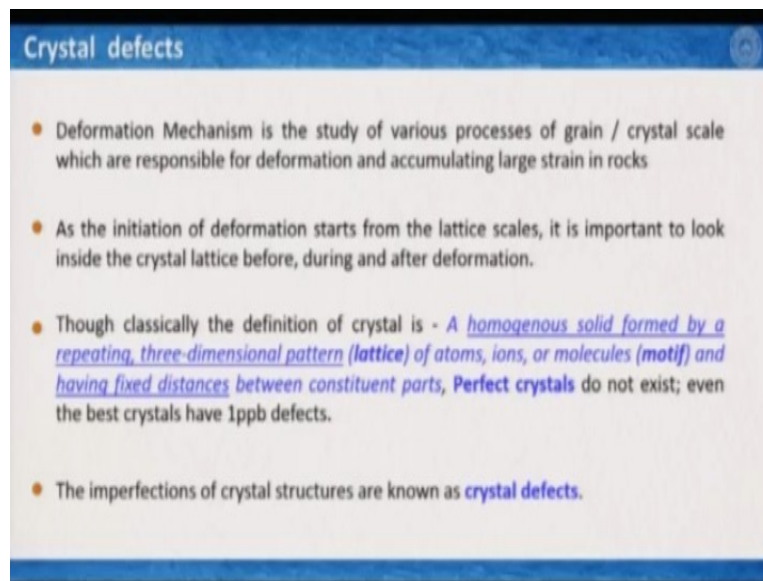
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Hello everyone! Welcome back again to this online structural geology NPTEL course and today we are in a new week and we are going to start deformation mechanism part one where we will study crystal defects and associated structures and we will cover the topics which are mostly an introduction to crystal defects and then we will classify the crystal defects and describe some of their associated features which are important for studying structural geology and in particular microstructures.

We talked about the deformation mechanism very briefly at the very end of this last lecture. It is very important to realize the fact that the deformation that will see, the strain the rocks do accumulate, sometimes these Trends are extremely large. So the question always being asked that what is the mechanism, what is the process by which these strains are being accumulated within the rock mass and most of the time we see that the entire rock is not getting strained but it is localized or channelized along a very narrow area or narrow zone what we call deformation localization.

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Now to comprehend this process it is the study of deformation mechanism that deals with the various processes of grain and crystal scale deformations, which are responsible for deformation and at the same time accumulating the large strain in the rocks. Now why grain and crystal scale? Why not in outcrop scale or in large scale or tectonic scale? Now at this time, we have to understand the fact that particularly in the ductile domain any deformation that we see that do initiate at a very very small scale. Very micro scale to be very specific and when we talk about the micro scale, we actually refer to the atomic scale.

So the deformation do initiate at a very very micro scale within the crystal. Most of the rocks as we know are crystalline solids poly crystalline solids. So it is therefore important to understand what is happening inside the crystal when we apply some sort of stress. How the crystal is accommodating this strain? What sort of features we should see within the crystals which are probably going to trigger a large scale deformation.

Accordingly in this lecture to understand this behaviour within the crystal, the deformation behaviour within the crystal, we need to understand first, what is inside a crystal? Now, we know that the crystal is generally that you need we call it a lattice and within the lattice we have the elements which we call motif. Now, when we define a crystal or what you have learned so far from our chemistry or physics lectures that classically a crystal is defined as what is written here, a homogeneous solid formed by a repeating 3 dimensional pattern which is the lattice of atoms, ions or molecules, which are your motifs.

And they have fixed distances between the constituent parts. Now, this sound like that it is very homogeneous solid or they have equal or fix distances between their constituent parts, their compositions or individual motifs are very similar and so on, which this looks like a very perfect place.

Unfortunately the perfect place inside the crystal hardly exists. What I mean by that the perfect crystal if we talk about then it does not exist. So the best crystal that you can think of would have around 1 part per billion defects. Now all these defects or imperfections that mix a crystal to deviate from its actual original definition are known as crystal defects or what is written here, the imperfections within the crystal structures are known as crystal defects and crystal defects are very very important in the deformation of rocks particularly in structural geology and at the same time in many other subjects also in material science and other mechanical processes.

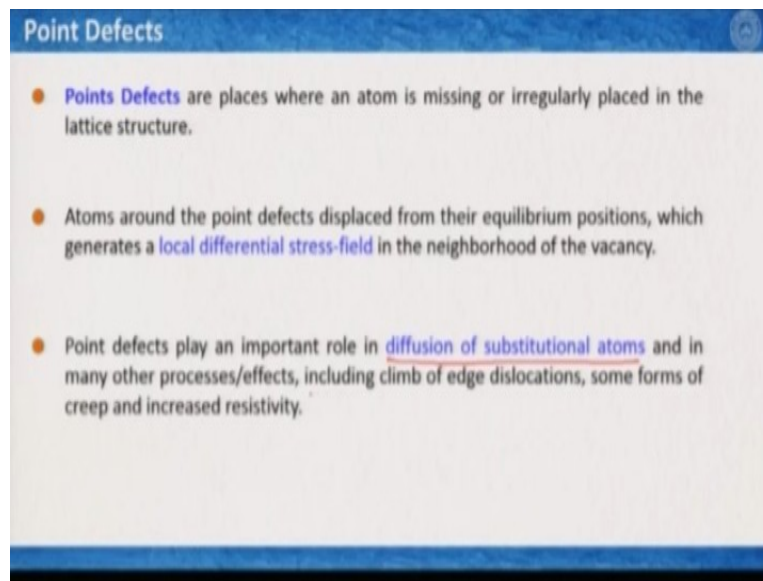
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Crystal defects		
Classifications -		
DEFECT	DIMENSION	EXAMPLE
Point	0 D	Vacancy / Interstitial
Line	1 D	Dislocations
Surface	2 D	Free surface / Grain boundary

So to classify crystal defects generally people do classify in three different ways. So the first one we call it point defect or it is also known as zeroth dimension and examples will see all of them vacancy or interstitial. The second category is line defect because it is line. So it is 1 dimensional and the examples of line defects are dislocations and then we have finally surface defects. Surface defects are as the name suggests, it is a surface. So it is two dimensional and examples are either free surfaces or various types of grain boundaries.

So in this lecture actually we are going to explore these three types of defects. So first we will take over vacancy interstitials and so on, that means point defects. Then we will go to line defects and finally we will conclude the lecture with the surface defects.

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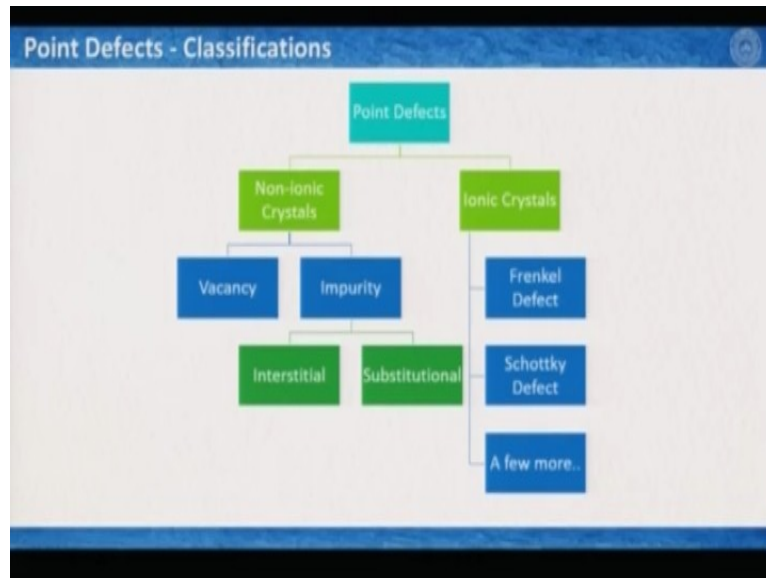


Now what is point defect? Point defects are places where an atom is missing or irregularly placed within the lattice structure. So atoms around the point defects are displaced from their equilibrium positions, of course if the crystal is not in equilibrium that means there must be something wrong and this wrong thing is either one atom or one element is missing or it is placed somewhere where it should not be.

