Phase Transformation in Materials
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Lecture - 21
CSL boundaries

Students we have been continuing our discussion on interfaces. And I am going to wind up today with few examples of different kind of interfaces. So, last thing which I started in the discussion in the previous class was coincidence side boundaries. As you know I have shown you that it is possible to have some lattice points of both the crystals, in a inter phase interface type interfaces to match if not all of them. And one such concepts is coincidence side boundaries. To given example that I start in the last class here I am showing you 2 units.

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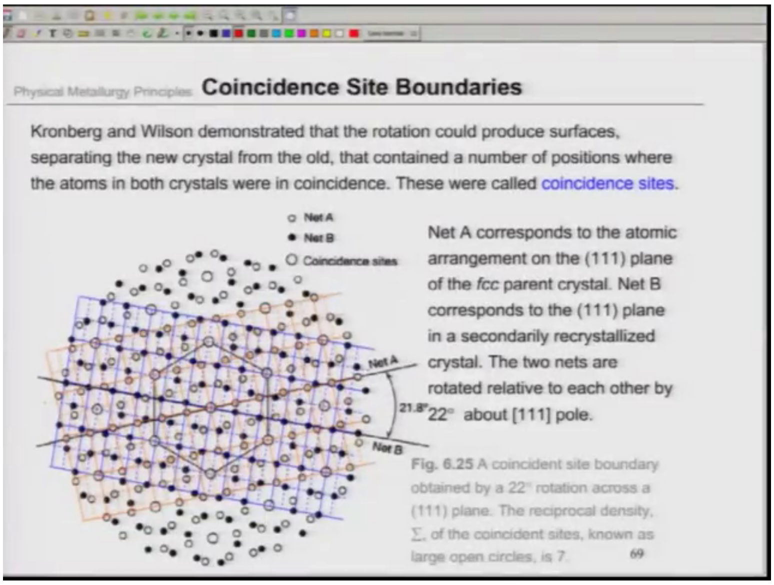

Physical Metallurgy Principles **Coincidence Site Boundaries**

Kronberg and Wilson demonstrated that the rotation could produce surfaces, separating the new crystal from the old, that contained a number of positions where the atoms in both crystals were in coincidence. These were called coincidence sites.

Net A corresponds to the atomic arrangement on the (111) plane of the *fcc* parent crystal. Net B corresponds to the (111) plane in a secondarily recrystallized crystal. The two nets are rotated relative to each other by 22° about [111] pole.

Fig. 6.25 A coincident site boundary obtained by a 22° rotation across a (111) plane. The reciprocal density, Σ, of the coincident sites, known as large open circles, is 7.

One corresponding to the small white circles you see here this are this small white circles, other one correspondence to the black dots. Now it is possible to align these 2 nets falling on each other by giving a rotation, around certain axis. And this big white blobs actually corresponding to the coincidence lattice you see here these are the white blobs. So, finally, it is possible to generate are make 2 lattices some points of the lattices fall on each other by rotation of the net B with respect to the net A by 21.8 degrees Celsius that is about 22 degree Celsius by one axis of the net A.

So, this is what is known as coincidence lattice; that means, what we have basically doing here is that if I have 2 different crystals side by side, we can have the bonds formats form between the atoms of the 2 crystals by rotating the one of the lattice with respect to the a major axis of crop crystals by certain amount by certain degrees or rotation. If In fact, this rotation is basically done to coincide this points or the atoms sitting on each other. So, the they can from bonds, but not all that comes actually is for only for certain number of atoms these kind of coincidence possible; obviously, if all the atoms are actually following on each other this will be a complete coherence interface.

Or even some atoms are falling on each other and some dislocations will be semi coherent type of interface, but we can actually generate basically semi coherent type of interfaces which is not exactly semi coherent, but partially semi coherent type of interfaces by doing such a kind of simple rotation of the crystal lattices. So, in this detailed grad actually you know there are few things which was governed in the literature and one of the important thing of coinciding lattices is the fraction of atom in coincidence at a boundary is always known as the density of the coincidence sides correct. Basically of all the atoms are not actually coincidence with each other along the boundaries.

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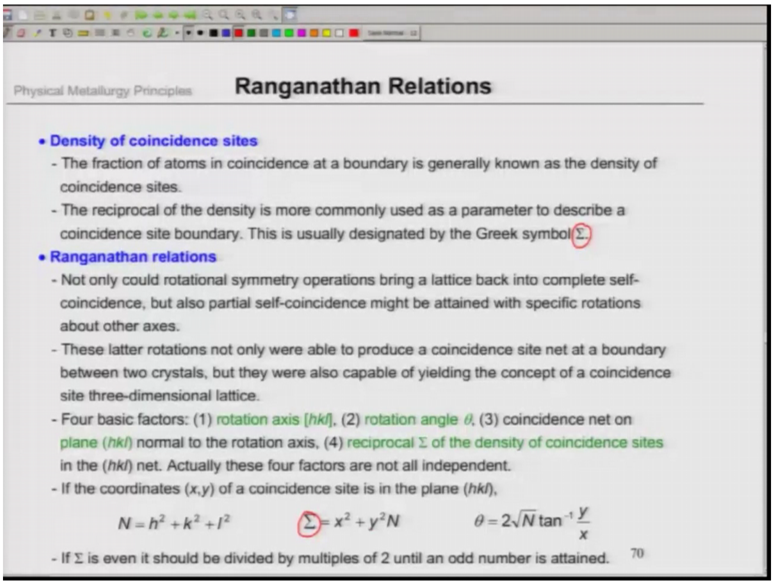

Ranganathan Relations

- **Density of coincidence sites**
  - The fraction of atoms in coincidence at a boundary is generally known as the density of coincidence sites.
  - The reciprocal of the density is more commonly used as a parameter to describe a coincidence site boundary. This is usually designated by the Greek symbol Σ.
- **Ranganathan relations**
  - Not only could rotational symmetry operations bring a lattice back into complete self-coincidence, but also partial self-coincidence might be attained with specific rotations about other axes.
  - These latter rotations not only were able to produce a coincidence site net at a boundary between two crystals, but they were also capable of yielding the concept of a coincidence site three-dimensional lattice.
  - Four basic factors: (1) rotation axis [*hkl*], (2) rotation angle θ, (3) coincidence net on plane (*hkl*) normal to the rotation axis, (4) reciprocal Σ of the density of coincidence sites in the (*hkl*) net. Actually these four factors are not all independent.
  - If the coordinates (*x*,*y*) of a coincidence site is in the plane (*hkl*),

$$N = h^2 + k^2 + l^2 \qquad \Sigma = x^2 + y^2 N \qquad \theta = 2\sqrt{N}\tan^{-1}\frac{y}{x}$$

  - If Σ is even it should be divided by multiples of 2 until an odd number is attained.

