

Phase Transformation in Materials
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Lecture - 20
Interphase interfaces in solids (cont.)

So, we have seen in the last lecture how we can create lattice registry across the interface. And that is how we can create coherence and on the interface. But you know it is may not be always possible to maintain this lattice registry. If and if is that is mainly because the plane spacing along the interface may be varying too much, and this will lead to large you know difference to make spacing. And this can lead to a situation where it is no longer possible to maintain the coherency.

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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 (δ) between α and β lattice.

$$\delta = \frac{d_\beta - d_\alpha}{d_\alpha} \times 100\% \quad (3.30)$$

d_α : interplanar spacing of matching plane in the α phase,
 d_β : interplanar spacing of matching plane in the β phase.

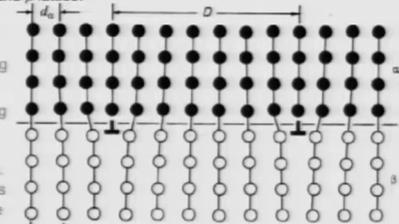


Fig. 3.35 A semicoherent interface. The misfit parallel to the interface is accommodated by a series of edge dislocations.

So, that is what I have written here strain is basically taken from the book (Refer Time: 00:50) strain associate with the coherent interface, will increase the interfacial energy system. But surface energy large misfit large misfit means sufficiently large variation of the inter planner spacing, it become energetically more favorable is become energetically more favorable to replace this coherent interface with semi coherent, in which lattice the registry is spiritically taken by the dislocations ok.

Basically what does it mean to say is that, suppose if we keep on increase these difference of the lattice you know planes I mean; so if the distance of the lattice planes

here and there in alpha and beta if we keep on increased that. After certain time it will may only it will be possible to maintain the interface coherency, but bonds we will get distorted too much. So, you can not actually accommodate so much of the strain in the distortion of the bonds is not possible. If the bonds are getting distorted too much along the at because the interface it is better for the system to actually create dislocations in the in another interface, A few dislocations.

So, that this distortion can be accommodated, other places a complete lattice registry can be maintained. So, that the distortion which is happening across the plane from left side to the right side for all the atomic planes and now reduced only to the dislocation course. That is the major difference which can happen. So, matching in the interface almost perfect, you see here this perfect here, perfect there, perfect there. A many places except dislocation course, where structure is distorted. So, instead of making the all the planes that could the interface distorted we are making only few places distorted. That is energetically more favorable. So, let us first described because we need to go into different formalisms, what do you mean misfit? Misfit is sophisticatedly coming from the difference of the inter laminar inter planar spacing.

So, as you see delta is always defined as a symbol for the misfit it is defined as $d_{\beta} - d_{\alpha}$ by d_{α} . So, d_{β} is the higher value; that means, spacing is higher for the beta and alpha. It can be other way also negative or positive both misfits are possible. So, d_{α} is inter planar spacing of the spacing of matching plane in the alpha phase and d_{β} is a same thing for corresponding that. If so, then we can defined delta as the misfit. And there is the always miss terms as a percentage. That is why you write 100, that is what is the way it is defined.

Now, how does it affect the boundary energy?

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Interface Coherence

- In one dimension, the lattice misfit can be completely accommodated without any long-range strain fields by a set of edge dislocations with a spacing D .

$$D = \frac{d_\beta}{\delta} \quad \delta = \frac{d_\beta - d_\alpha}{d_\alpha} \quad (3.31)$$

In other words, in a unit length, there are $1/d_\alpha$ and $1/d_\beta$ arrays of α and β respectively. Therefore, there are $(1/d_\alpha - 1/d_\beta)$ vacant arrays of β in a unit length, which is equal to the number of misfit dislocation in a unit length.

The spacing of edge dislocation equals to $1/(1/d_\alpha - 1/d_\beta)$

$$D = \left(\frac{1}{d_\alpha} - \frac{1}{d_\beta} \right)^{-1} = \left(\frac{d_\beta - d_\alpha}{d_\alpha d_\beta} \right)^{-1} = \frac{d_\alpha d_\beta}{d_\beta - d_\alpha} = \frac{d_\beta}{\delta}$$

- For small δ

$$d_\alpha \approx d_\beta$$

$$\Rightarrow d_\beta \approx \frac{d_\alpha + d_\beta}{2} = b$$

b : Burgers vector of the dislocations.

$$D \approx \frac{b}{\delta} \quad (3.32)$$

In one dimensional lattice space it is completely accommodated with without any no longer long range strain field by set of dislocations. And the dislocation; obviously, has to be accommodated this basically looks like a low angle grain boundary where lot of dislocations. And the spacing between dislocation is defined by d_β by δ where δ is the misfit. So, as the d_β increases that mean distance between the difference between the 2 α and β planes, spacings increases this d will becomes smaller.