So therefore, if an element within the lattice is staying somewhere else or is missing then the crystal always tries to make things in equilibrium but it cannot do it. So therefore there is a local differential stress field that is generated in the neighbourhood of the vacancy and this local stress field is very very important in determining many processes that primarily include the diffusion of substitutional atoms and in which we can think of many other processes that these vacancies are responsible for. These are flying of edge dislocation, some forms of creeps and increased resistivity.

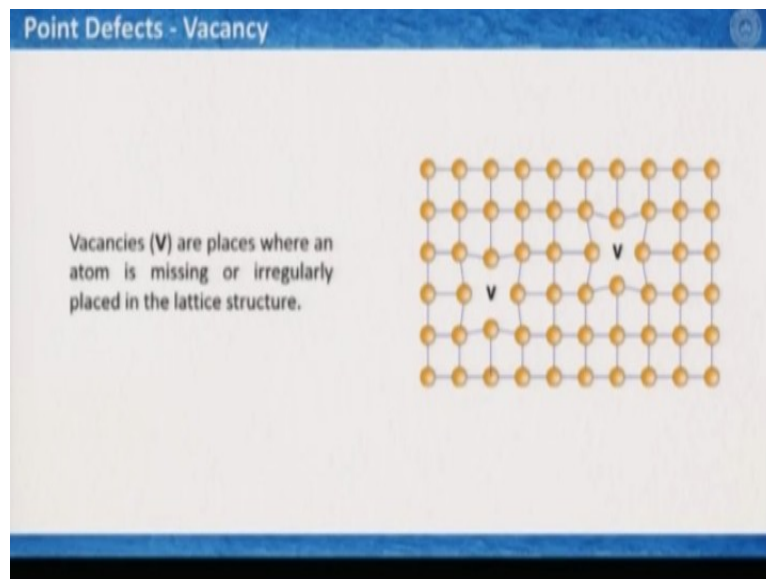
We learn particularly diffusion and substitutional atoms very briefly in this lecture but we learn more later on diffusion creeps when we learn the particular mechanism. I bet today we will look at how the flying of edge dislocations do happen with the assistance of point defects.

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So point defects are classified in this manner what is given in the slide so first they classified whether your crystals are ionic or non-ionic and if your crystals are non-ionic then you have vacancy and impurity and within the impurity, we have interstitials and substitutional vacancies. Within the ionic crystals there are mostly two categories one is Frenkel defect, another is Schottky defect and there are few more but we will mostly look at Frenkel and Schottky defect very briefly but before that let us go to the non-ionic crystals and first take over the vacancy.

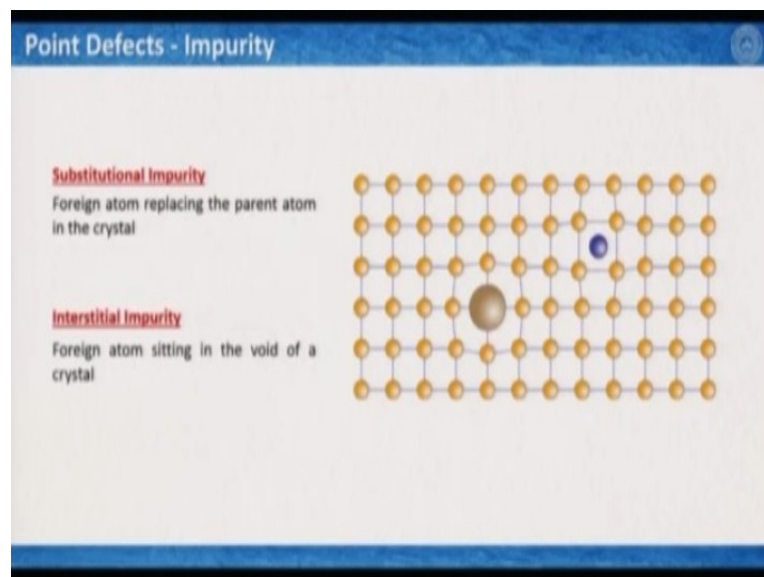
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So vacancy that we talked about as we see in this illustration that if I look at this area in particular, the atoms within this particular segment of this lattice are distributed very homogeneously, their inter atomic distances are constant and so on. However, if we see this place in particular or this place in particular one atom or one element is missing. So vacancies are therefore the places where an atom is missing or irregularly placed within the lattice structure. What is important to you see that this straight connections that we see where there is no vacancies as such are now somehow distorted and they are distorting towards the vacancy side.

Now this is where these bonds or these lines as you can think of stretched, deformed or distorted and these are the places where you generate some sort of differential stresses.

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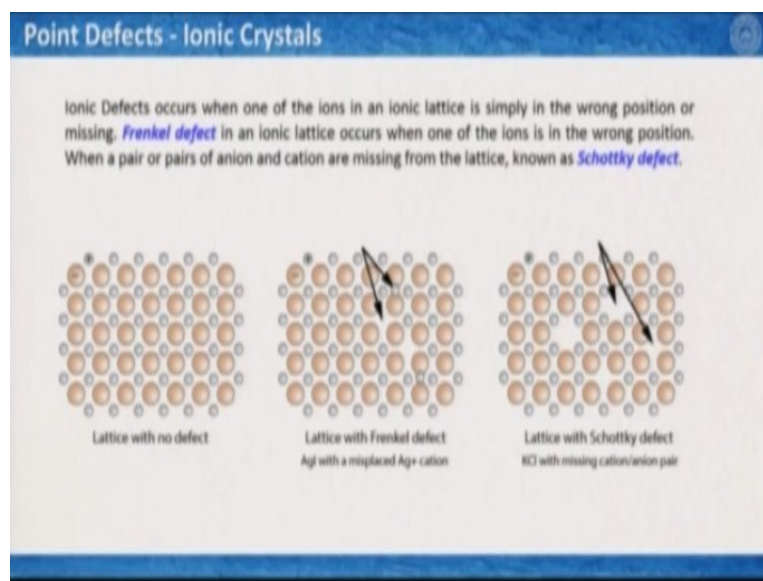


So these are vacancies and let us talk about the impurities. There are two kinds of communities as we have learnt one is substitutional impurity. That means you have a vacancy but vacancy is not vacant, it is occupied by some foreign atom. So a foreign atom came, it replaced the parent atom within the crystal, so this is known as substitutional impurity. And interstitial impurity is when a foreign atom sitting in the void of a crystal. So somewhere within the crystal it disturbs the lattice structure but it does not omit or remove any atom from the lattice. So here this one is an example of substitutional impurity and this one is an example of interstitial impurity.

