

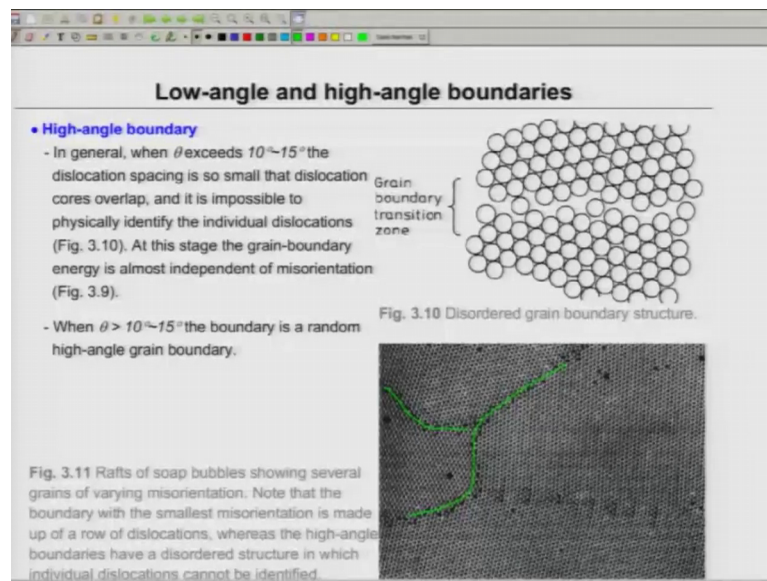
**Phase Transformation in Materials**  
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**Lecture – 19**

**High angle grain boundaries, Equilibrium in poly-crystalline materials, Interphase interfaces in solids**

So, in the last 2 lectures I have given you some idea about different types of interfaces. At least I could convince you that interfaces between crystals of similar compositions and structure can be different types one of these is basically considered as a low angle grain boundaries. And I discussed you about different types of low angle grain boundaries tilt and twist. So now, as I just told with the angle between the 2 grains, either it may be tilt or twist is more than 10 to 15 degrees, then no longer the dislocation to accommodated along the grain boundaries can be 10 above.

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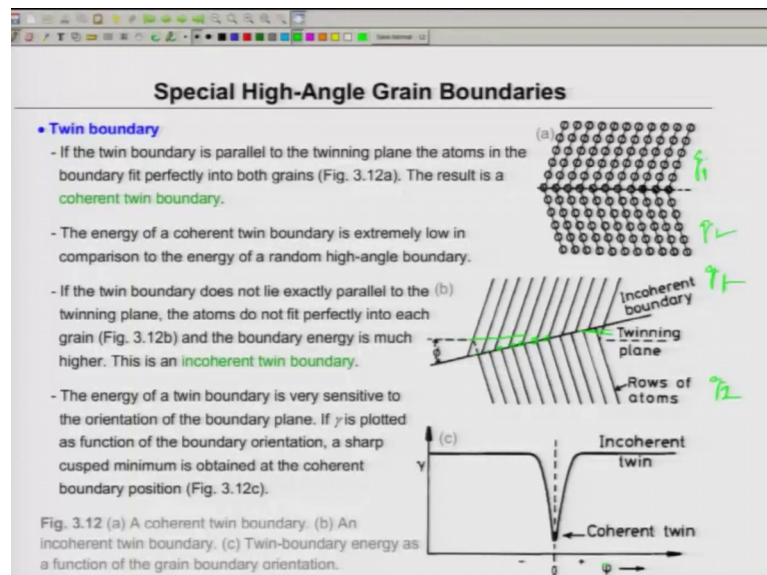
So, general when the theta exceeds this value then dislocation spacing is become very small, and the cores were dislocation start overlapping and therefore, we can no longer have dislocation arranged in a parallel row giving rise to a low angle grain boundary.