So, therefore, we have to consider the important factor that is the fraction of atoms which should coinciding with each other on the boundary.

In fact, we do not take into that consider, we take into considers reciprocal of the density and reciprocal of the density is usually consider as a parameter to describe the coincidence sides boundary. And the reciprocal is basically did designated by a letter called Greek letter called given here like this, this is summations. Now that is basically tells you how many of lattices are actually falling on each other. In this regard one of my teacher has actually extensively worked on in his young days and he gave pure relationships which are valid. This can be obtained and forget is given in the books how this can be obtained relationships are not you know very difficult.

Not only could the rotational symmetries operations which we have done in the last slides, can bring by the lattice with some kind of a self-coincidence, but partial self-coincidence also can be attained with specific rotations along the about other axes. That is what I have being telling about it partial coincidence is always possible. These latter rotations are not only able to produce coincidence side nets at a boundary between 2 crystal, but also their capable of building concept of coincidence side 3 dimensional lattice; obviously, in 3 d if these points are matching some of them not all of them or productions of them then we can call then as a different type of 3 dimensional coincidence lattice.

So, there are 4 factors which are responsible for making these coincident possible. One is the; obviously, the rotation axis along which we are rotating that one crystal lattice just rather. Second one is the angle that I have already discussed. Third one is the coincident net on the plane h k l normal to the axis; these obvious because if I have a one axis whether the coincidence plane is 1 1 1or some other plane that will dictate what kind of things. And obviously, the important parameter which I have just now told you is the rotational reciprocal of the density that is see important aspects. So in fact, all these 4 parameters are not independent.

Mathematically it can be shown that this all this 4 parameters are related suppose if I define the coordinates of a coincidence lattice in h scale plane any coordinate of a point and the h scale plane, as a you know n is h square plus k square plus l square then sigma oh sorry not sigma. This is this is one kind of a one kind of a summation term is equal to x square plus y square n and angle is 2 root n tan inverse y by x. Therefore, we can actually relate you can see that if I know n n can can be a easily related because n is nothing but the plane or the directions in a cubic lattice, they are there are similar same and x and y basically your coordinates on which this coincidence lattice will happen they are related to each other.

So, by doing this by actually by using these relationships, we can actually generate even kind of sigma boundaries different kind of boundaries. Sigma 9 and sigma 27 or sigma even other boundaries also possible to generated. Sigma this boundaries whichever the coincidence thing happens is basically some of the twin boundaries nowadays called.

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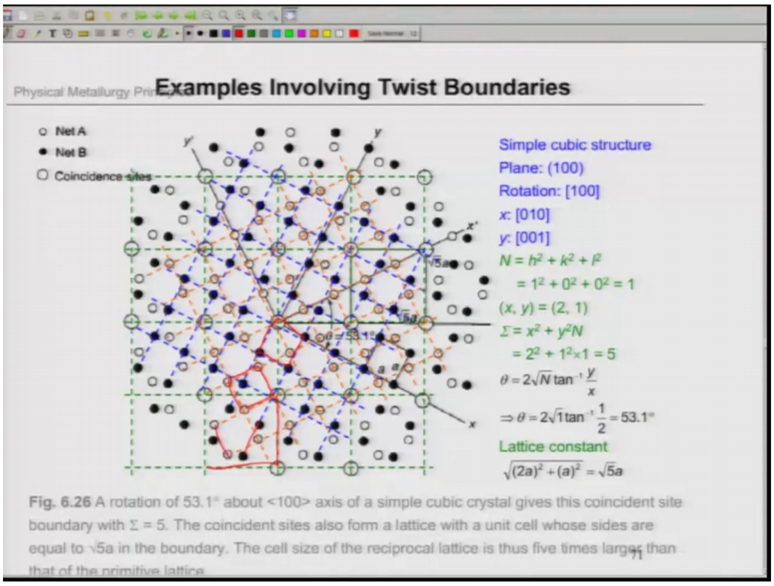

Examples Involving Twist Boundaries

Simple cubic structure

Plane: (100)

Rotation: [100]

x: [010]

y: [001]

$N = h^2 + k^2 + l^2$

$= 1^2 + 0^2 + 0^2 = 1$

$(x, y) = (2, 1)$

$\Sigma = x^2 + y^2 N$

$= 2^2 + 1^2 \times 1 = 5$

$\theta = 2\sqrt{N}\tan^{-1}\frac{y}{x}$

$\Rightarrow \theta = 2\sqrt{1}\tan^{-1}\frac{1}{2} = 53.1°$

Lattice constant

$\sqrt{(2a)^2 + (a)^2} = \sqrt{5}a$

Fig. 6.26 A rotation of 53.1° about <100> axis of a simple cubic crystal gives this coincident site boundary with Σ = 5. The coincident sites also form a lattice with a unit cell whose sides are equal to √5a in the boundary. The cell size of the reciprocal lattice is thus five times larger than that of the primitive lattice

Fine example of a twist boundary; so let us give a example of relations how relationship can be used. First look at the right side you know if I consider simple cubic structure and consider 1 o o plane and axis is perpendicular that there is 1 0 0 plane 1 0 is the axis and x and y; obviously, will be x axis and z axis here that is a 0 1 0 y axis and 0 axis, there will given little bit different way.