Now most of the gemstones that you see or that we are aware are actually results of substitutional impurities. I give you an example of ruby. We know ruby is a fantastic gemstone is red colour, but the host mineral of ruby the actual mineral of ruby is nothing but corundum. It is aluminium oxide. Now the chromium atom it replaces, if it replaces 1 percent of the aluminium's inside this corundum crystal, then it becomes red and that is why it becomes very important to us or very precious to us because of this red colour.

So it is not a pure crystal that will see as ruby. It is actually a corundum aluminium oxide and in one side, the metal side we have aluminium replaced by chromium and therefore we see the red colour and that is why it is expensive. Now for the interstitial impurity you can think of the carbon steels that most of our soft steels that we use nowadays including our cars and so on. The carbons are doped inside the ferrite crystals, which is a BCC crystal and these you can think of a carbon atom inside the ferrite crystal. So carbon steel is a perfect example of interstitial impurity.

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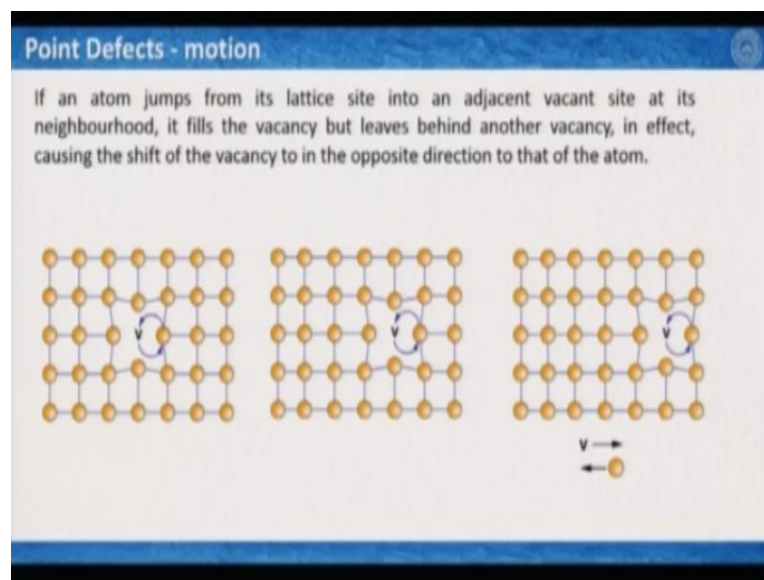


When we learned about substitutional and interstitial impurities let us move on to point defects will read to ionic crystals and as we have classified there are two types of ionic crystals defect. One is Frenkel defect and another is Schottky effect. Now ionic defects they do occur when one of the atoms in an ionic lattice is simply in the wrong position or missing. In this context of Frenkel defect in an ionic lattice that occurs when one of the ions is in the wrong position. So what we see here, this is a lattice structure without any defects. So this is a perfect crystal as you can think of and then you have some ions with positive charges and some ion with negative charges.

Now what we see here positive charged ions are missing from this side and they are sitting somewhere here and the same example you can see the ion is missing and it is sitting somewhere here. Now the basic idea or one of the properties of crystals with Frenkel defect which we are discussing now is that that nothing is missing in this frame. So number of atoms or number of ions if we count, these remain constant. Therefore even if there is vacancies different type of vacancies the density of the crystal does not change. On the other hand, Schottky defect is when you have a pair of anion and cation are missing.

For example, as you can see here this one and this one. An anion and cation are missing from this crystal or this lattice and again here. A pair always they have to disappear from the system as a pair and if that happens then it is known as Schottky defect and you can imagine that if this happens then the density of the crystal varies. So the example of Frenkel defect is you can think of as the example is given here silver iodide which is a kind of material or complex where in this case the Ag plus ion, the silver ion is missing from the actual site and it is sitting somewhere else and Schottky defects we mostly see in different kinds of salts where for example here the KCl ion, the KCl salt where both K and Cl K plus and Cl minus they are missing from the crystal.

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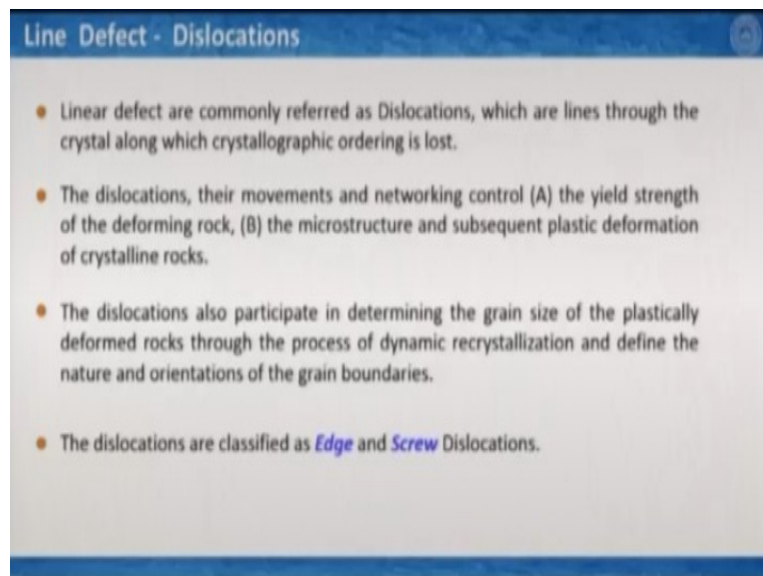


Now how point defects are important to us. We will learn more about it but points defect are if there are some sort of differential stress externally or some sort of disequilibrium been they try to move from one side to another side. So if an atom jumps from its lattice side into the adjacent vacant side at its neighbourhood, it fills the vacancy but because there is no extra atom so it leaves behind another vacancy.

So in effect that it causes the shift of the vacancy to in the opposite direction to that of the atom. What I mean by this or reading this text is explained in this illustration. So what is see we have a vacancy here and we have a neighbouring atom. Now if this atom has to move then the best place to move is to come to this vacancy side. So what it decides, it moves to this place and the vacancy then comes back the position of the atom.

So therefore in the next lap, again the next atom moves to this vacancy side and the vacancy comes back or vacancy moves to the position of the atom and here is the same case. So what we see here that in this illustration back that vacancies are moving in this direction and atoms are moving in this direction. So therefore their movements are opposite. It is very similar to the way electricity moves or the electricity goes. So electrons move the direction opposite to the electricity. So this is a very interesting idea that we will explore more and it involves also the volume changes or shape changes of the crystal during or due to the movement of vacancies and atom in the system but for the timing will stop here. We will learn more about it when you learn more about diffusion creep and diffusion mechanism.

