Phase Transformation in Materials
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Lecture – 18
Boundaries in single-plane solids

So, now, we will discuss about the boundaries in a single phase solids. So, we have only discussed boundaries between solid and vapor remember I am skipping the boundaries between solid and liquid which I will discuss in solidification. So, now, I am going to discuss boundary between solids solid single phase solids or let us assume that the grain boundaries. So, there are different types of boundaries we will consider, but we will not be able to deal all of them today.

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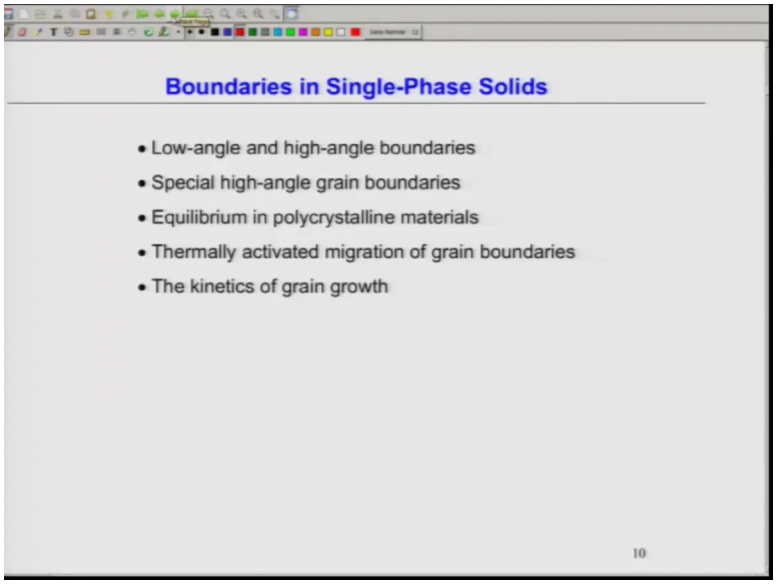

Low angle high angle boundaries special grain boundaries and there are other things like equilibrium polycrystalline material we have polycrystalline then what will happen polycrystalline is a mixture of all kinds of boundaries.

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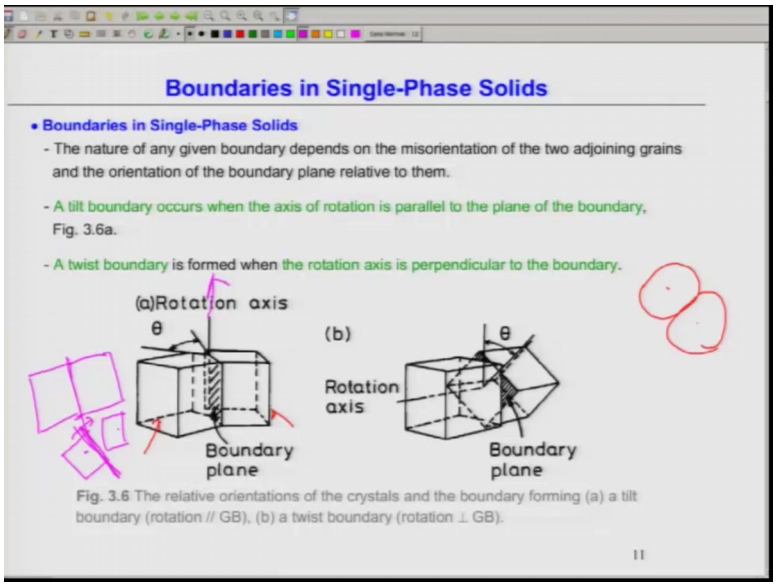

Now, well before I deal with let me see what is basically if you consider a single copper suppose we have a copper and there are main grains so; that means, each grain has same chemistry only consist of copper atoms. Difference between the 2 grains is what orientations one grain is oriented in one way, other grain is oriented other way that is why the boundary between the 2 grains will have orientation change. So, nature of many boundary depends on the most miss orientation of the 2 adjoining grains that is what it is been that is what exactly I told you.

Basically if I a single grain a grain is a single crystal that is assume that now single crystal of one grain in touch with a single crystal of another side of the grain. This is one grain this is in tough with another grain you can see here their orientations are different so; that means, nature of this boundary depend upon the miss orientations of these 2 grains nothing else other than that will matter to them. So, how can I create that I can create in many ways these miss orientations.