You can actually define x and y depending on a reuses, but there has to be permitted to the plain one o o o that is what is 0 1 0 and 0 0 1, that must be permitted to this plane. Now n square is nothing but a square plus k square pus l square that is is equal to 1 and suppose x and y is 2 comma, one that is see coincidence point coordinate of the coincidence point. So, therefore, sigma is basically 5 and theta is basically 53.1 . So, if I rotate 53.1 degree one, degree one of the net will respect to the other. Then I will get a sigma 5 boundary that is what it says if it is the simple cubic structure.

So that is the known a rotation of 53.1 degrees about 1 0 0 axis of a simple cubic lattice gives the coincidence side boundary of sigma 5. This both sides also form a lattice with this unit cell who sides actually root 5 a or the boundary the cell size of the (Refer Time: 08:06) lattice is a 5 tends (Refer Time: 08:11) primitive lattice. Let us see here net A is basically small y dots you see here small y dots and net B is small black dots. And now the net B is rotated respect to the net A by 53.1 degrees. Therefore, they come in coincidence with each other some of them points and this gives you these black the white big blobs where the coincidence such happened.

You can clearly see this is this was the unit cell of A atom and this was the unit cell of B atoms; the black ones. So compare to that unit cell of these new is 5 root 5 times bigger. That is what is happen that is can be calculate easily because as you know this distance I know. So, therefore, we can calculate this distance I know we can easily calculate the values of that and A. We can actually generate different kinds of boundaries by using such as say these formulae. And this is widely used in the literature noun. So, this is basically special boundary let me tell you this boundaries do not exist in all crystals.

So, therefore, these boundaries are very special and they can be actually generated by using different options in the crystal structure.

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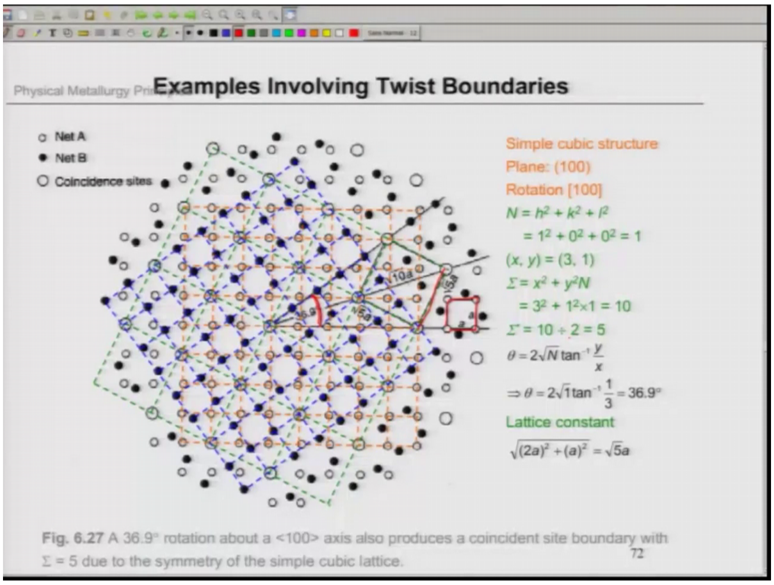

Examples Involving Twist Boundaries

Simple cubic structure

Plane: (100)

Rotation [100]

$N = h^2 + k^2 + l^2$

$= 1^2 + 0^2 + 0^2 = 1$

$(x, y) = (3, 1)$

$\Sigma = x^2 + y^2 N$

$= 3^2 + 1^2 \times 1 = 10$

$\Sigma = 10 \div 2 = 5$

$\theta = 2\sqrt{N} \tan^{-1} \frac{y}{x}$

$\Rightarrow \theta = 2\sqrt{1} \tan^{-1} \frac{1}{3} = 36.9°$

Lattice constant

$\sqrt{(2a)^2 + (a)^2} = \sqrt{5}a$

Fig. 6.27 A 36.9° rotation about a <100> axis also produces a coincident site boundary with $\Sigma = 5$ due to the symmetry of the simple cubic lattice.

72

Now, another one this is actually of a another twist boundary, where again the plane the same and now this is the exactly same no this is different. So, x plane is same rotation x is 1 0 0. And if suppose coincidence point coordinate of this 3 comma 1, then what happen this place becomes sigma become 10. In fact, 10 and 5 they are not much difference is only actually the lattice parameter will be divided the points will be divided by number of points will be less in 5 by half the coincidence points. And the angular rotations are will be exactly 36.9 degrees.

So, if I if I actually rotate 36.9 degrees of the cubic axis we can also generate a sigma 5 boundary where the coincidence points will be similar to that what I have shown you in this case also it is easily seen 36.8 is what is the rotation axis required a cubic crystals to do that and here. You see a unit cell things are shown it is it is root 5 a easy distance of the new lattice parameter fine.

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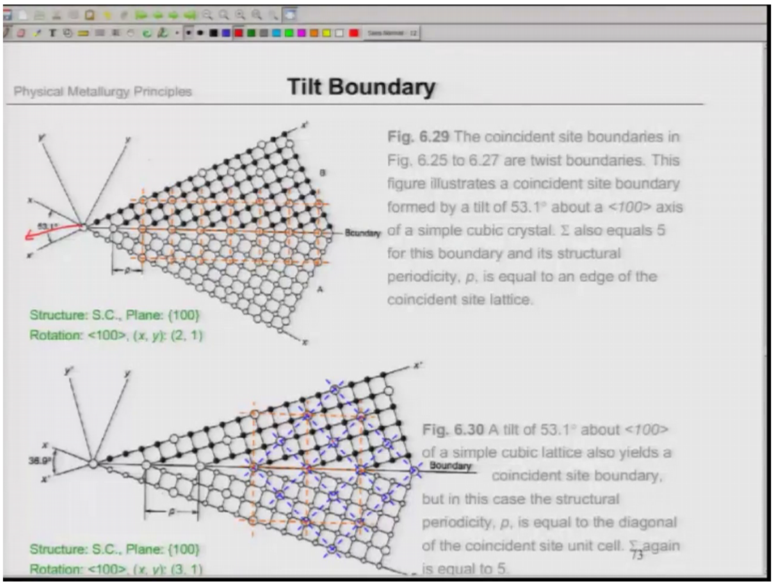

Physical Metallurgy Principles

Tilt Boundary

Fig. 6.29 The coincident site boundaries in Fig. 6.25 to 6.27 are twist boundaries. This figure illustrates a coincident site boundary formed by a tilt of 53.1° about a *<100>* axis of a simple cubic crystal. Σ also equals 5 for this boundary and its structural periodicity, *p*, is equal to an edge of the coincident site lattice.