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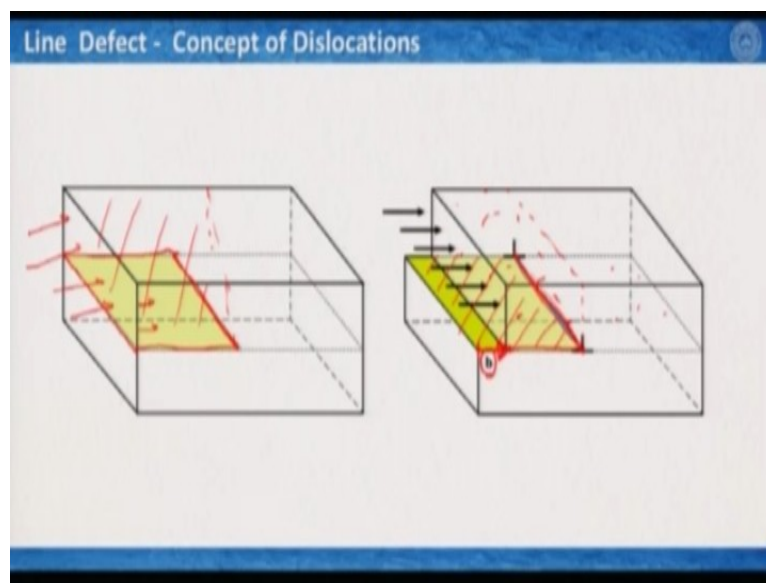
Let us move to the next part of this lecture is line defect or dislocation that we have learnt. Now vacancies as you have learnt are zeroth dimension that means they are point defects but line defects are linear defects and linear defects are commonly referred as learnt dislocations and dislocations are nothing but the lines through the crystals along which a crystallographic ordering is lost. We will learn more about it soon. So these dislocations are very very important in terms of structural geology. So their movements and networking control many

many things which are responsible for the formation of the structures that we see inside the thin sections or even large scale structures.

One of them is the control the hill strength of the deforming rock. So strength of the rock is controlled by dislocations and their movements. They also can produce various types of micro structures and subsequent plastic deformation of crystalline rocks. The dislocations also do participate in determining the grain size of the plastically deformed rock. So a plastically deformed rock has larger grain size or smaller grain size is actually controlled by dislocations and this happens to a process called dynamic recrystallization. This will also learn in the next lecture and it also defines the nature and orientations of the grain boundaries.

So, dislocations are one of the most important crystal defects that we deal regularly in looking at micro structures and so on. The dislocations are classified in two segments one is edge dislocation and another is screw dislocation. Now we will first look at edge dislocation and then we will understand the screw dislocation. Edge dislocation is much easier to understand and comprehend but before we go to actual scenario, let us get a concept that what is dislocation.

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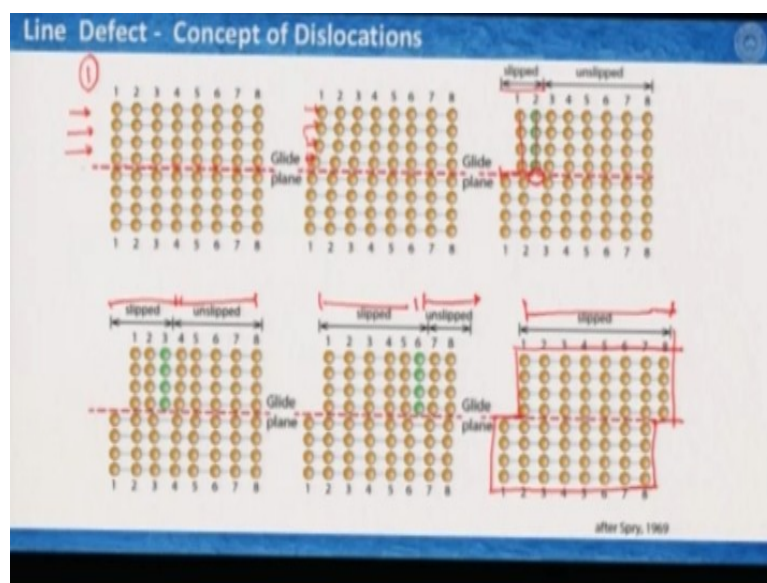


Now what we have here in this illustration? We have a block say a crystalline solid and then by some means we made a cut. Halfway cut to the middle of this block. Now because this would be deforming plastically let us assume that to understand, to visualize better let us assume that this is a piece of rubber and then if you push it this side top part only, leaving not at the base so it could try to squeeze in this direction but because this part is fixed so at this segment this material would be much denser.

So eventually it would look like something like this where this edge of this cut is fixed. There is no displacement and then along this line everything but slipped along the plane that you made cut or you can call it a glide plane. Now, this has to move following a vector and if we consider that this is a vector because we are applying the force in same direction so we can term it as b . We learn what is it later but this is the basic concept of dislocation that one side of this cut or one side of this line has got a slip and another side is not slipped.

So this part experienced slip and this part not. Now as the volume or other things has to be constant. In this segment, you might have some rearrangements of the atoms within the lattice so that it can accommodate this unit vector displacement within itself. As a result the lattice, the atoms they are arranged accordingly to accommodate the deformation when the other parts are not deformed or not disturbed as well. Now this line is known as dislocation line that separates the slip and non-slipped part.

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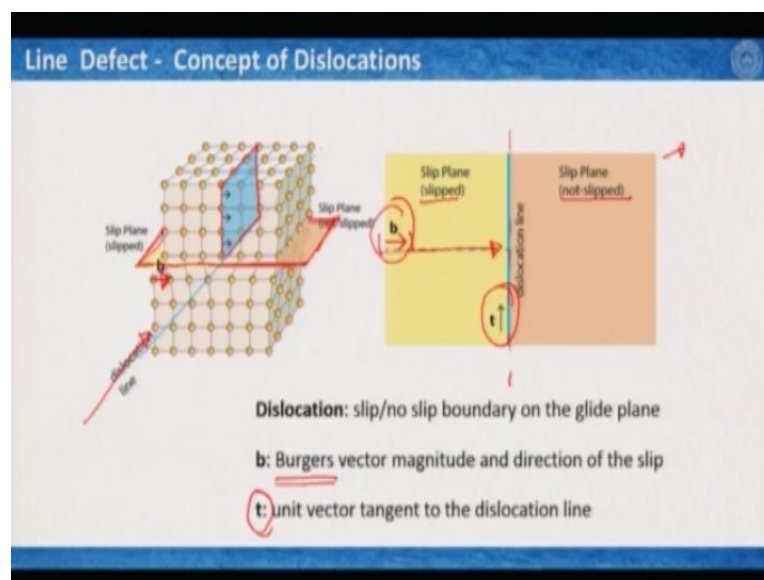
So now if we all try to look at in our actual diagrams or actual illustrations so what happens when a dislocation moves? Now in this first illustration what we see it is a perfect lattice structure there is nothing and then we apply some sort of force in this lattice above this line, which we will refer as glide plane. So initially when we apply the force will certainly push the crystals or atoms, I am sorry, the crystals on this side. So these crystals will move a little bit. Now here comes the very interesting part.

Now it can happen that all atoms in this area, it can receive the stress. They can move at the same time and they end up by slipping each and every plane to give you shape like this which you will see is going to happen at the very end but if you have to do it at one time the stress you require is significant and experimental studies showed that the actual stress that requires to deform this few orders of magnitude less.

So there must be something happening or the lattices are accommodating the strength or moving the stress such a way within themselves that reduces the strength of the rock yield strength of this system or the crystal. Now this is how it happens. So what happens that this line of atoms, they move but then they displace a single set of atoms as well. So therefore it does not have any connection at the bottom and this is where we produce our first dislocation or the cut that we talked about in the previous slide that before this the material got slip and after that it is unslipped and then this dislocation moves one after another and finally it achieved to this shape where we actually see that an unit length has got displaced.

Now this is how this slip and unslipped lengths got changed continuously and finally, we get in that top part slip, but it did not slip in a single process, but step by step. The movement of dislocations is very similar the way silkworms move or the earthworms move on the surface.