In other what is an unit length there are 1 by the d_α and 1 by D_β arise of α β respectively dislocations. So there are 1 by D_α minus 1 by D_β we can arise of arise of β in the unit cell is equal to the number of misfit dislocation in unit cell. Well what does it say? See d is nothing but what if you put down d what is become. You can clearly see d is 1 by α minus 1 by D_β basically d is like this, 1 by α minus 1 by D_β . Now if I do the mathematics properly I do get d_β by δ . So, when δ is small that is misfit is very small, then d_α will d_β .

So therefore, the then is d_β become burger vector. So, that is why when misfit is very small you know that is you need only one or 2 dislocations to along the boundaries to a crates as a kind of interfaces. And then energy of the boundaries (Refer Time: 05:28) and higher than the coherent boundaries, but not much. That is what happen when we have this (Refer Time: 05:36) where this misfit is so, small that either one or few dislocation

enough to create such a kind of boundaries. And these actually are you know there is stable boundaries.

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Interface Coherence

- In practice, misfit usually exists in two dimensions and the coherent strain fields can be completely relieved if the interface contains two non-parallel sets of dislocations with spacings $D_1 = b/\delta_1$ and $D_2 = b/\delta_2$.
- If the dislocation spacing is greater than b/δ (3.32), the coherency strains will have been only partially relieved by the misfit dislocations and the residual long-range strain fields will still be present.
- Interfacial energy of a semicoherent interface
It can be considered as the sum of 2 parts: (a) a chemical contribution, γ_{ch} , as for a fully coherent interface, and (b) a structure term γ_{st} which is the extra energy due to the structural distortions caused by the misfit dislocations.

Fig. 3.36 Misfit in 2 directions (δ_1 and δ_2) can be accommodated by a cross-grid of edge dislocations with spacings $D_1 = b_1/\delta_1$ and $D_2 = b_2/\delta_2$.

$$\gamma_{\text{semicoherent}} = \gamma_{\text{ch}} + \gamma_{\text{st}} \quad (3.33)$$

- For small values of δ , the structural contribution to the interfacial energy is approximately proportional to the density of dislocations in the interface.

$$\gamma_{\text{st}} \propto \frac{1}{D} \propto \delta \quad (D = b/\delta) \quad (3.34)$$

Well, I am talking about only one dimension right. Only along one directions, but crystals are not they are (Refer Time: 05:58) dimensions.

So, let us talk about only 2 d what happens; in the practice actually misfit actually existing 2 dimensions or in 3 dimensions. In some cases, but for the sake of understanding let us assume is speech some only existing along 2 dimension. And along one dimension z axis let us suppose let us no misfit is perfect match is a coherency. So, the coherency strain field can be comparably reliefs if you have then you to you want to relief that we need 2 sets of dislocations. One set of dislocation along the x axis other sets (Refer Time: 06:28) and the y axis, that is what you shown here in you see there is this there this is along x this is along y ok.

That is what is shown sorry this is along x, now this is along y that is shown delta 1 and delta 2, because both the directions I will be lattice planes may not be perfectly matching the misfits. And therefore, based of the misfits we need to sets of dislocations. The movement of dislocations spacing is more than beta b is basically burger factor of the dislocation, by delta the coherence system will have see been only perceives relief by the misfit dislocations. And there will be residual stands residual stand did mainly because of the distorted bonds. Because it is more than v further vector by delta if this dislocation,

spacing still some bonds which little bit shown here I can go back here. This although with these dislocations are created relieve the strain, but still there are few bonds like this one, this one, along the core of the dislocation of this one, they are having distortion.

All though dislocations are existing only in 2 places, but the bonds are still some bonds are still distorted. This can only happen when the spacing between the between the dislocation between these dislocations basically more than burger vector b by δ . So therefore, interfacial energy of semi coherent interface will have 2 parts, right. One part is chemical contribution that we have seen for the co interface that see defines of the atoms in the across the plane. On the beta side you have one kind of atom white atoms on the alpha side of a black atom. So, that is leads to chemical part second part is known as structural plot what is given as γ_s , which is the extra energy due to structural distortion cross by the misfit dislocations.