Structure: S.C., Plane: {100}
Rotation: <100>, (*x*, *y*): (2, 1)

Fig. 6.30 A tilt of 53.1° about *<100>* of a simple cubic lattice also yields a coincident site boundary, but in this case the structural periodicity, *p*, is equal to the diagonal of the coincident site unit cell. Σ again is equal to 5.

Structure: S.C., Plane: {100}
Rotation: <100>, (*x*, *y*): (3, 1)

So, actually in this way we can actually make tilt boundaries or twist boundaries depending on that. You can see here it is much clear here much clear here if I have 2 2 lattices one shown there one shown this is the top A and B type and you want to have a coincidence of the atoms, we can tilled say a or actually we are tilt a here respect to B respect to these axis these axis by 53.1 degree Celsius.

Then, these are the points on which the lattice of a will be falling on lattice of points of B. Other points it will not fall. So, therefore, there will be fraction of slides on which sides in the lattice of a lattice of B actually will be forming bonds with the atoms of a other sides it is not form bond element angling or there will be answer is 5. So, by that way we can actually create a simple steel boundary which is known as coincidence science steel boundary.

Again same thing has shown it is a much detailed way how the coincidence sides forms you can actually rotates 36.9 degrees and create another type of sigma 5 boundary tilt boundary 36 of 5 will lead to at A angular. You can see here this points are at an angular shape angle with respect to the B lattice not exactly following on the B lattice right in the case of in the first case where the rotation of 53.1 degree Celsius.

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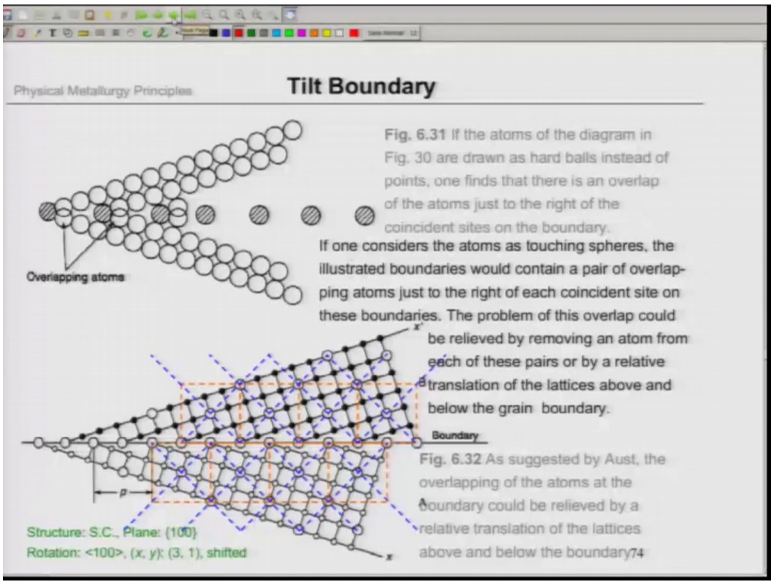

Physical Metallurgy Principles

Tilt Boundary

Fig. 6.31 If the atoms of the diagram in Fig. 30 are drawn as hard balls instead of points, one finds that there is an overlap of the atoms just to the right of the coincident sites on the boundary.

If one considers the atoms as touching spheres, the illustrated boundaries would contain a pair of overlapping atoms just to the right of each coincident site on these boundaries. The problem of this overlap could be relieved by removing an atom from each of these pairs or by a relative translation of the lattices above and below the grain boundary.

Fig. 6.32 As suggested by Aust, the overlapping of the atoms at the boundary could be relieved by a relative translation of the lattices above and below the boundary

Structure: S.C., Plane: {100}
Rotation: <100>, (x, y): (3, 1), shifted

Last one I like to say you that, you know if one can say atoms as touching fair the illustrated boundaries should contained only pair of over lapping atom just to the writes of the each coincidence lies side slides on this boundaries. And the problem of this overlap could be relieve a reviving one atom from each of these pairs or by a relative translation of the lattices about the below the grain boundaries. That is what is shown here. We can actually instead of coincidence this are these actually sitting one each. So, nstead of coincidence we can actually move these points, this one here or this one there like that way or this one there or this one here and crate a boundary that is also possible.

So, there are many such option exist you need not go into details of that if you are really interested to creates such a kind of boundaries you can look at this atomic constructions along 1 o o this is along one one a simple cubic and do this kinds different of different options can be generated, and these all done actually in the literature.

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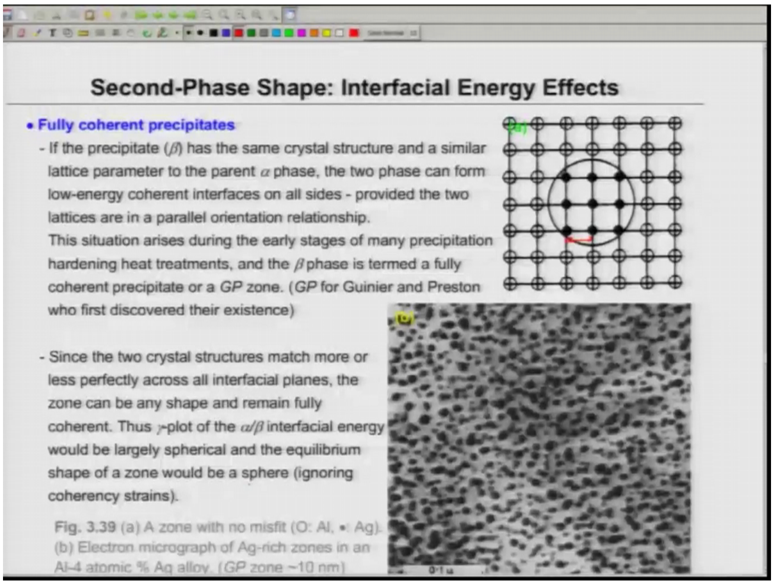