But we have going to deal with only 2 simple cases remember that there are many ways you can do this miss orientations between the 2 grains, but we are going to deal with only 2 simple cases and these 2 simple cases such enough for you understanding for the material science phase transformations one is a tilt boundary. So, one is important suppose I have a grain on the left side which is shown as a block like you and I have a grain on the right side and they oriented differently that is what is shown here one grain

is looking like this way other grain is looking like other way and I want to bring them together and from a boundary.

So, what I can do I can actually tilled one respect to other to have a coincidence and this steel boundary occurs whenever the axis of rotation the axis of rotation means you see here this is what is how its rotated. So, if this 2 are the same this 2 have been like this and like this the same orientations, but they are not same. So, what will happen or let me draw it in a different way may if it is not visible if this 2 are same one is like this other one is like this, then you do not call this is a boundary because there are same orientations only when one guy is like this other guy is like that then there in different orientations.

So, if this is the 2 orientations of the grains and I want to bring them to boundary what I can do I can actually tilt this one this pa primary one along this axis tilt to bring it to same or that on the right side one and that is it tilt happens along a common axis of the 2 and this common axis is this one which is shown here this one is a common axis and this tilt is given by theta is just like tilted by amount theta you have 2 cubes one cube is tilt with respect to other by theta that is that is what is tilting and this; this is I know how is very not easy to understand basically; what I have 2 separate grains, they are all single crystal grain in different way and they are coming together and that is why the boundaries forming.

When they come together form a boundary in order to have a coincidence of the atoms otherwise bonds will be remain all broken that is not possible because bond has to be you know bonds has to be matched little bit otherwise energy will very high to do that you can actually tilt the atoms or planes actually in one of the crystal. So, that it atoms on this boundary falls on the other crystal that is what it is a tilt boundary and to do that we need to have a tilting of one of these crystals with a common axis parallel to the common axis.

So, this is the common axis; we have tilted parallel to the common axis that is what it is known as a tilt axis tilt grain boundary now twist one is same thing, but you know twisting is what twisting is something like this way this is the way of twisting. So, rotation axis is parallel perpendicular to the boundary; that means, what I am twisting one crystals to the other in such way the rotation axis along the rotation such this is our rotation axis that is actually perpendicular to the plane of the boundary here the plane of

the boundary or remaining constant is the axis rotation axis was parallel to that, but here rotation axis perpendicular.

This is the rotation axis; you will see that is the perpendicular to the boundary. So, that is the main difference between a twist and tilt boundary and these are all seen most of the boundaries in the in the in the crystal you see are mixer of thee 2.

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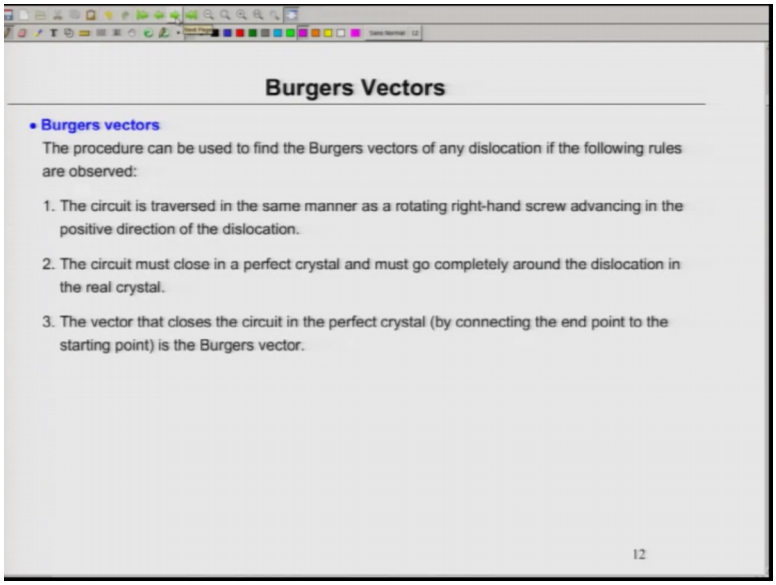

So, when you tilt and twist you are basically creating what creating deformations or you are deform in distorting this atoms actually and distortion is done by dislocations as you know basically whether you tilt or twist whether you have tilted this way that way or a twisting it if when you twist this pen this way what you doing a deforming it basically if you take a rod and try to twist it or try to tilt it this way.