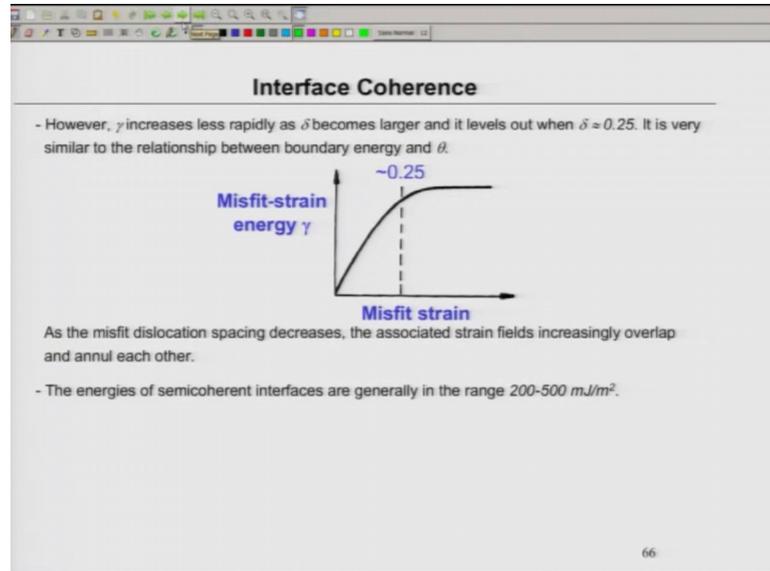
So, chemical semi coherent in a interface we will have chemical part and the structural part. Now chemical part is; obviously, because of the change of the bonds type. A b bond has being is the mone main bonds across the interface, but a structural type structural part which is these γ_s , the small value of δ that misfit the structural contribution to the interfacial approximately proportional to the number of dislocation or density of dislocations; obviously, more number of dislocation more is the dislocation course and more is the energy of the structural part. So, that is basically understandable.

Therefore I have written here γ_s the structural part is proportional to $1/D$, $1/D$ is the difference distance between the 2 set to dislocations or is basically proportional to δ , because $1/D$ is proportional δ because these proportional to $1/\delta$ d is equal to b/δ . So therefore, D is proportional δ . So therefore, more is the distortion more is the structural part. That is understandable clearly, because the δ is the misfits more is this difference between the inter planar spacing of alpha and beta more is number of dislocations are required. But you can also have semi coherence and interface along the $3 \times y \times z$. Then you need another set of dislocations along z axis also.

So, the more number of dislocation along the 3 axis says more is the energy of the system that is the structural plot of the of the interface energy will increase, as you have such a kind of situations. But in metallurgical system normally coherence is perfectly

mention along one of the axis other x y z, and other 2 axis can semi coherent or it can be completely incoherent.

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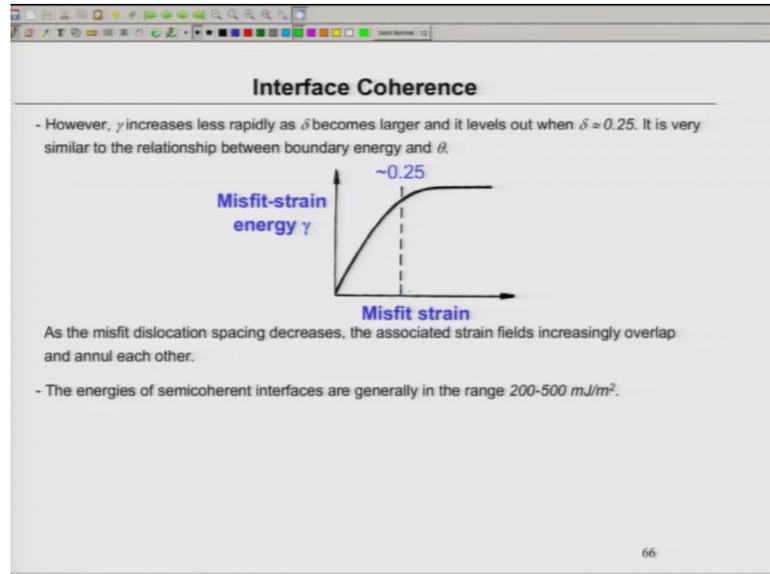
So therefore, I can actually do a little bit of maths, this is basically coming from literature or whatever; understanding of their measurement of the energies or calculations. You know gamma actually when the misfits are increases gamma and increases rapidly.