And at this stage most the grain boundaries actually are known as high angle grain boundaries. And there are actually random. They cannot be treated as a very systematic way lectures like normal low angle grain boundaries. Basically in a low angle grain

boundaries there are regions of fit that way fit in most by cases only at the cores were dislocations atomic fit, the fit between 2 grains are no toppe. But in high angle random grain boundaries the number of this unfit regions where the atoms of the 2 grains are not able to fit each other are more. And in a bubble wrapped model that can be easily seen, that you see along the grain boundaries of high angle this is what I am marking by using a pen is there are large number of misfit regions where atoms for the growth both the grains to not meet fit each other.

And this is basically the future of random high angle grain boundaries. That is why and the high angle grain boundaries are not discussed much in the literature. Because exact atomic matching or atomic as been sell on this grain boundaries and not yet resolved nobody understands how atoms can actually coexist along this boundaries. What we can do is the next few you know slides to make you understand there are some special cases of these kind of boundaries, where the angles are more than 10 to 15 degrees, but atomic fitting or atomic match is possible. That is what I am going to show you for the next few cases ok.

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Let us take the special high angle grain boundaries. Once has high angle grain boundaries was a twin boundary. As you have seen in the low angle grain boundaries the misfit between the 2 grains orientation misfit can be accommodated by arranging dislocations at a particular interval. Since same way twins can also be used to form

special high angle grain boundaries. Let us discuss or what is the twin. You know twin is nothing but a special arrangement of atoms when one part of the crystal in becomes mirror image to the other parallel crystal along a boundary.

And this is a one of the dominating deformation mechanism in the many of the hexagonal crystals. Few cubic crystals also so twinning, but there may be different types of twins, but whatever it is twin is a one of the predominant mechanisms or deformations in many of the metals or even alloys. So, if a twin boundary, we are talking about twin boundaries that right. So, the twin boundaries parallel to the twin planes. So, what is the twin plane? Here it is shown here there is a twin plane along these in a dotted line. You can see here the atomic planes have distorted or rather deform in such a way that if you if I place a mirror and the twin boundary the one set of planes become mirror image to the other set of planes that is what is a twin boundary is.

So, if this twin boundary actually is parallel to the twinning plane. Twin boundary is mean boundary along the grain boundary. If it is parallel to the twin plane then atoms will fit perfectly along in the both the grains. Suppose this is grain one and this is grain 2. So, what is happening here? Along this twin boundaries which is parallel to the twin plane also here, the atoms fit exactly nicely. There is not even a single you know misfit along the boundary; that means, you do not need any misfit dislocations to accommodate any kind of reference in the atomic fitting such a kind of boundaries known as coherent twin boundaries, because atoms are matching perfectly with each other atomic planes.

Only thing which makes the different is that orientations are changing from one grain one to grain 2, and the change the orientation is basically twin related. So, this kind of grain boundaries where there is a exact match of the atomic planes will have very low energy. In fact, energy can be as well as one mille joule per meter square. So, energy of a coherent twin boundary extremely low in fact, in the literature nowadays people are working on mechanical behavior of material, such a way that boundaries can a made like a coherent twin boundaries.

Then energy of the boundaries are very low. So there my grains will not grow, not even that we can actually make the many interesting you know phenomena understandable like grain growth or recrystallisations, if you creates such a kind of grain boundaries predominately in the material. But this is basically such a kind of situation when a twin

boundary is exactly falling on the twin plane is a very, very odd situation. Normally is very really happen, but you do happen in some cases excuse me. So, if a twin boundary does not lie. Suppose parallel to the twin plane what will happen on such thing is shown here you see a twin boundaries here. This is a twin plane; this is the plane twinning is one. And the boundaries somewhere solid line this is the boundary.

So therefore, twin plane and the twin boundary are not same. They are at an angle each other. So, that angle is given by  $\theta$ . Now in such a case what happens? If such a case happens you will see there are places where the atomic planes match suppose here I am marking. So, marking here they are you see it is matches you as you go away from this that twin where the planes are not matching. There is a distance there is a basically definite mismatch of the atomic planes coming from the grains  $g_1$  to  $g_2$  very clearly seen.