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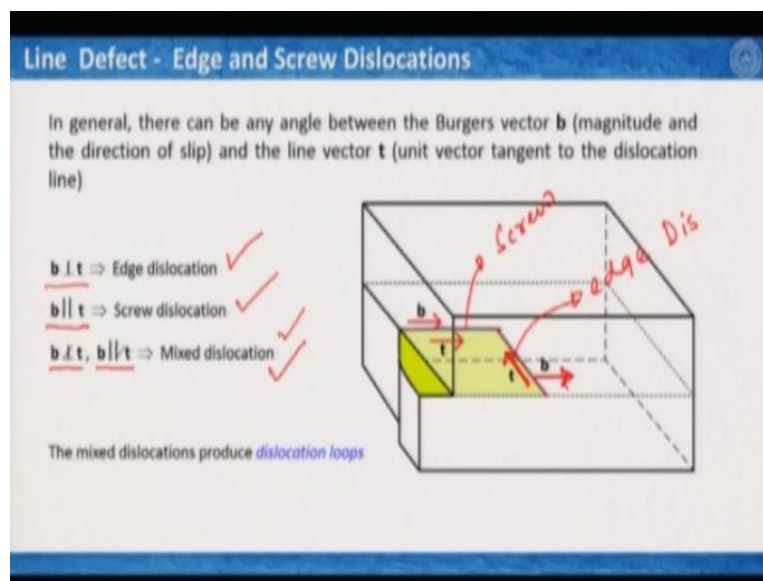
So if we try to look at in a different way this dislocations so imagine that this is our dislocation line with blue line here and then this is our glide plane and this unit vector that the dislocation move on the slipped side along the slip plane is an unit vector and it is known as Burgers vector. So Burgers vector is the magnitude and direction of the unit slip. Now this Burgers vector, though the spelling is very similar, b u r g e r that we eat as snack, is

absolutely different to what we call Burgers vector. Burgers vector is named after the Dutch scientist physicist. So do not confuse this Burgers to what we eat burger.

At present, this is the plane along which we have that separates the slipped and non-slipped part. So if we can project this plane in our flat area, then we see that this is the dislocation line. So you are projecting on this area on this surface. So the yellow side is the slip plane and this light pink is our non-slip plane. So these parts are slip and these parts are non-slip and what is separating slip and non-slip is dislocation line.

Now dislocation moving along this direction with that unit vector, unit Burgers vector. We can introduce another vector here, which is T that tells about the unit vector tangent to the dislocation line. Now in this case, this Burgers vector and this tangent vector are perpendicular to each other. When they are perpendicular to each other this is known as Edge dislocation or the propagation direction of the Burgers vector or direction of the Burgers vector is perpendicular to the dislocation line.

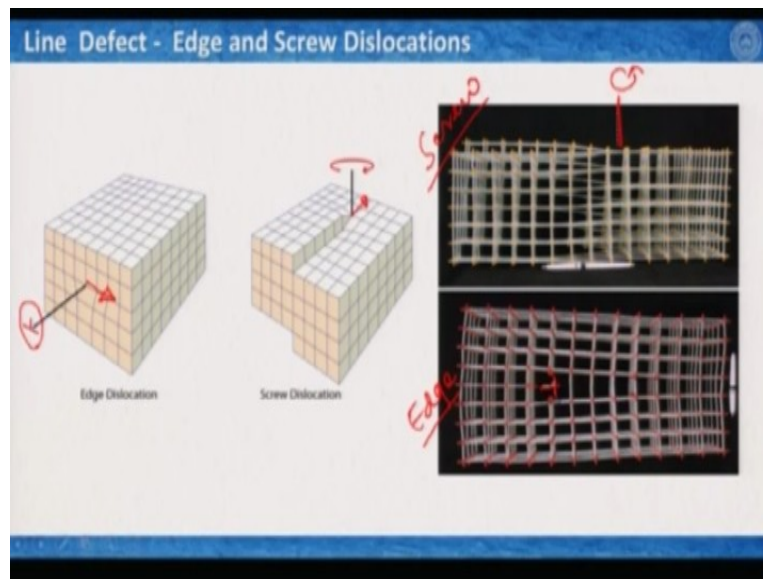
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This slide gives an example, what we see that therefore this $B \& T$ their directions their vector directions could have any angle. So between the Burgers vector which is the magnitude and the direction of the slip and the line vector T , which is the unit vector tangent to the dislocation line. So as we learnt that if B is perpendicular to T , then we call it edge dislocation.

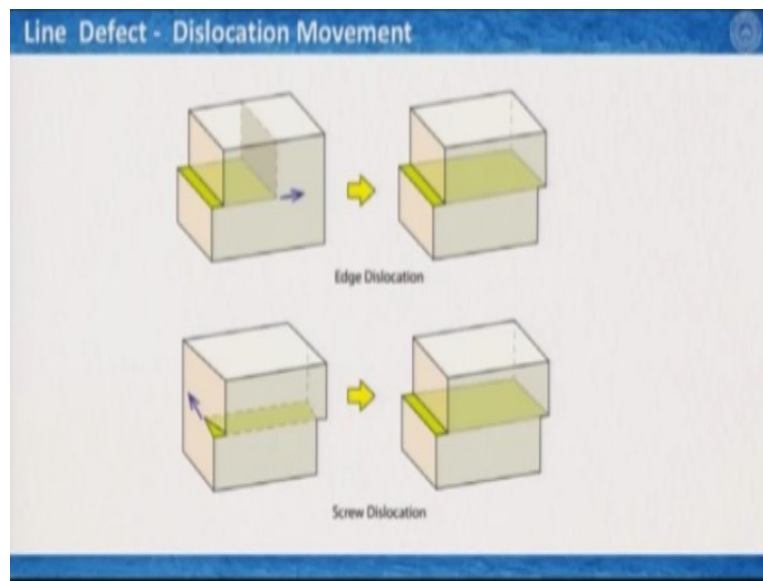
If B is parallel to T then we call it screw dislocation and if B is neither perpendicular nor parallel to T , then it is mixed dislocation. So what we see in this illustration and this is what we have learnt, this vector where B is directed this way and T is directed this way their mutual relationship is perpendicular. So this is my edge dislocation, but here as we see that V and T these 2 are parallel to each other. So this is screw dislocation. Now if there are other relationships like for mixed dislocation, then they form something called dislocation loops. We just learned the term we will not go much detail of this.

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This slide shows how they look like if we try to draw them. So edge dislocation is something like this and now we know that it is defined with this T either flipped or straight where screw dislocation looks like something like that where the dislocation is moving in this direction and here dislocation is moving in this direction for edge dislocation. Here are two models that you can see. This one is edge location, I am sorry, this one is a screw dislocation and this one is the edge dislocation where this is the rotation axis and here this is the dislocation line.