As you see here that because you are creating dislocation in one side, other thing your create making this some of the planes atomic plane bonds distorted. But it is has been seen that when the delta, delta has a critical value which is known as which is about 0.25, when these reaches then the misfit energy there part becomes. Constant no if does not increase further well the misfit dislocation as the misfit dislocation decreases associates strain field, that is mainly because again from coming from the lower can grain boundary discussion. As you create more number of misfit dislocations are the chrisom is misfit dislocation distances, after some you know increase the number of dislocations they are strain field start overlap. And the moment will stain fully star overlap what will happen?

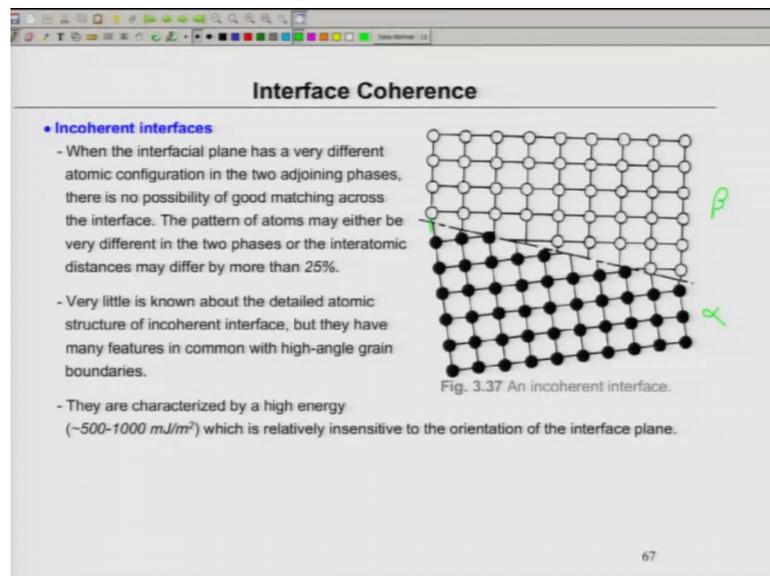
Negative and positive strain field may cancel each other. And these can lead to labelling of the misfits energies. So, that is what you see the misfits strain is about 25 percent is 1 to 5 sorry 2.5 percentage is not 25, 2.5 percent is the misfit strain is what is 2 phase

normally does the interface misfit energy increases after which it becomes constant. Energy of a semi coherent interface is normally 200 to 500 mJ/m².

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Now, let us discuss of this third case which is known as incoherent interface. We have coherent we have seen semi coherent what is see in coherent interface when the interfacial plane has a very different atomic configuration the 2 adjacent phases. Different complete different atomic configuration existing between the adjusting phases, and there is no possibility of good matching. Is impossibly do that and such a kind of

pattern of atom can either be very different in both the phases or it is possible that interact with distances, may differ more than 25 percent.

One so, is shown such a kind of thing you see here the atomic as when is atomic configuration in both the phase's alpha and beta, this is beta and this is alpha, is such that there is no we can match deep atomic planes. There is a little match here, but slowly with the matching has done completely out of the way. So therefore, the all almost most of the atoms across the interface not satisfied by the other side of the crystal, other side of the phase. So, alpha atoms that is black atoms or not at all forming any bonds across the interface, so that is why (Refer Time: 13:08) interfaces actually call incoherent interface, because there is no lattice registry at all we can think about it.

Please try to understand there is very little has been this research on such a kind of interfaces, we know the such a kind of interface do exist, but little atomic structure of these things are not know it. And they will very high energy about 500 to thousand mille joule per meter square, which is important thing is that that is insensitive to the orientation. It does not matter what is the orientation energy will remain constant same. We have seen that depending on the orientation of the crystals, as show the phases across the boundary in both in coherent and semi coherent the energy can vary, but here that is not the case. Is just like a high angle grain boundary, high angle grain boundary also energy of the boundary it does not matter what is the orientation of the crystals across the boundary.

Same thing happens here also. Now upon give you some idea.