So, what I that means, what that means, this bonds here sitting atom sitting at the positions are not this satisfied by the bonds by the atoms on the grain 2. And this is known as incoherent twin boundary. Because at an planes are not matching for all the at for the all the planes. Roles of atoms on the grain  $g_1$  sorry,  $g_1$  is not matching with many of the (Refer Time: 07:21) those of atoms are not matching with grain  $d_2$ . And this leads to increase of the interfacial energy a grain energy, because this un you know satisfied bonds which are there along the boundary will lead to increase in the energy.

So, energy of a twin boundary is sensitive to the orientations. That is what you see here. In such a case of first case where this a coherent twin energy will be very low, but the movement I change the twinning plane and the boundary plane, that the they are distinctly different then the energy will be higher. So that means, it depends on the this value  $\theta$ , which is the angle between the twinning plane and the boundary plane. And you know it is energy is in certain value if I plot a  $\gamma$  versus  $\theta$  were versus  $\phi$  here, for certain values of the  $\phi$  half of this  $\theta$  were not  $\phi$   $\theta$  actually, this  $\theta$  you see that. So, the energy becomes very low. And that is why the coherent means from. So, that were coherent twins will have what are So, magnitude lower even values than compared to incoherent twins.

And this is where is very important. That is why it is better actually we create grain boundaries which are semi coherent type. And so, that this kind of situation this kind of energies energy this can be preferred. So, this is a very special grain boundary ok.

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**Special High-Angle Grain Boundaries**

Table 3.3 Measured boundary free energy for crystals in twin relationships (mJ/m<sup>2</sup>).

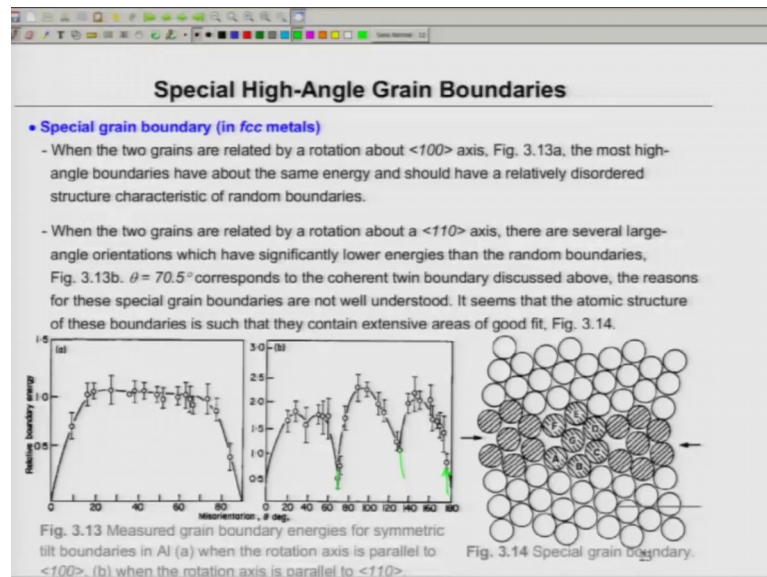
Crystal	Coherent twin boundary energy	Incoherent twin boundary energy	Grain boundary energy
Cu	21 (3.4%)	498 (80.0%)	623
Ag	8 (2.1%)	126 (33.4%)	377
Fe-Cr-Ni (stainless steel type 304)	19 (2.3%)	209 (25.0%)	835

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Now, to give we some energy values, but different crystals like copper silver or may be stainless steel stainless steel is say one of the classic case. In the coherent twin energy boundary as you see here is basically for the copper is basically only 2 and 21. Silver means slower for stainless steel is about 19 very close to 20 mille joule per meter square. Now in coherent twin boundary on the other one order miniature is higher is about 500 or 100, and is 100 and normal grain boundaries which are actually even much higher.