What you are doing you are you are making the atoms deform; they are making the atoms move actually and this displacement of atom is defined by dislocation we know that and dislocations is actually characterize by dislocation means the displacement of dislocation characterized by what is known as burgers factor you know burgers vector is basically well defined you all should know that.

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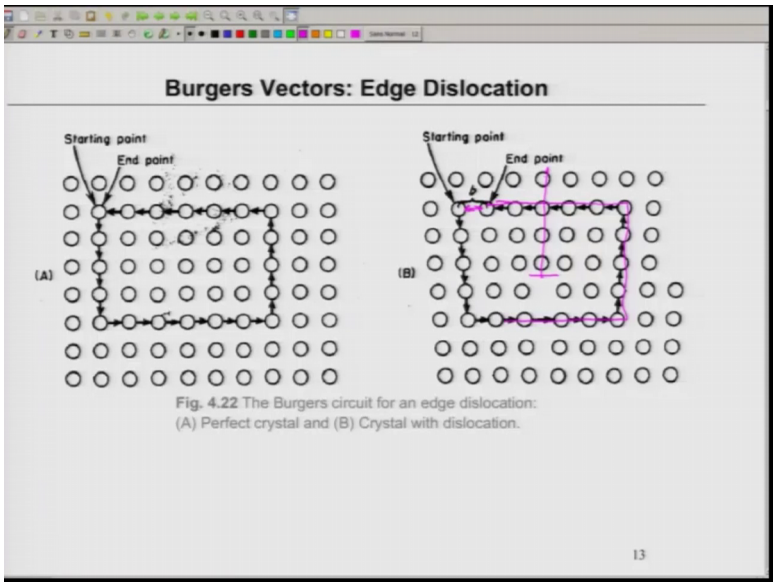

This is nothing, but what if I draw a burgers circuit the failure of closer of the burger circuit is what is known as a burger vector that is what is shown here you see in a perfect crystal there is no dislocation there is no extra plane. Now there is no failure of the closure.

But the when you have a dislocation which is sitting here this is a dislocation and if I start from here mope like this mope like; this mope like this; there is a closure here.

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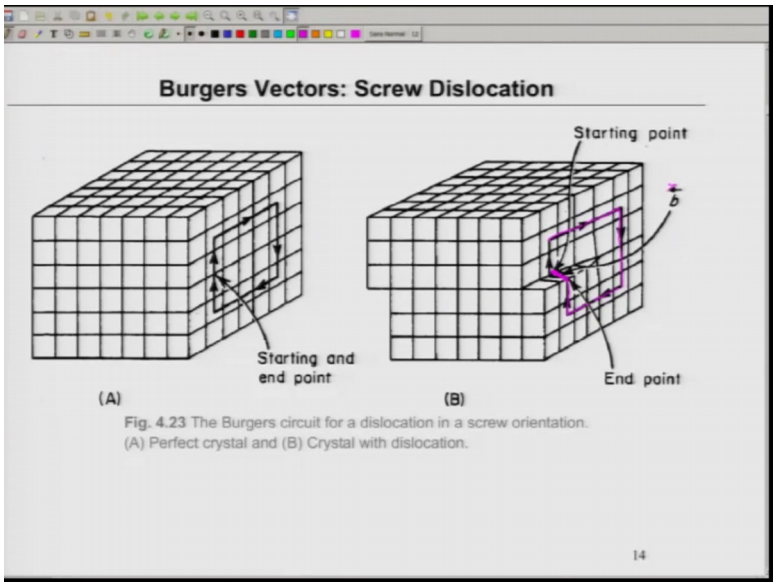

That is what it end this is the closure failure that closure burger is what is known as the burger factor direction of that tells you direction of the factor and the magnitude to value of that tells you the value of the burger factor this is very important in a 3 dimensional space; that means, you can either have a you know screw dislocation case you can see this is a perfect crystal; there is no closure problem, but in a screw dislocate is place; there is a closure problem here you go you can start from here, then go there, then go there go there go there go there further moment is here you cannot reach here. So, there is a closure problem.