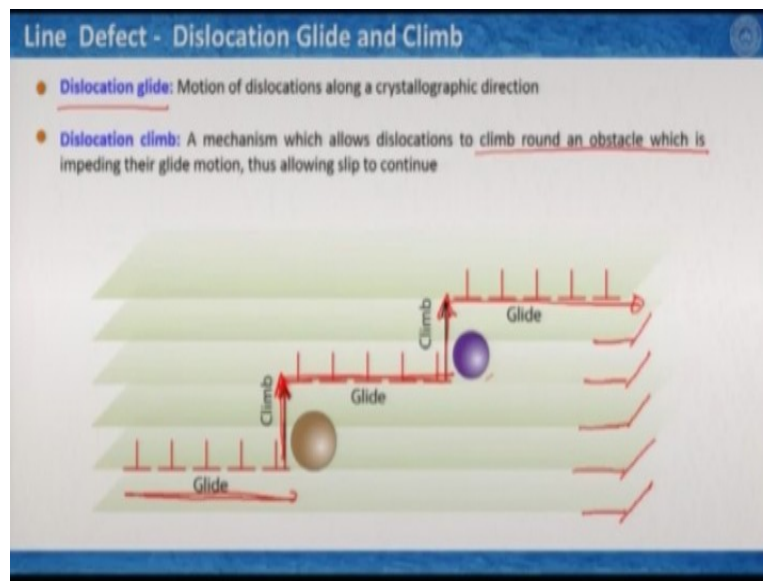
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Now the event does not matter whether we are dealing with edge or screw dislocation the end products or the slip more or less they appear very similar. At least we understand for our lectures this way they could be very complex, but we understand it this way that when we have edge dislocation this is the propagation direction and this is the dislocation line so they are perpendicular to each other but because it continues to move so eventually get a slip of unit vector, burger Burgers vector but here it slips this way so propagation direction of the dislocation is this and it also move in this direction so, they are parallel to each other but eventually we end up with this Burgers vector.

Now does not matter at least from a very basic idea we can have these diagrams in your mind that does not matter whether this is edge dislocation or screw dislocation, we end up with the same type of deformed structure for our basic understanding but actual thing is much more complex or it could be even complex.

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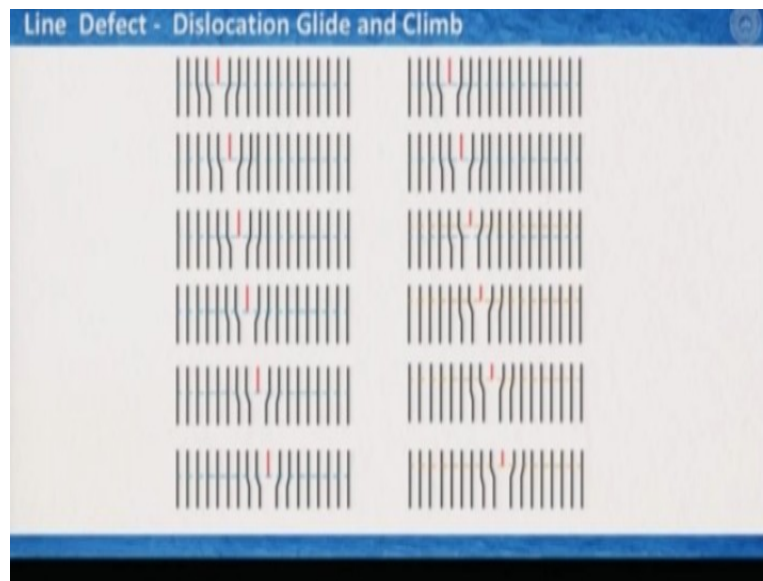
Let us talk about that how do this dislocations move from one side to another side of the crystal. We had a very basic idea when we saw that one term is moving relative to the next we saw the also the movement of the vacancies. So one vacancy moves and then one atom moves to support the opposite direction, but for dislocations as we have understood so far that it has to move along a particular crystallographic plane or what you have learned as a glide plane. Now not necessarily dislocations could move along the glide plane always life is not always happy.

So sometimes on the glide plane, we have some obstacles in the form of interstitials and the interstitials are sometimes so big that dislocations individual dislocation do not have the energy to move or to sort of ignore this obstacles and move further on the same glide plane. If that does not happen then it has to find one way to move to another glide planes and move accordingly.

So when it moves along a single glide plane is known as dislocations glide. Motion of dislocations along a crystallographic direction what we see here that it is gliding. So these are your individual glide planes stacked in a crystal. Now a climb happens when you have an obstacle, which is impeding their glide motion it stops the glide motion and allows the dislocations to jump to another crystallographic plane and then continue glide. So this is glide, then climb, glide, another obstacle, then again climb and then it glides again.

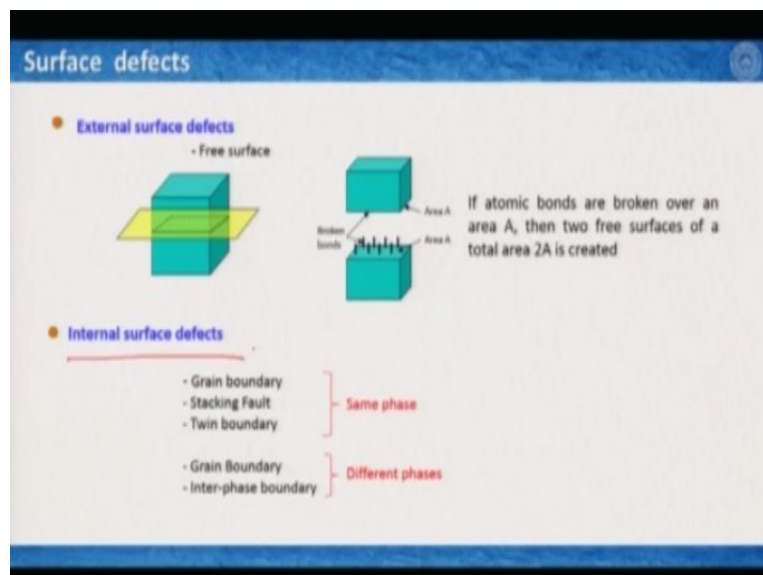
This is how it occurs continuously? Now you clearly understand at this point that glides requires less energy than climb just has to climb so it requires some more energy and energy can come from various sources. We will learn about it later.

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So eventually if I look at in a different form, it looks like this. So this is the glide entire place, so you see a fix crystallographic plane and the dislocation is moving from one array of atoms to another array of atoms without changing the crystallographic plane but here in this case you just see in a different way probably here there was an obstacle so the dislocations move to the next level and it changed this glide plane and continued moving as we see here. So this is how the dislocation glide and dislocation climb are conceived.

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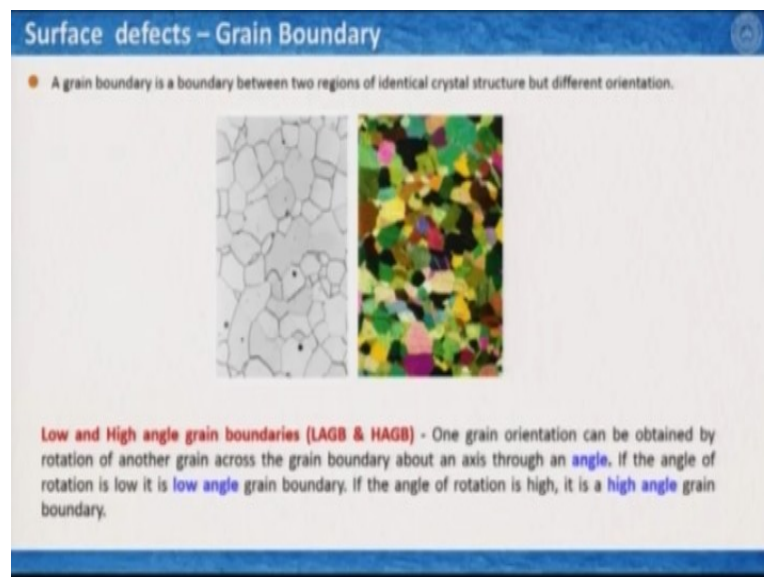


Now let us talk about the surface defects. Surface defects are classified in two segments, one is external surface defect and another is internal surface defect. We will not talk about much or we will not consider the external surface defects but just to know that if atomic bonds are

broken over an area then you create two free surfaces and the area is double of the area you had. It has some other implications but we are not going to deal with this but we are mostly concerned about internal surface defects and within the internal surface defects, we have we can have surface defects between the same phases and between the different phases.