So therefore, it is very clear that if you have twin orientated grain boundaries which even the angles are high 10 to 15 degrees are higher, steel I can actually have a very low grain boundary energy, that is one part.

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Now, let us look into in (Refer Time: 09:37) detail about these special grain boundaries. And let us suppose let us considered FCC crystals. You know when 2 grains in FCC crystal are suppose related by rotation along 1 0 0 axis. That is what is shown here. Now the most angle grain boundaries have the same energy and it should be should have a relative disorder structure. That is because of you know that is mainly because of the random these a random boundaries.

Now, when the 2 grains are related by rotation about 1 1 0 axis, there are several large angle grain boundaries which can be significant low energies. So that means, what I am talking now is orientation dependence, if 2 grains are suppose related by rotation along 1 0 0 axis. That is the one of the cube axes, then this very difficult to actually make them you know low angle or say low energy, because they will be very little very little anyway to create such a kind of grain boundaries but when they are related by rotation along 1 0 0 1 1 0 axis.

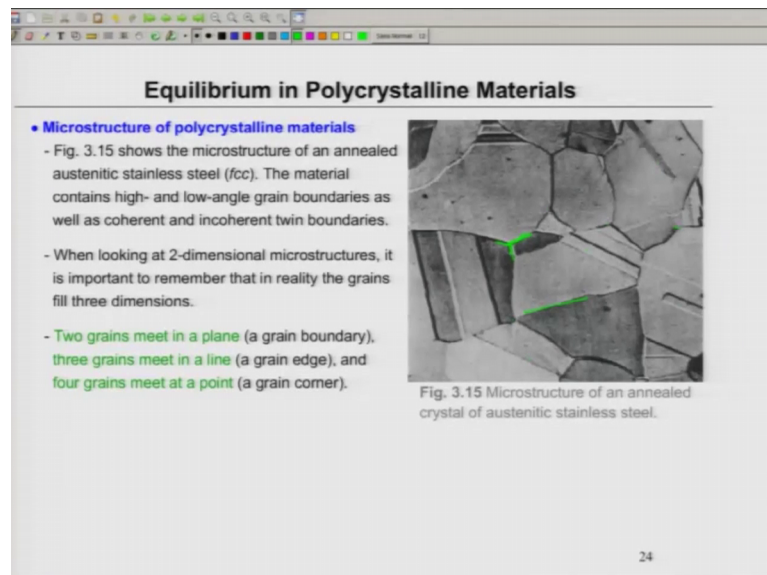
That is one of the phase tangles then what will there are several I think grain boundary orientations which can have lower energy. Like one which is shown as 70.0 degrees, 70.0 degrees is specific case. This corresponds to a coherent twin boundaries. We know that the FCC crystals between it tell related by 1 1 0 the angle becomes actually 70.5 degrees.

The reason is for this boundaries not yet understood, why? Because whether is really that this boundaries has a perfect atomic match or not people are try to do some electron

microscopy, but it is not clear. But it seems the atomic bar the planes do match nicely that is why they can be created. And these are things which is shown here you see here, this is you see this is the gamma plot again. Here this is gamma verses related boundary energies persist the orientations. You see this is one low another low. And similarly So there will be another low here. So, these angles which this is 70 point this is about 140 141 actually.

And the other one is about 100 and a 78. So, these angles it boundaries are related along 1 1 0 axis, then they actually form very low energy boundaries in FCC crystals.

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Now, upon give you. So, I have given you fair amount idea one low. I have it is not possible discuss about all the high angle grain boundaries, some of them are really varied complex. But you know real micro structure consist a many grains, they are not actually only one boundary or 2 boundaries there are thousands of grains in real microstructures. And each grain is oriented differently from the other grain. So, well therefore, the boundary nature of the boundaries up all these grains which will have with the neighbors, will change based on type of orientations they have even chemistry also.