Second-Phase Shape: Interfacial Energy Effects

- **Fully coherent precipitates**
  - If the precipitate (β) has the same crystal structure and a similar lattice parameter to the parent α phase, the two phase can form low-energy coherent interfaces on all sides - provided the two lattices are in a parallel orientation relationship. This situation arises during the early stages of many precipitation hardening heat treatments, and the β phase is termed a fully coherent precipitate or a *GP* zone. (*GP* for Guinier and Preston who first discovered their existence)
  - Since the two crystal structures match more or less perfectly across all interfacial planes, the zone can be any shape and remain fully coherent. Thus γ-plot of the α/β interfacial energy would be largely spherical and the equilibrium shape of a zone would be a sphere (ignoring coherency strains).

Fig. 3.39 (a) A zone with no misfit (O: Al, •: Ag). (b) Electron micrograph of Ag-rich zones in an Al-4 atomic % Ag alloy. (*GP* zone ~10 nm)

So, now after discussing about different boundaries, let me tell you that this boundaries actually dictate the interfacial energies. What type of boundaries that is a coherent incoherent semi coherent special semi coherent boundary or it depends it dictates actually interfacial energy?

So, by interfacial energy dictates these shapes of the second phase. Now in a fully coherent precipitates, what will happen? This is what you shown here. You see here this white atoms are actually the atoms of the matrix and the black atom actually precipitates phase let us suppose. And the way they are forming that there is a exact coincidence of the points or the atoms sitting on each other. And not only that it seems the inter laminar inter planes facing of the black atoms is same as that of the white atom white atoms.

So, because of that the interface created by this kind of matching is basically coherent fully coherent precipitates. And if you know the precipitate has the same crystal structure and similar lattice parameter that can happen. In; that means, what energetically the all the along the all the surfaces the precipitate and the matrix has the coherent interface and they have a very specific orientation relationships, crystal of a planes has to match on each other each of these precipitate on the matrix. Situation happens in real situation actually happen in case of aluminum, copper alloy. So, aluminium nothing silver, aluminium, silver alloys also when the precipitates actually start to from at the beginning and these actually known as we will discuss in detail known as guinier preston zones g p zones.

G p zones actually are it is solid atoms sitting on a matrix surface few layers of solid atoms. They have not here from the precipitates which will discuss in detail manner when you talk about the second phase precipitates from the matrix. You see here in that cases shape of the precipitate can be anything it basically to it is spherical because there is no you know preferential interfacial energy change along any of the interfaces. So, this must be a spherical precipitate. So, gamma plot of the alpha beta interface will be largely spherical and equilibriums shape of the zone could be a sphere

Obviously, when we are doing that we are assuming there is no coherency strain. What is the meaning of coherency strain where assuming that the bonds actually are straight between A and B atoms between the black and white atoms that is may not be the case because atomic sizes of silver and co aluminum may be different? So, therefore, the bonds may not be exactly of the integrally state when they are following on each other there will be little distortion, but while doing. So, we are ignoring that coherency strain the strain due to this distortion of the bonds which required to maintain the coherency across the interface. But still normally we see this this precipitates just spherical with norm in the in the experiment also you see.

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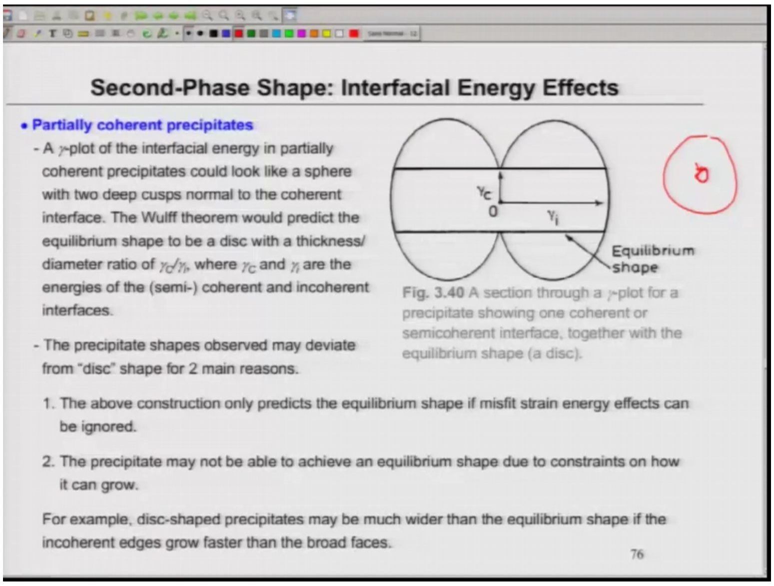

Second-Phase Shape: Interfacial Energy Effects

- **Partially coherent precipitates**
  - A γ-plot of the interfacial energy in partially coherent precipitates could look like a sphere with two deep cusps normal to the coherent interface. The Wulff theorem would predict the equilibrium shape to be a disc with a thickness/diameter ratio of γ_C/γ_i, where γ_C and γ_i are the energies of the (semi-) coherent and incoherent interfaces.
  - The precipitate shapes observed may deviate from "disc" shape for 2 main reasons.

Fig. 3.40 A section through a γ-plot for a precipitate showing one coherent or semicoherent interface, together with the equilibrium shape (a disc).

1. The above construction only predicts the equilibrium shape if misfit strain energy effects can be ignored.
2. The precipitate may not be able to achieve an equilibrium shape due to constraints on how it can grow.

For example, disc-shaped precipitates may be much wider than the equilibrium shape if the incoherent edges grow faster than the broad faces.