Between the same phases we have grain boundaries, stacking faults, twin boundaries and so on and we call so can have grain boundaries within different phases and also a different kind of interface boundaries. So from now on we will mostly look at grain boundary and twin boundaries, also kind of grain boundary. We look at mostly these two. We will ignore stacking fault for the time being.

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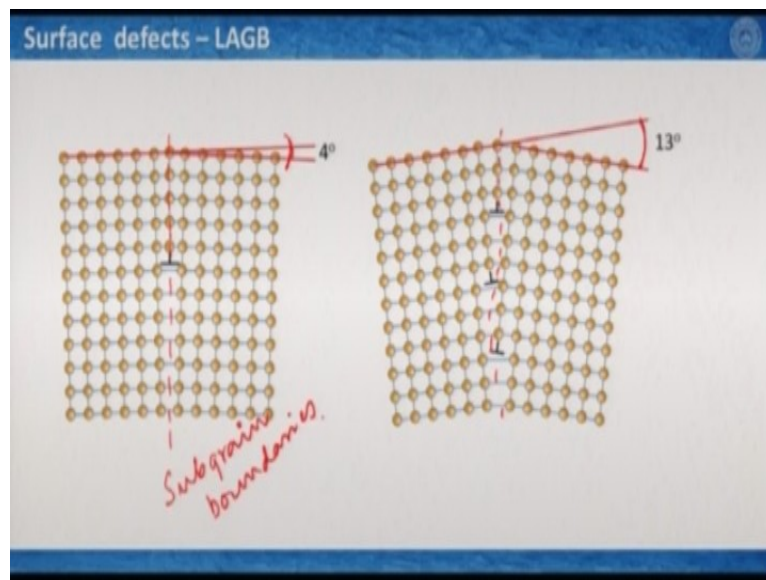
So what is grain boundary? You all talk about that the grain boundary is straight, grain boundary is curvy. And grain boundary is serrated and so on. From the crystal point of view or crystallographic point of view a grain boundary is a boundary between two regions of identical crystal structures, if we are dealing with same phases but different orientations.

Here we have two examples. This is iron oxide and this is calcite. You see that their composition are very same but because they are differently oriented maybe this grain here is oriented differently compared to this plane here and this is why probably we see some lines in between them. We see different colours here. This is cross-polar, this is calcite. Through cross-polarized light this is a thin section and we see different colours because the grains are oriented differently, we see different colours. This we have learned from our optical mineralogy classes or mineralogy classes.

When we talk about different orientations, there are possibilities of various orientations from 0 to 90 degrees or more. So we classify them mostly in two categories, low angle grain boundaries or LAGB or high angle grain boundaries or HAGB. There are also classification tilted and twisted twin boundaries. We are not going in that right now. Now low angle grain boundaries as it suggests that one grain orientation can be obtained by rotation of another grain across the grain boundary about an axis so an angle. So that means I have for example two grains.

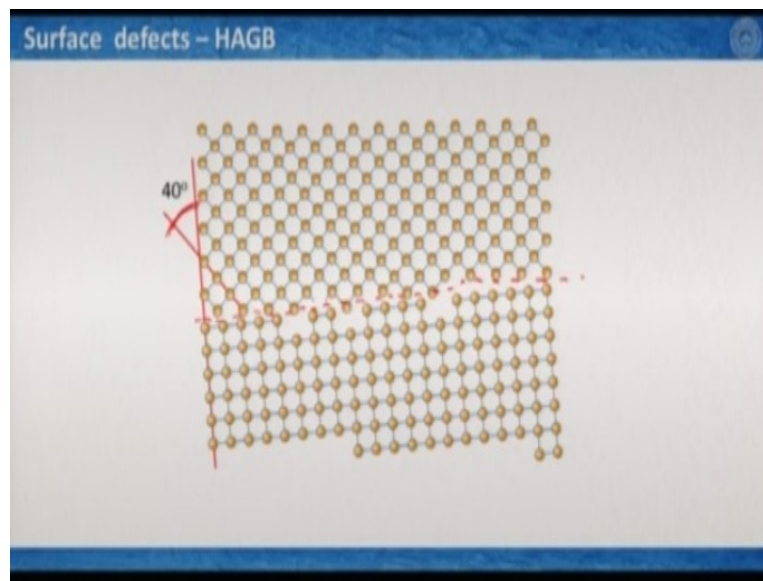
Now if my finger traces are the lattice orientations, then they can have differently oriented by this angle and this is the rotation axis. Okay? So if this angle is low, then this is low angle grain boundary. If this angle is high, then this is high angle grain boundary. So how do they look like.

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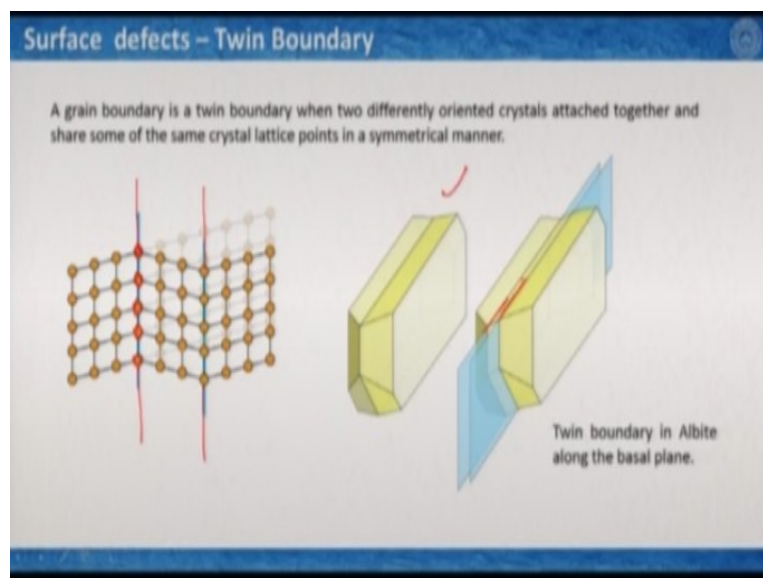
So these are low angle grain boundaries. I have given two examples. As you can see that this probably is defining one very low angle grain boundary where this and this 2 different areas or 2 different lattice structures are not staying in the grain stem yet but their angle is only 4 degrees, very less. So these are known as some sort of sub-grain boundary with higher grain boundary angles and what is important that this could be probably your grain boundary. What is important is that these grain boundaries are marked by dislocations and if we have dislocations at the grain boundaries that means grain boundaries are also a storage or a places where you can find more or more dislocations.

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Then high angle grain boundary. As we can see here this is your grain boundary and in this case the grain boundary angle or high angle is 40 degrees. Therefore this is high angle grain boundary. Now how high you need to make a high angle grain boundary or how low you need to make a low angle grain boundary that varies from studies to studies but generally 15 degrees or low is low angle grain boundaries and 15 degrees or above is high angle grain boundary. That more or less the convention but sometimes this 15 degree shifts to 10 degrees and so on.