So, it shows austenitic stainless steel on the right side you see, what do you see here? You see it contains low angle grain boundaries high angle grain boundaries as well also twin boundaries you see these are the twins. You see in case of stainless steel there are many twins exist. So therefore, you have all kinds of boundaries. But remember we are

looking at when you looking at a micro structural in optical I c m, we are looking at 2 dimensional pictures. It is it is not that we are looking at 3 dimension. So therefore, but most of the grains are actually 3 dimension in the entities. So, the boundary we need to need to look at if you really want to get the characteristics of the atomic matching we need to look at the z axis also not only action y, but z axis also.

So, in a 2 dimensional picture what I will you see you see the grains can meet along a boundary or in a plane that is what a grain boundaries. This is a grain boundary in a 3 grains can meet as a a at a line, I do not know whether is there or not yeah is there is one grain here there is another grain here there is another grain. See the 3 grains are meeting along this line. And also 4 grains can meet at a point, whether it is there or not let see 4 grains meeting at a point somewhere there. 1 2 3 4 yes now it is not there most of the cases.

So, very rarely you see that kind of 4 grains meeting at a point, but you can see many times 3 grains are meeting at a point these are the points that is 3 grains meets. So therefore, these the what is important point I am trying to convey is that not only the boundaries, but also this edges or the corners actually or the meeting points. They also lead to an energy of the system. Because it is not possible to always are perfect or the semi perfect atomic matching at this points. So, finally, energy of the whole polycrystalline material will be summation of the boundaries different boundaries. Whether it is say high angle low angle or twin boundary or even and additionally and this points in which this grains to will do meet 3 grains or 2 grains.

Remember when you are trying to have 3 grains meeting and alloying a line or a point it is extremely unlikely that the atomic planes will be at a you know very low energy configurations at this points. So therefore, finally in a natural what I can say is that real polycrystalline crystals are much more complex than we think about it. Although we can talk about interfaces separately like grain boundaries and other things, but real grain structures are much more difficult. That is why actually lot of engineering comes into picture. You can do many, many engineering to modify this boundaries and create different kinds of materials ok.

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### Equilibrium in Polycrystalline Materials

- **Torque of grain boundary**
  - The boundaries are all high-energy regions that increase the free energy of a polycrystal relative to a single crystal. Therefore a polycrystalline material is never a true equilibrium structure.
  - The grain boundaries in a polycrystal can adjust themselves during annealing to produce a metastable equilibrium at the grain boundary intersections.
  - Let us consider a grain-boundary segment of unit length  $OP$ , Fig. 3.16. If the boundary is mobile, the force  $F_x$  and  $F_y$  must act at  $O$  and  $P$  to maintain the boundary in equilibrium.
 
$$F_x = \gamma \quad (\text{from Equation 3.3})$$
 If  $P$  is moved a small distance  $\delta y$  while  $O$  remains stationary, the work done will be  $F_y \delta y$ . This must balance the increase in boundary energy caused by the change in orientation  $\delta \theta$ .
 
$$F_y \delta y = l \left( \frac{d\gamma}{d\theta} \right) \cdot \delta \theta$$

$$\therefore \delta y = l \delta \theta \quad (\delta y \text{ is very small})$$

$$\Rightarrow F_y = \frac{d\gamma}{d\theta}$$

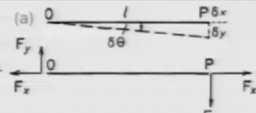
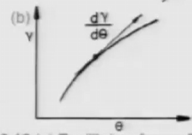



Fig. 3.16 (a) Equilibrium forces  $F_x$  and  $F_y$  supporting a length  $l$  of boundary  $OP$ . (b) The origin of  $F_y$

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So, I will not I will skip this part because this will come later. So, what I will do is now I will go to the interfaces, boundary between interfaces. These are things which will come later when you discuss about the recrystallisation and grain growth.

So, let me just start and say that. So, far we have discussed about the boundaries between crystals of same type same chemical compositions that like in pure metals. But you can have boundaries between 2 different phases, and these are the boundaries. Which are more important by the way before I go into details of that you know the boundaries, Which we have seen so for high angle low angle boundaries also will exist in these.