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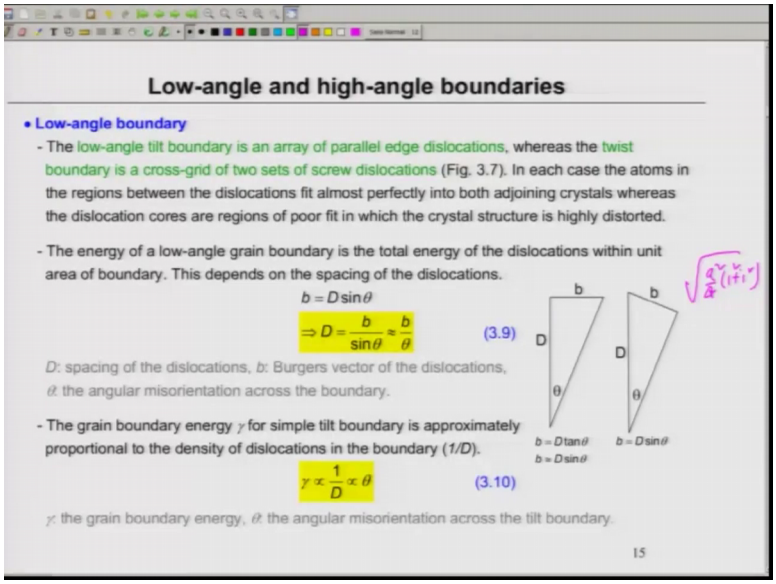

That is what is your burger factor in the screw dislocation I hope because in a what is called normal dislocation that is what is your edge dislocation; that is what, I shown you here, this is a edge dislocation this is very easy to understand. So, screw is little bit difficult that is what I want to discuss. Now people actually most of the scientist, they have actually discuss that I can considered the tilt boundary or twist, even tilt boundary easy to understand 2 types; one is the low angle other one is the high angle boundary low angle means the theta which we have tilted if you go back that here theta by which you have tilted is very small.

High angle means theta is large we will define the theta small and high very soon what is the high angle values we can assume that basically W D; they have actually considered that a low angle grain boundary where the tilting angle is very small can be considered to

be to be consisting on of array of parallel edge dislocations; whereas, the twist boundary is a clause kid of 2 sets of 2 dislocations we will come back to those figures which is taken for early from the book.

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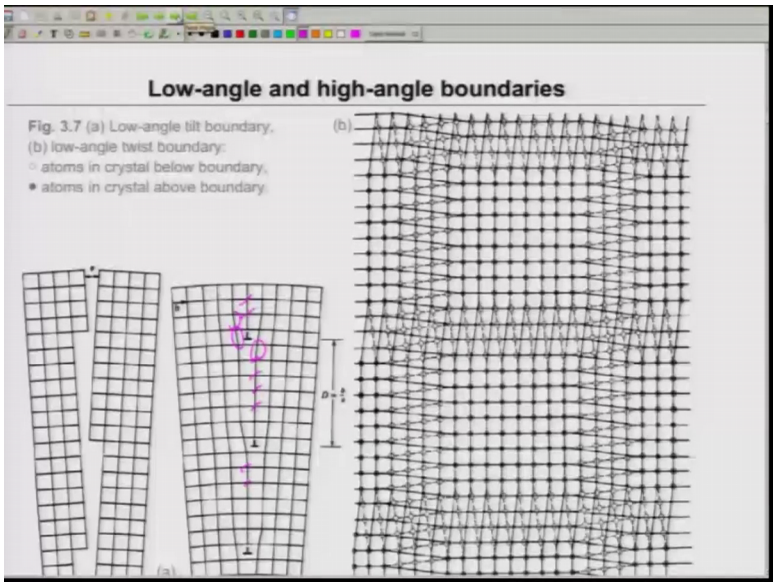

Now, let us considered the tilt boundary tilt boundary is very easy to understand I hope it is there is a picture there yes on your left side you see consider this first one do not look at the right side.

First you look at your left side you see there are 2 crystals and they are miss orientations are actually theta and I have to put them together to form a boundary and they are tilted already by certain angle theta if I put them together; what I found is nothing, but a array of dislocations 1, 2, 3, correct; that is what is basically a small angle tilt boundary looks like this is what W T G; it an others have thought about very easy to understand; now few things you to understand very clearly if I do that.

Now, energy of the low angle boundaries; so, total angle dislocations nothing, but dislocation energies correct before I go that let me see each case atoms in the region between the dislocation fit almost perfectly in the both as an crystal whereas, dislocations cores are regions of poor fit in which crystals structure highly distorted what is the meaning of that it says you know most of the part crystal is fit nicely here crystal fits nicely see the bonds are very nicely not broken not even distorted here also. Similarly, here, there, here, here, here, wherever here only in the core where dislocation

it is little bit distorted bonds are broken and also distorted you see distortion here; this is the core distortion bonds are distorted bent.