But you know when it is partially coherent things to gets change completely if it is partially coherent; that means, some of some of the surfaces of the precipitates is coherent and some of the surfaces are not coherent. Suppose we have a matrix and you have a precipitate which is like this, these are surfaces which are coherent and these surfaces is not partially coherent the flat surface is perfectly coherent, but on the other hand the curve surfaces partially coherent.

So, what will happen them normally such a case the gamma plot. The surface energy plot will have will be you know looks like a fair with cusps you see on the normal surfaces; that means, the along these surfaces normal surfaces flat surfaces, there will be curves sitting on that. That is what you shown here this is spherical on there is a minimum value on the flat surface. That is what is known as a cusps. Now the whole theorem predicts that equilibrium said of these things will be plate or a disc not a plate with a thickness to diameter ratio given by the 2 interfacial energies one is the gamma c that is and gamma I.

Where these are actually gamma c is basically semi coherent surface precipitate and this other one is the incoherent interface gets energies. And precipitates says observe may deviate they are normally this separate, but it can deviate from this separate little bit because of 2 reasons one is that in the above construction you have not considered misfits energies effects. Because of misfit along this semi coherent interfaces there are dislocations and this dislocation lead to strain energy which we have not considered. Second is that precipitate rule construction does not consider anything due to strain energy it only considered the interfacial energy effects, precipitates may not be able to reach the equilibrium state.

In that case also this may not have a these statement. So, these are precipitated may be much wider than the equilibrium say if than coherent energy edges grow faster than the coherent energy that will see in few slides. Finally, if one of the few of the surfaces are semi coherent type, and pure co incoherent type than we will have a disc shaped precipitated like this. You know this is just like a saucer on which we sometime drink tea or coffee you have seen that.

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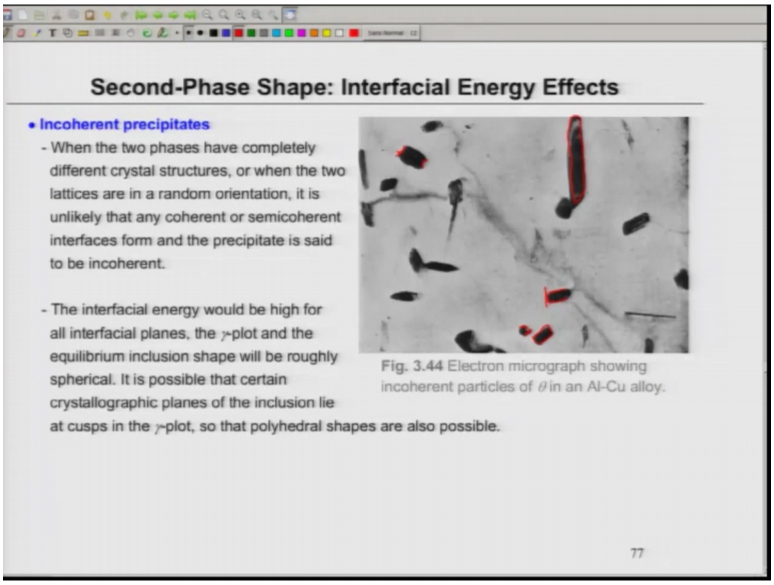

Second-Phase Shape: Interfacial Energy Effects

- **Incoherent precipitates**
  - When the two phases have completely different crystal structures, or when the two lattices are in a random orientation, it is unlikely that any coherent or semicoherent interfaces form and the precipitate is said to be incoherent.
  - The interfacial energy would be high for all interfacial planes, the γ-plot and the equilibrium inclusion shape will be roughly spherical. It is possible that certain crystallographic planes of the inclusion lie at cusps in the γ-plot, so that polyhedral shapes are also possible.

Fig. 3.44 Electron micrograph showing incoherent particles of θ in an Al-Cu alloy.

Now, if it completely incoherent you can see here there all kinds of things are presents here in this microstructure which is basically precipitates of theta in aluminum copper alloy.

Suppose is completely incoherent; that means, 2 phases are 2 phases are no complete different crystal structure and they have no lattice matching. So, there actually random orientations, it is very likely unlikely that coherent or semi coherent interfaces form and the precipitate is said to be completely incoherent. So, in such a case you know the precipitate can have any steps. It can have actually says interfacial energy would be high for the inter for all the interfacial planes a gamma plot the equilibrium inclusion shapes will be roughly spherical it is will be roughly spherical means it will not be exactly spherical just like in case of coherent, but there will be distortion.

The once which is shown here is the see this is a plates for a precipitate. So, you can see here this a plate, this is one is a they have a coherent interface here, but there is no in co coherency here. Similarly, there is a coherent here which is semi coherent such semi coherent here in coherent there. And the one which is shown as a big one is basically has lost all kinds of coherent semi coherency that is why the surface looks like a curved one. Similarly, here also you see here there is the surface is slowly getting curved so; that means, the co semi coherence is getting lost. So, as the precipitates become bigger the strain energy effect becomes stronger and they lose the semi coherency or coherency with a matrix.

So, in a normal picture in normal tea a micrograph, if you look at all the aluminum copper precipitates, you can see all kinds of orientation relationships and different kinds of a interfaces presence on these kind of this kind of precipitates which we will discuss in many detail when we talk about the precipitates. Well, just to give an better idea.