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Interface Coherence

- **Complex semicoherent interfaces**
 - Semicoherent interfaces can also form between phases when good lattice matching is not initially obvious.
 - Example: $(111)_{fcc}$ and $(110)_{bcc}$ Nishiyama-Wasserman (N-W) relationship
 - relationship
 - $(110)_{fcc} // (111)_{bcc}$
 - $[001]_{fcc} // [\bar{1}01]_{bcc}$
 - Kurdjumov-Sachs (K-S) relationship
 - $(110)_{fcc} // (111)_{bcc}$
 - $[\bar{1}\bar{1}\bar{1}]_{fcc} // [\bar{1}0\bar{1}]_{bcc}$

The only difference between these two is a rotation in the close-packed planes of 5.26° .

- A coherent or semicoherent interface between the two phases is impossible for large interfaces parallel to $(111)_{fcc}$ and $(110)_{bcc}$. Such interfaces would be incoherent.

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Fig. 3.38 Atomic matching across a $(111)_{fcc}/(110)_{bcc}$ interface bearing the NW orientation relationship for lattice parameters closely corresponding to the case of fcc and bcc iron.

Let me talk about very special cases semi coherent interfaces. As you see it to have a semi coherent phase you need to have certain kind of a orient you know atomic planes across the interface between the 2 phases must have certain kind of a arrangements. But you know semi coherent interface can also form between phases when good lattice matching is not initially obvious. That is these are the system who existing in metallurgical systems. Let me give an example. Let us talk about you know in a iron steel FCC is a gamma phase gamma iron gamma solid solution of carbon in gamma FCC iron, and this BCC is suppose alpha ok.

So, 1 1 1 of FCC is a closest pack plane, but 1 1 0 is not a closest pack plane BCC. But there is a orientation relationship in which has been given by long back magnesium and washer man, that says that 1 1 0 plane of BCC will be parallel to 1 1 1 plane of BCC. Whenever such a planes will parallel across the interface that has to be one direction which will also parallel otherwise it is not possible to dictate exact orient relationship. So, in 1 1 0 0 1 directions in contained in the 1 1 0 BCC structure is also parallel to 1 bar 0 1 or a contained in the 1 1 1 FCC plane. Or it can be that the first relationship is maintained like in kurdjumov and sachs relationship which is k s type, but the planes the directions containing in the both the planes parallel in these case are different.

Here actually 1 1 bar 1 in the BCC is parallel to 0 1 bar 1 plane in FCC. The only different between these 2 is rotation. You try to understand these are (Refer Time: 16:03)

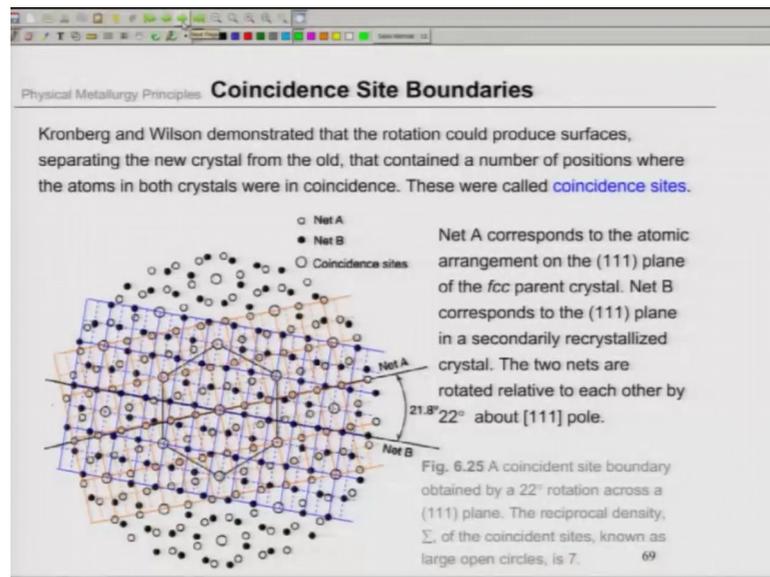
difference between these 2 you know in both the cases actually difference between the both cases basically at the closest pack planes actually (Refer Time: 16:12) about 25.26 degree celcius let me explain to carefully, if you look at carefully here this is 1 1 1 plane of BCC. This is 1 this is 1 1 0 plane of FCC. This difference between these 2 orientation is about actually about 5 5 degrees. That means, I can I say super impose atom, in the FCC crystal with the BCC crystal in such way that the directions will be only where it little bit; that means, atoms are there existing across the plane, but directions are about at an angle. If they are falling on each other then it was a perfect match, but in such a case which is not possible because of the atomic planes and such orientated.