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### Interphase Interfaces in Solids

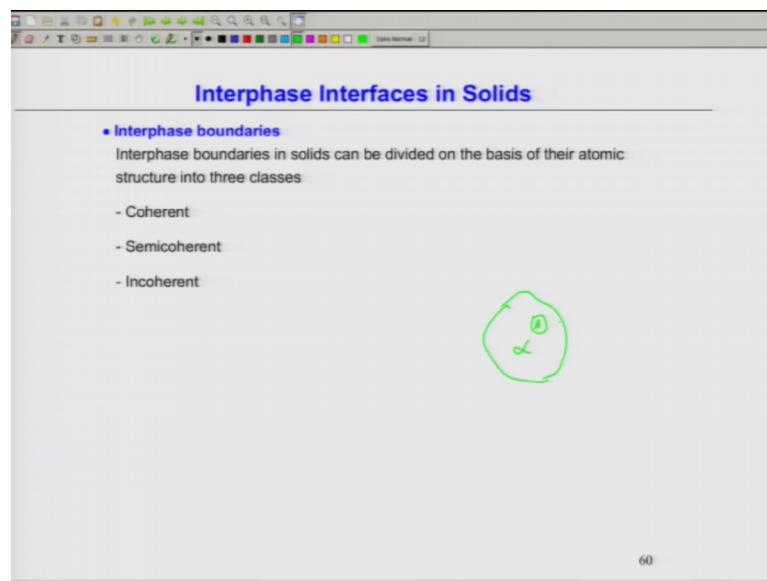
- Interface coherence
- Second-phase shape: interfacial energy effects
- Second-phase shape: misfit strain effects
- Coherency loss
- Glissile interfaces
- Solid / liquid interfaces

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In this solids, but in addition to that there will be boundaries, which will be between 2 separate phases ok.

So there are different types of things which will be talking about it we will talk about first of all talk about whenever we have 2 different phases what is the interface coherence. How the interface between the 2 phases will be can be met coherent? And if they are not coherent well what are the what are the different possibly it is exist. Whether we can actually discuss I do not know whether we will get time in it is lecture on the next lecture, but we have do discuss some higher because specific hardening depends on second phase size, and how we can actually get those. And whether we can have a coherency loss, what will happen if I have a loss of coherency along the boundaries? And finally, possibly we will discuss about the glissile interfaces.

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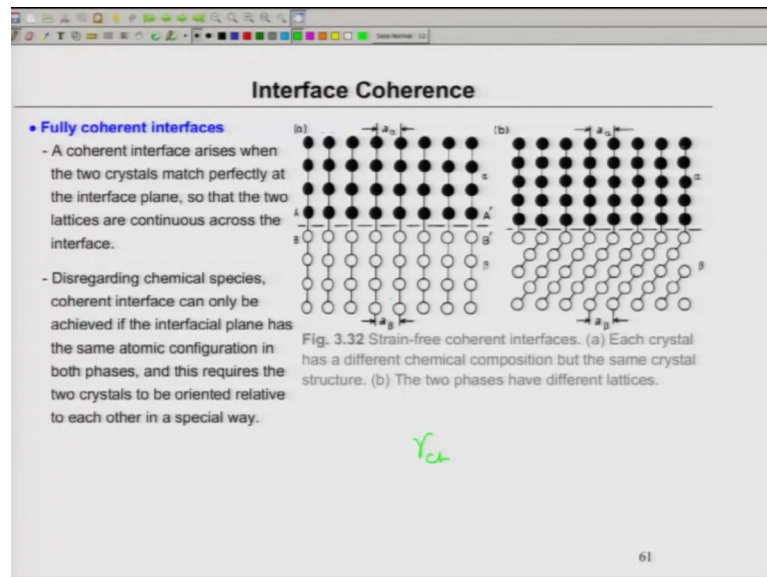


You know interface boundaries in solids basically interface boundary means with a alpha phase suppose and we have inside we have beta.