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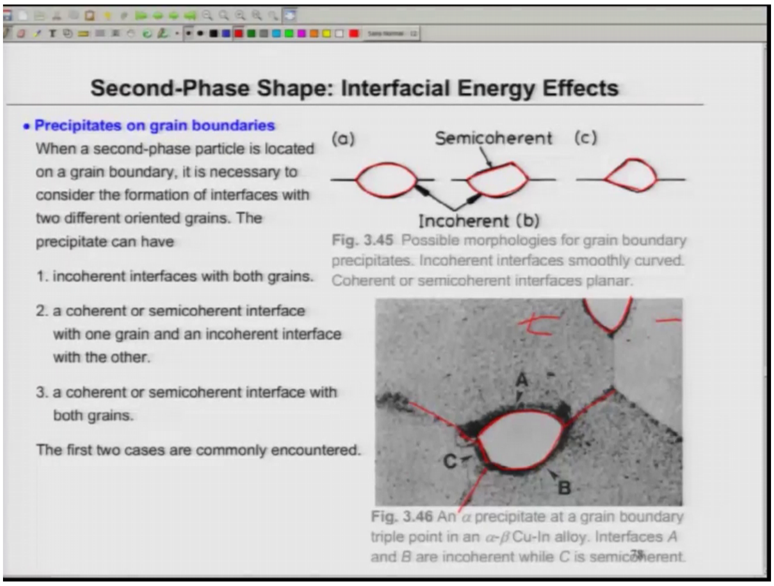

Second-Phase Shape: Interfacial Energy Effects

- **Precipitates on grain boundaries**

When a second-phase particle is located on a grain boundary, it is necessary to consider the formation of interfaces with two different oriented grains. The precipitate can have

1. incoherent interfaces with both grains.
2. a coherent or semicoherent interface with one grain and an incoherent interface with the other.
3. a coherent or semicoherent interface with both grains.

The first two cases are commonly encountered.

Fig. 3.45 Possible morphologies for grain boundary precipitates. Incoherent interfaces smoothly curved. Coherent or semicoherent interfaces planar.

Fig. 3.46 An α precipitate at a grain boundary triple point in an α-β Cu-In alloy. Interfaces *A* and *B* are incoherent while *C* is semicoherent.

Suppose a precipitates may set on a grain boundary then what will happen? A precipitates sets on a grain boundary the one which is shown here we see here there is a surface here there is a this is flat, but these 2 surfaces are actually curved and this is a boundary, this is a boundary this is a boundary the 3 grains 1 2 3 3 grains are actually.

So, this is sitting on a grain boundary we are very sure. So, that is one of the case then we need to consider what is the orientation relationships or rather what kind of interface of the precipitates with having with different grains 2 different grains; so if is you know if it is completely in coherent with the both the grains then this is what it will look like. The precipitate to will have such a kind of shapes. If it is semi coherent or the one grain this is; what it will be incoherent with the normal grain. Similarly, here semi coherent with one grain semi coherent with both the grains here one part and other part is incoherent with the both the grains. All kinds of possibilities do exist. First 2 cases are very commonly encounter the one which is shown if here this is basically in a aluminum copper alloy precipitates.

Here you see this is another one, where it is a completely incoherent with the both the interfaces with both the grains the precipitate phases. Obviously, if it is coherent or semi coherent along certain interface the precipitate to like to keep that coherent incoherent interface intact, because that interfaces the lowest energy interface or low energy interface. So, precipitate will not grow along that because if it grows and becomes bigger there is a highly likely chance or it is highly likely that this interface will lose the nature of coherency or semi coherency. So, that is what precipitates always grow along the incoherent interfaces where the energy is already very high.

So, there is no loss of energy in as far as the growth of the precipitate is concerned. This is normally see in in the aluminum copper precipitates.

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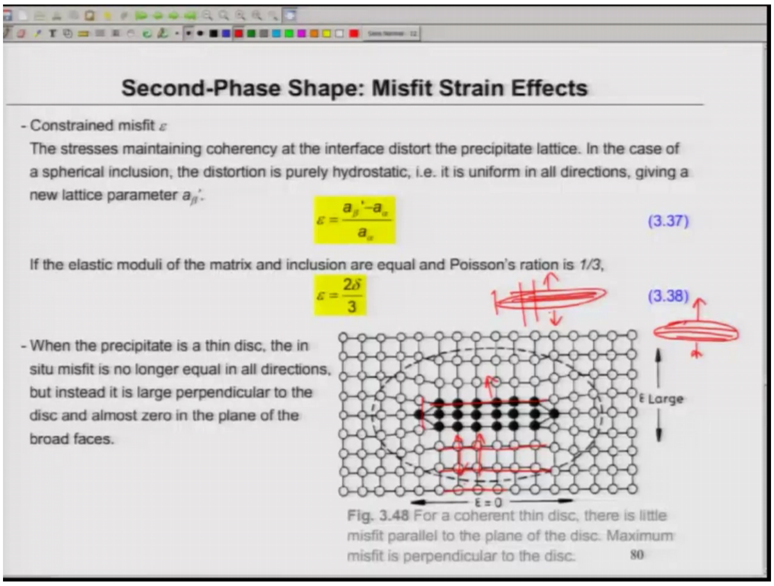

Second-Phase Shape: Misfit Strain Effects

- Constrained misfit ε

The stresses maintaining coherency at the interface distort the precipitate lattice. In the case of a spherical inclusion, the distortion is purely hydrostatic, i.e. it is uniform in all directions, giving a new lattice parameter a_β'.

$$\varepsilon = \frac{a_\beta' - a_\alpha}{a_\alpha} \qquad (3.37)$$

If the elastic moduli of the matrix and inclusion are equal and Poisson's ration is *1/3*,

$$\varepsilon = \frac{2\delta}{3} \qquad (3.38)$$

- When the precipitate is a thin disc, the in situ misfit is no longer equal in all directions, but instead it is large perpendicular to the disc and almost zero in the plane of the broad faces.

Fig. 3.48 For a coherent thin disc, there is little misfit parallel to the plane of the disc. Maximum misfit is perpendicular to the disc.

80

Well, just to give you some idea, what about time we have in this lecture you know we have not considered misfits strain effect at all while talking about the last few examples, but what is it is effects? You know let me go back.