So, only possibility that to create a semi coherent interface here is to have a little bit of angular distortion between the directions in the FCC and the BCC crystals. So, they are naturally not parallel. Exactly specifically telling they are parallel in such way, but there are actually in one direction other direction that will angular relationship. So, at the because of that you see here that the here if some reasons some reasons they atomically planes are not matched. Here you see here not matched the, but here they are matching. There actually we are looking from the top. If you look from the top across the interface the wherever the black and white atoms are falling in each other; that means, they are perfectly registered perfectly at a at an and bonding each other perfectly there is no distortion much.

Wherever they are falling apart; that means, in this place or in this place there falling apart; that means, they are not matching each other there is a dis gap between the 2 planes. So, even after angularly distorted, angularly distorting the directions of the plane where 5 degrees it is not possible to have a perfect match of the atoms platinum planes, across the interface. Some places atoms that mean planes will match some places there will not match, but still it is better than a complete incoherency. In incomplete incoherency there will be no match at all, we have seen that. Compare to that this is much better situation energy can be still lower that is why they are said complex semi coherent interfaces, the special diagram.

A coherent semi coherent between the 2 bound phases is impossible for large interfaces parallel to 1 1 1 in FCC and 1 1 0 FCC such interfaces will be a; obviously, incoherent if the distances are very large ok.

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Now, there is another important concepts let me just another few minutes I will just introduce the concepts, and this is basically coming from book of radial physical metallurgy principle robert radial. You know, this concepts actually known as coinciding sites boundaries. Long back both kronberg and Wilson actually did. So, that the (Refer time: 19:16) can produce surfaces. Separating the new crystal from the old that contain the number of positions where atom in both crystal were coincidence. Let me just go back here.

The reason I what up these concepts in these case both n w and k s relationship is basically that, even in this atomic you know this atomic distribution or atomic configuration some places atomic places are matching some places there not matching. So, wherever these atomic planes are matching, they are means they are atomic bonds actually coinciding. Wherever they are not they are falling apart they are not coinciding each other. That is exactly is the idea of kronberg and Wilson. They said that rotation can produce surfaces separating the new crystal from the old or maybe 2 phases that contain a number positions where atoms in the both crystals will coincide. But so other places they will not coincide.

And these positions are no known as coincidence sites. The kind of lattice we create is known as coincidence site lattice. Net A I do not know whether you can see net A correspond to, correspond to white atoms and net B correspond to black atoms. Here say

net A correspond the atomic as man. So, on 1 1 1 plane So, FCC 1 1 1 a plane in FCC, are actually you see there are (Refer Time: 20:38) oriented, if you carefully look at it. And net B also corresponding to 1 1 1 plane in a secondary re crystallized crystal out of FCC. I do not know no the now you have no idea will crystallization, but let us suppose something has formed from the crystal a you know first FCC parent crystal. These 2 nets are rotated related to each other by 22 degrees.

Across 1 1 1 directions; that means, if I 2 nets one net other net like this I rotate by 22 degrees one net respect to the other along one of the axis. And let us suppose if the axis the body is diagonal of the FCC (Refer Time: 21:21) is along 1 1 1. So, if I rotate along 1 1 1 one of the this you know nets then I can bring some of this planes some of the atoms coinciding with the parent crystal. That is what is known as coincidence site lattice. So, I can actually rotate in certain angles this angles are will be you know will be particular values, you can rotate along certain all angles I will be certain angles in which you can rotate one of the lattice planes with respect to the other lattice plane in a certain axis, and bring this kind of coincidence. This is possible actually in many many is cases.

And whenever when I do that I create special boundaries in there will be cases which I will show the next class the boundaries will be perfectly matching atomic registry will be perfect. And obviously, because of that energy of this boundary should be lower. The basic idea is that I can rotate the one plane respect to other. Just like you see in n s and k s type of relationship as I discussed in the last slide, where the 5.2 60 rotations of the 1 1 1 you know the planes along 1 1 along 1 1 1 directions it can lead to certain kind of match of the lattice planes in certain positions. So, that leads to (Refer Time: 22:43) of the interfacial energy. This is possible to extent this idea can be possible to extent to further to create different kind of boundaries. And these boundaries are also known as coincidence site boundaries or special boundaries.

Let me stop here because these concepts are actually very difficult, and in the next class we will talk about how we can create such a kind of boundaries and how can actually you can discuss about the different relationships in the next lecture. I fact, in next 2 lectures, I am going to complete rewind of interfaces and start discussing about real phase transformations afterwards.