That is what it says. So, right so; that means, basically energy of this bond is nothing, but co energy of dislocations correct there is one thing you must take care from these lecture one thing that energy of a low angle grain boundaries nothing, but energy distortion energy of the core dislocations because if you assume that dislocation the grain boundary is consisting of parallel row of dislocations second thing is that if I increase the theta what will happen if I increase keep on increase the theta, then means this angle, I have to look more and more number of dislocations you remember; the planes will go the atomic planes will go further away as you increase the theta.

Theta increase means you are put taking this is theta initially then you are taking you see going away. So, more and more dislocation is replaced another boundary now how many dislocation you can put it that depends on dislocation will interact dislocation cores will try interact you know the once a time will come or the situation will come in which core of dislocation will try to overlap one each other in such a situation you cannot accommodate any more dislocations and that is the maximum value of theta which we can have in a low angle grain boundary because the movement core over dislocations fall on each other; that means, the whole boundary is distorted because every bond will be distorted.

That is that is where the energy was energy of the boundary will very high. So, there is a limitation of value of theta and that values normally ten to 12 or 10 to 15 degrees that is why tilting you can do if you tilt more than that then it has becomes a different-different thing depend situation that is call high angle high angle grain boundaries which we will discuss later, but for the sake of your understanding for a small angle grain boundaries you cannot have theta more than 15 degrees that is why whenever you do a experiments and the characterize grain boundaries you always measure what is the miss orientations if it is less than 15 degrees you call as a low angle grain boundaries if it is more than 15 degrees call as a high angle grain boundaries that is the way we defined things.

So, if I go back little bit here that is one thing second thing is that another is a low angle grain boundaries I told you is nothing, but total energy of the dislocations now it depends on a spacing of dislocations as you see from this picture if this is the burger factor this is

your distance between the 2 dislocation and this is the angle theta then is b is nothing, but D sin theta or rather distance between the 2 dislocation is b by sin theta theta is small; obviously, is not as small as you can think of it then is b by theta where theta is in radiant. So, therefore, if I know the miss orientations and if I know the burger factors in the crystal that is one known for a F e 3 crystal is a by 2 1 1 0 where a is the lattice parameter. So, therefore, b is nothing, but a square by within route a square by 2 1 plus 1 ok.

Now, nothing, but is what happens is becomes a by square by 2 4 1 square plus 1 square. So, this become a by 2; 2 that is the burger vector and if you know the theta let us suppose theta is five degrees that is the radian; you get the distance between 2 dislocations. So, grain boundary energy is simple for the tilted by uppers mainly proportional to density of dislocation in the boundary more number of dislocations higher is the energy more is distortion so; that means, its inversely proportional to the distance more the number distance is smaller.

So; that means, if proportional to theta. So, gamma is nothing, but proportional to theta again you see in the normal crystal surfaces we see this is solid and vapor where gamma was a function of theta; theta was the orientation of this boundaries with respect to the crystal here theta is the tilting angle. So, therefore, gamma is proportional to theta which is the angular miss orientation across the boundary that is very clear and understandable now what happens to the twist boundary as I said here again go back twist boundary is nothing, but cross kid of 2 sets of screw dislocation what is it lets see here; you see here this is twist boundary you have twisted one crystal with respect to other.

So, because of that what you have form a line number of screw dislocations no longer edge screw dislocations because if you look at a screw dislocation from with top they look like a screw you see from this; this you see this is screw here lets right handed screw you have distorted the screw. So, this boundary is nothing, but a cross the of the 2 sets of screw dislocation one set is shown by this the solid other set is shown by the dotted lines that is what you see and that that is little bit difficult to understand that is why the experimental work on twist boundaries is very less most the experimental research has been done on tilt boundaries and luckily many of these screw boundaries actually tilt boundaries in the actually experiments and therefore, it is easy to understand

why actually they are tilt; the tilt boundaries are much easy to form than the twist screw dislocations are actually little cause more distortions compare to your edge dislocations.