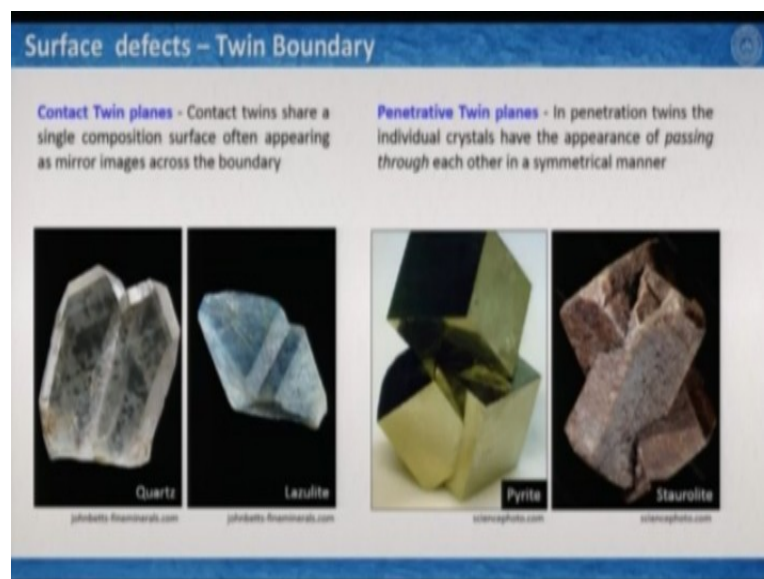
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Now there is another type of grain boundary where which is known as twin boundary when two differently oriented crystals so it has a grain boundary but they are attached together such a way that they share some of the crystal lattice points in a symmetrical manner. What we have seen in other images, for example, if we come here the previous slide, the lattice of this grain and the lattice of this grain they are not sharing any of the atoms of the neighbouring grain but if it is a twin boundary then they share. So this is the twin grain boundary. So they share, so this line of atoms is shared in both grains and if that happens then this is a twin boundary.

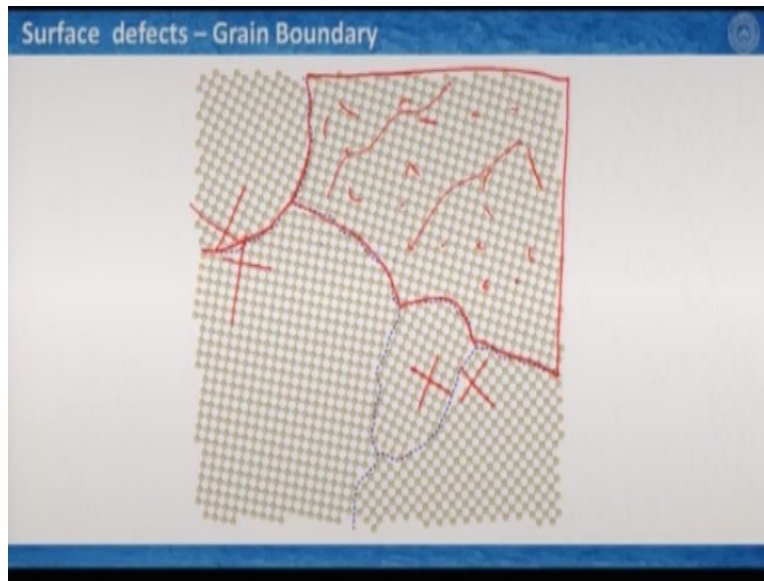
Twin is very common in most of the geological minerals. For example, this is a sketch of an albite mineral. So this is crystal without twinning and these two blue planes are your twin planes and these are your twin boundaries.

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Now twin boundaries we can also classify in two different ways. One is contact twin boundaries or contact twin planes and penetrative twin boundaries or penetrative twin flames. So contact twin boundaries they share of a sort of single composition surface often appearing as mirror image to each other. For example, we see here a quartz or this is a lazulite but in penetration twins the individual crystals have the appearance of passing through each other like they sort of penetrate one crystal and of course it has to be done in a symmetric manner. So here are 2 examples. What we see here this one is for pyrite and this one is for staurolite. As you can see from this it seems that it almost went inside the crystal but that happened in a symmetrical manner.

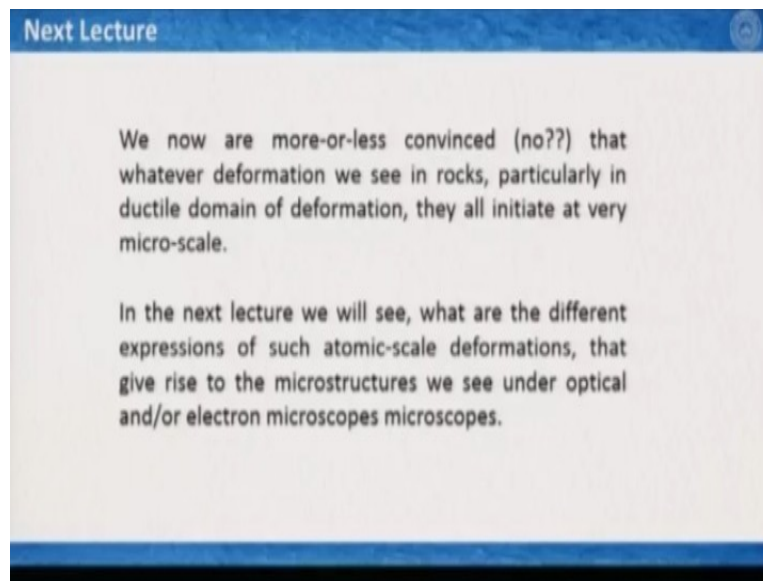
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So this is how we conceive so far a grain boundary. We have seen probably under microscope different crystals their grain boundaries and so on but actually if you can scan it or if you can x-ray it with some inner eyes, then the individual grain boundaries are like this the blue lines and they are separated even if their compositions are very similar, they are separated because their orientations for example, here the orientation is like this and here the orientation is like this. So they are essentially different. For example, here the orientation is like this and here the orientation is somehow like this. So they are somehow different and that is why we see them in a different way.

Now this grain as it appears here, for example, if I consider these grains is extremely homogeneous. There is no dislocation inside in this area. There is no vacancy inside, there is nothing so it is perfect but that is not the case always so this individual place can also be deformed. It may have also some sort of sub-grains and so on and therefore we see different kinds of features. For example, blows extinctions in quartz. We learn more about it soon.

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Now we have reached the end of this lecture so I believe as per the today' you are now more or less convinced that whatever deformation we see in rocks particular in ductile domain of information, they all initiate at a very very micro-scale atomic scale. Now how to feel them how to understand that yes these are there because they are in atomic scale and unless you have some sort of very very high resolution microscope like TEM or so on you do not see them.

So in the next lecture actually we will see and learn what the different expressions of such atomic scale deformations are and their typical arrangements and what are the different kinds of microstructures which are responsible for all these arrangements and deformation. So this is the topic in the next lecture. We will divide it in three segments. First we learn cataclastic processes that are not really some sort of study that involves all these things to learn but this is very important in structural geology but then we will go to intra crystalline deformation and diffusion creeps where these things that we learned today will be very important. So till then goodbye. Thank you.