That between them the boundaries known as interface boundary, because there are 2 separate phases they have different crystal structures. They have different chemistry. So therefore, we cannot no longer talk about this is a boundary grain boundary between alpha and beta with always say this is a boundary phase boundary between alpha and beta. So, these such boundaries can be have 3 different types. At least we have some idea about that in basis material science. Depending on the atomic structure across the

boundaries we can be other coherent type semi coherent type in coherent type. Right now it is not possible for it to understand what are these for there the 3 division classes, which will be talking about it in next. Well, whenever you talk about 2 crystals.

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See alpha is a crystal beta is a crystal because alpha is a grain of alpha type beta is a there in a beta type. So there 2 separate crystals because that is why 2 there is separate grains of different phase different chemistry. You know it is possible that in a very nice situation where the planes of alpha across the boundary will be exactly matching the planes of beta, that is what it, is shown here. You see there is a boundary a prime and b, b prime. Between the alpha and beta phases and you see the atomic spacing in such way the oriental the suppose that can happen. That can happen actually do happen I will give example also.

In such a way that a alpha that is the distance between the planes of the atoms in the alpha phase, and a beta distance between the plates in the beta phase are exactly same. So obviously, if this can happen many cases, it does not require the both of them should have similar crystal structure. If it is good if it is not still it can happen. So, this such a kind of boundary where the atomics bonds are exactly satisfied is known as the fully coherent interface because 2 lattices are continuous across the interface. Now what is the energy of the boundaries due to mainly due to the chemical difference is across the boundary?

So, here in the beta phase only atoms are white color, white kind of a balls on the all the phase they are actually black. The So therefore, inside the alpha phase the bonds are basically between black and black inside the beta phase between white and white. But that interface the bonds on basically between alpha and black and white. So therefore, bond characteristic has change. So, such a kind of energy we will have such a kind of boundary we will have energy because of these kind of interface in the bonds; that means, the bonds are actually varying across the across these boundary to changed the chemistry.

So therefore, basically energy of this kind of system energy of this kind of what do I say this kind of structure of boundary structure will basically because of chemical type which is known as gamma chemical because bond type has changed across the boundary. So, disregarding the chemical species crystal interface can only be achieved if the listen carefully, if interfacial plane has a same automatic configuration the both phases and; that means, this requires the 2 crystals to be oriented relatively each other in a very special way. They has to be related in a very special way otherwise this kind of situation will not occur.

You know in a copper, silicon systems such a kind of thing happens silicon ridge phase which is called kappa, is basically having hexagonal crystal structure. On the other hand copper silicon phase has a FCC crystal structure. Whenever kappa phase which is silicon ridge for forms within this copper silicon FCC phase the interfaces arranging such way 1 1 1 plane a FCC is copper silicon will be parallel to 0 0 0 1 plane of a c p cup kappa phase. And this 2 planes it seems they are so nicely match they are this facings the devalue of the 1 1 1 planes in the copper silicon FCC phase. Exactly same as a devalue of 0 0 0 1 plane of a a c p kappa phase. And because of that there is a complete lattice registry; that means, the planes exactly follow on each other across the interface.

And that is why that is what I you say such a kind of configurations possible when 2 crystals are oriented related to each other in a very special way. You know this is you see this is what one situation another situation is saw in the right side that is known as b, where the planes are not parallel, but atomically matched. You see the planes in the alpha phase they are actually coming down from the top to bottom, but on other planes in the beta phase they are moving around angle would respect to the interface, but still the

satisfy all the bonds at the interface. So therefore, either such a kind of orientation I am saying only over 2 there may be some other possible.

Either is first type of orientation when planes across the boundaries are parallel to each other or the planes across the boundaries are actually at an angle to each other, but when the both the cases the certain planes has to be oriented parallel to each other. Then only this kind of coherency you can happen. So, coherency means that atomic planes must be satisfying the bonds across the interface. All the bonds then only coherency is possible. Otherwise coherency has no meaning. So, whatever in the situation whether a or b exist in the real crystal actually there and interfacial energy of the energy of the boundary basically coming from the chemicals say part of that.