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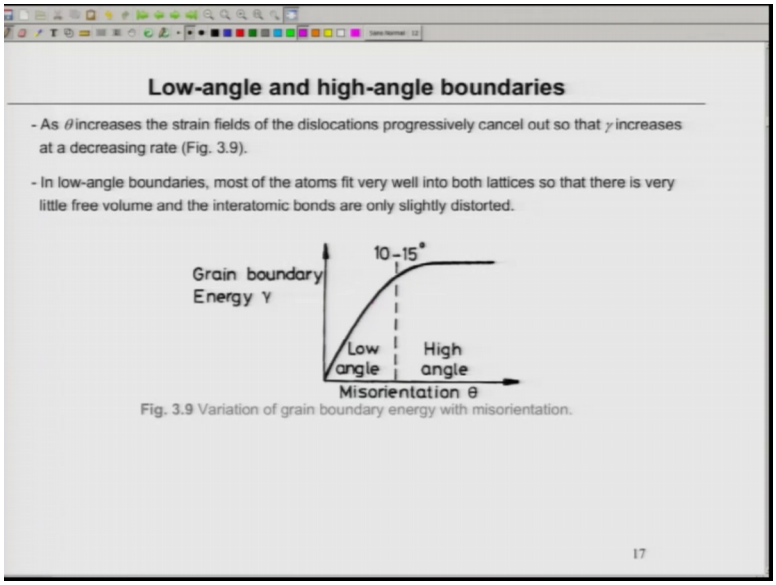

And that is why they are much less, but as I said correctly in sometime back most of the boundaries are mixture between screw the tilt and twist. So, that is why analysis becomes little bit difficult now as you see. So, gamma is nothing, but a function of theta the tilt boundaries correct. So, if you carely see when angle is very low number of dislocations also low the gamma is low when the angle increases gamma slowly increases, but after 10 to 15 degrees gamma tapers off why as I said you after 10 to 15 degrees you cannot put more number of dislocations dislocations cores have overlapped.

So, remember if dislocations core overlap what will happen if dislocations have different type of nature suppose one is positive one is negative they will try to cancel each other stain fields and because of that energy though system will be reduced or the slope of the curve will slowly reduce that is what you see it becomes it slowly tapers off as from this point onwards is slowly tapering off that is mainly because of this overlap of these dislocation cores and because of overlap of a dislocations cores sometime they will cancel each other and they cancel each other means therefore, the stain field will reduced as the stain energy reduces gamma energy interface energy or grain boundary will reduce.

So, most of the atom fits very well between the lattices. So, there is very little volume 3 volume and interacting bonds are highly distorted in a low angle grain boundary correct and I that is what we marked these 10 to 15 degrees high angle grain boundary because we cannot put more number of dislocations into the boundary that is where that they will start overlapping and they will start cancelling each other stain field. So, therefore, we cannot no longer considered a high angle grain boundary to be consisting of array of dislocations that is that assumptions which W T read analyze have done will not a valid when you have a theta more than 10 to 15 degrees thus the one of the important aspects.

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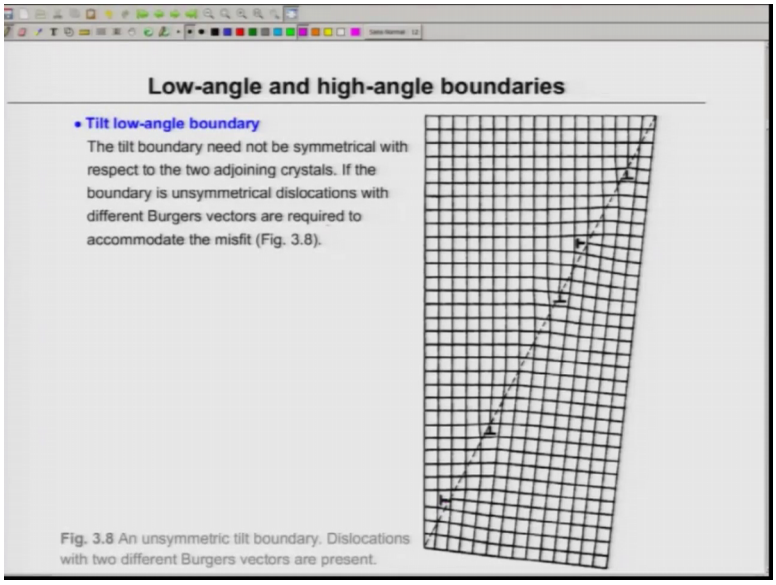

Now, you know I consider tilt boundaries that is what I am showing you here tilt boundary need not be symmetrical with respect to the adjoining crystals that is what you always think it can be angle also this un symmetrical with respect dislocations with different burgers vectors you see here the burger factor is different here than here this is one type this is another type this is the one type this is the another type. So, in actual crystal this is what will happen never it will be like a you know straight line and also symmetrical and all the dislocation will arrange one after another they can be in a at an angle and therefore, I know that is what you say different burger factor required to accommodate the misfits because misfits may be different at locally and that can accommodated by putting dislocations of different burgers vectors.

And you know that is only possible in crystals which have which can allow you to produce different burgers vectors not in many crystals it is not possible when theta that is what again I am telling you when theta exceeds more than 10 to 15 degrees dislocation spacing a. So, small dislocations cores overlap it is impossible to physically identity identify the individual dislocations that is what you see here it is not possible at this stage grain boundaries almost independent of miss orientations in many energy basically gamma is independent of theta.

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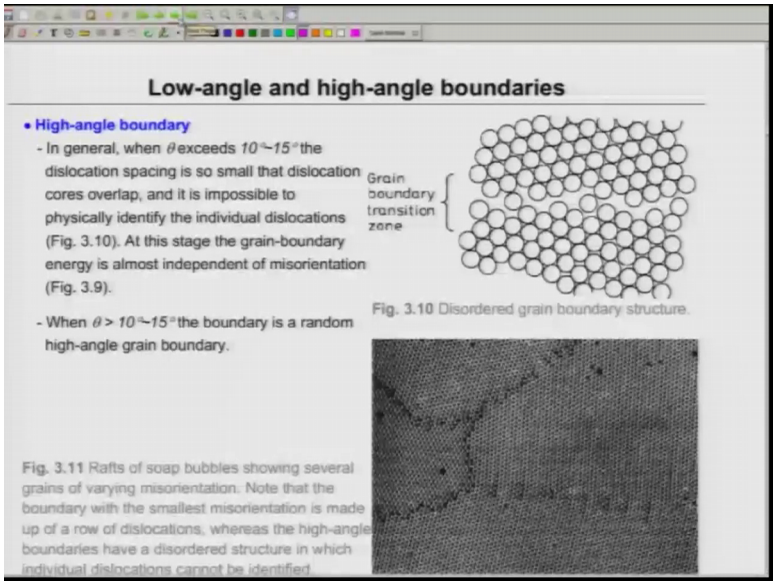

So, when theta is more than ten to 15 degrees boundary is say nothing, but a random high angle grain boundary you can no longer considered to be a consisting value of dislocations.

This is a rafts model which people use to describes as you see if it is a high angle, then number of number of you know miss joint take places are very large is a low angle, then it is possible to considered that way. So, one actually visualize the grain boundary system using a soap bubbles rafts of soap bubble models.

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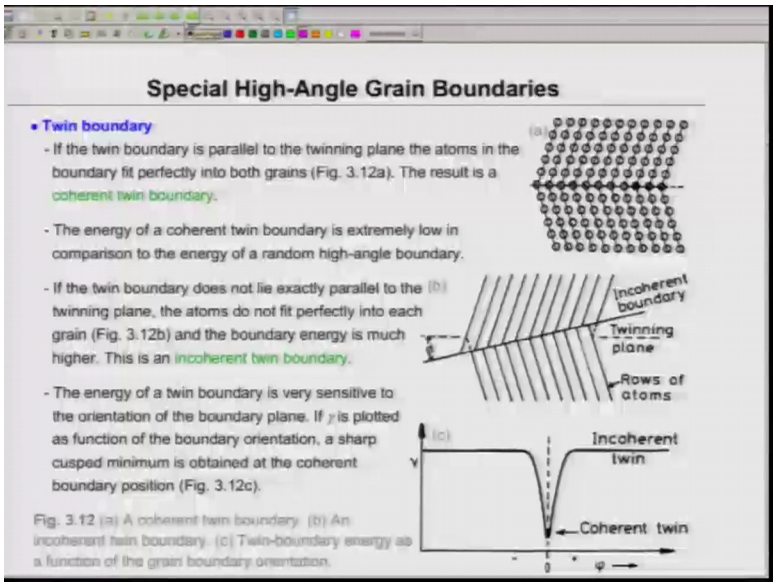

So, let us stop it here because I will start I will discuss high angle grain boundaries other things now that is what is the next. So, and the values and other things we will do it next class and we will discuss about this special high angle grain boundaries because high angle grain boundaries are very difficult to understand when only considered special boundaries which are easy to understand and the special boundaries are called sigma boundaries or coherent boundaries which you will see later on in the next class.