There is no structural distortion the bonds there is nothing, because of the perfect lattice registry. So, because of that structural part of the interfacial energy is not is basically vanishingly 0 small. Only chemical part exist in such a kind of situations. Well, let me see what is next there.

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**Interface Coherence**

- At the interface, there is usually a change in composition so that each atom is partly bonded to wrong neighbors across the interface. This increases the energy of the interfacial atoms and leads to a chemical contribution to the interfacial energy ( $\gamma_{ch}$ ). For a coherent interface, this is the only contribution.

$$\gamma_{coherent} = \gamma_{ch} \quad (3.29)$$

In general, coherent interfacial energies range up to about  $200 \text{ mJ/m}^2$ .

- When the distance between the atoms in the interface is not identical, it is still possible to maintain coherency by straining one or both of the two lattices. The resultant lattice distortions are known as **coherency strains**.

Fig. 3.34 A coherent interface with slight mismatch leads to coherency strains in the adjoining lattices.

So, you know as the interface let us complete this part then we can move on to the next class about the in coherent and coherent semi coherent interfaces. At the interface there is usually change in composition, that is what I told you just now. Because atomics atom such changing from the white to the black. And So therefore, energies only because of

chemical energies of these boundaries are basically normally maximum up to 200 mille joules.

It can vary from actually 10 to 200 mille joules per meter square when the interface between the atoms is suppose we can have a situation interface the distance between the atoms in interfacial not identical. Suppose in the alpha phase distance is this much beta phase little bit higher. Still it is possible to maintain the coherency by straining one of the lattice. Like here you can see beta has been strain more than the alpha. So, basically atoms at influence on the both the interface has been strain little bit; that means, bonds has been distorted little bit on the both sides and this kind of distortion we always different as a coherency strain, same in order to maintain the coherency across the interface.

It is better for the system to distort the bonds than to live behind unsatisfied bonds. This always better and that is why such a kind of systems it do happens in specific (Refer Time: 25:06) may alloys such a kind of situation actually arises like aluminium copper system. You know such a such a kind of boundary you can exist and this boundaries also has a low energy, but not as well as 200 mille joule per meter square little bit higher than that. And in this situation the obviously, the gamma the total interfacial energy between the 2 boundaries basically, because of both chemical part as well as structural part and structural part is coming from the distortion of the bounds.

That is basically strain energy. The and this strain energies are basically normally may not be perfectly plastic may be is the elastic also. Whatever may situation strain energy we will do exist along this boundaries and these things to increase of the boundary energy. So, interface coherency actually see can be steel attained even if the lattice planes spacings are not matching perfectly on the interface. System will like try to attains such a kind of configuration inner to reduce the energy of the system, but in many cases it may not be possible ok.

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## Interface Coherence

• **Semicoherent interfaces**

- The strains associated with a coherent interface raise the total energy of the system, and for sufficiently large atomic misfit, or interfacial area, it becomes energetically more favorable to replace the coherent interface with a semicoherent interface in which the disregistry is periodically taken up by misfit dislocations.
- The matching in the interface is almost perfect except around the dislocation cores where the structure is highly distorted and the lattice planes are discontinuous.

- Definition of misfit ( $\delta$ ) between  $\alpha$  and  $\beta$  lattice.

$$\delta = \frac{d_\beta - d_\alpha}{d_\alpha} \quad (3.30)$$

$d_\alpha$ : interplanar spacing of matching plane in the  $\alpha$  phase,  
 $d_\beta$ : interplanar spacing of matching plane in the  $\beta$  phase.

Fig. 3.35 A semicoherent interface. The misfit parallel to the interface is accommodated by a series of edge dislocations.

So, that is what I am showing here. So, let us stop here. And will carry over the discussions over the interference coherence and the semi coherent and the inter coherent boundaries in the next lecture.