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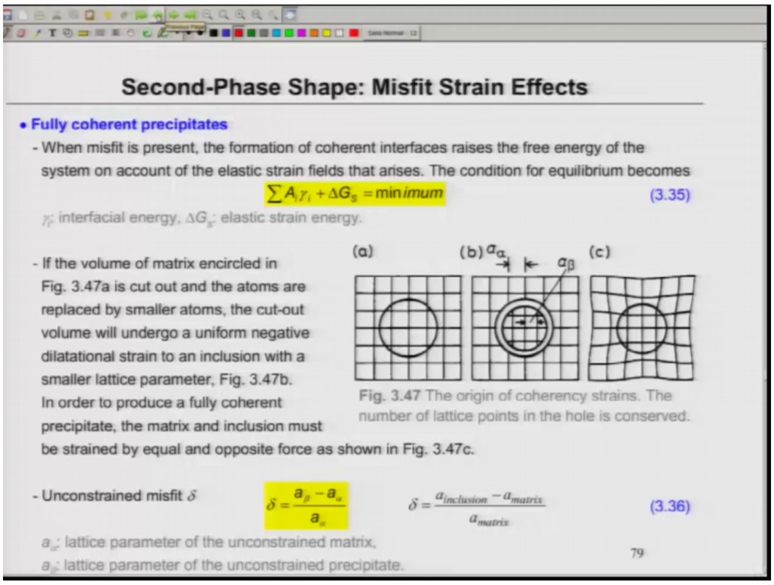

Second-Phase Shape: Misfit Strain Effects

- **Fully coherent precipitates**
  - When misfit is present, the formation of coherent interfaces raises the free energy of the system on account of the elastic strain fields that arises. The condition for equilibrium becomes

$$\sum A_i\gamma_i + \Delta G_S = \text{minimum} \qquad (3.35)$$

γ_i: interfacial energy, ΔG_s: elastic strain energy.

  - If the volume of matrix encircled in Fig. 3.47a is cut out and the atoms are replaced by smaller atoms, the cut-out volume will undergo a uniform negative dilatational strain to an inclusion with a smaller lattice parameter, Fig. 3.47b. In order to produce a fully coherent precipitate, the matrix and inclusion must be strained by equal and opposite force as shown in Fig. 3.47c.

Fig. 3.47 The origin of coherency strains. The number of lattice points in the hole is conserved.

  - Unconstrained misfit δ

$$\delta = \frac{a_\beta - a_\alpha}{a_\alpha} \qquad \delta = \frac{a_{inclusion} - a_{matrix}}{a_{matrix}} \qquad (3.36)$$

a_α: lattice parameter of the unconstrained matrix,
a_β: lattice parameter of the unconstrained precipitate.

When we have a suppose completely coherent precipitates fully and misfit is present misfit can be presents in many ways. So, it can be represent as a distortion of the bonds, now it can be present as a misfit dislocation also in case of semi coherent interface. When misfit represent format of formation of the coherent interfaces raises the free energy of the system. Because of the elastic strain energy effects; obviously, bonds are distorted right across the interface because of that there will be elastic strain energy.

So, energy elastic energy will be high. So, no longer we can actually consider the equilibrium condition to be summation of ai sigma a to be 0 ai is surface area and sigma is the energy of the systems. So, we have to add with that think delta g s which is nothing but a elastic strain energy because strain energy will play a role this is no longer cannot be ignored. And if the follow on the matrix which is shown here suppose this is the follow on the matrix in in circle is cut down if I take out the matrix, matrix was there already and this atoms are replaced this atoms were the sitting at replaced with the precipitated atoms or you know some other atoms smaller atom. Suppose then what will be there will be negative dilation negative expansion or they think; that means, the are the whole thing will shrink.

It will shrink to a smaller size that is what is called negative dilations and this dilation sent to inclusion with the smaller lattice parameter, that you can see because we are putting smaller size atoms we have taken out these atoms on the matrix and put smaller size atoms. So, there will be there will be dilation there will be you know smaller lattice parameter of that. And this will; so therefore, in order to produce a fully coherent precipitates the matrix and the inclusion must be strain that is what is shown here. Because of the atomic size is differences do not to form the bonds the between the precipitated and the matrix and keep the interface to be completely coherent; that means, all the atoms are bonds of the atoms are said to be satisfied then the bonds has to be distorted between the smaller atom and the bigger atom that is between the precipitated on the matrix.

And the as you see the un constant misfit is basically a beta by minus a gamma a alpha, but beta is the precipitation alpha is the matrix. Or is basically a inclusion minus a matrix by a matrix that is the way we defined the misfit that we have already discuss. Now if I look at it very carefully what is this you know constant misfit epsilon which we are talking about a that is basically nothing but a strain. So, the stresses maintaining this coherency of the interface will distort the precipitate lattice you can see here also they we clearly see that all the bonds are satisfied across the interface, but this is strained the whole thing is a strain you can see the region which is marked as a dotted line is strain.

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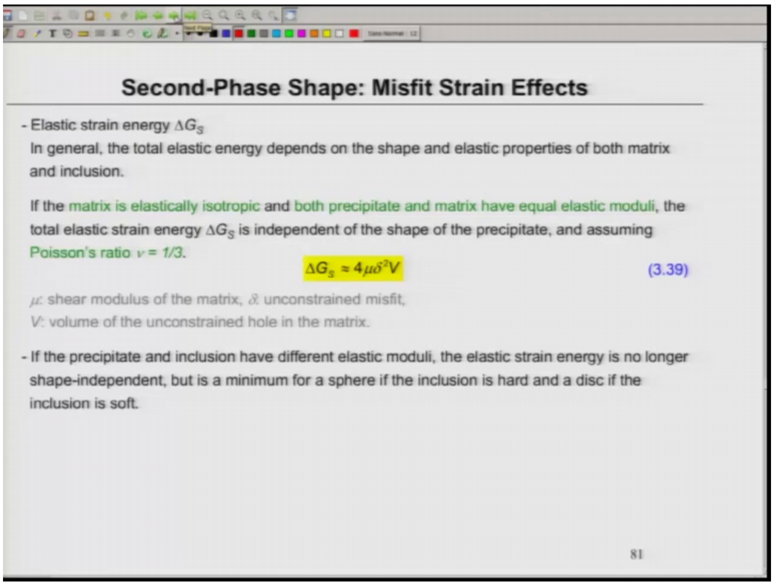

Second-Phase Shape: Misfit Strain Effects

- Elastic strain energy ΔG_S

In general, the total elastic energy depends on the shape and elastic properties of both matrix and inclusion.

If the matrix is elastically isotropic and both precipitate and matrix have equal elastic moduli, the total elastic strain energy ΔG_S is independent of the shape of the precipitate, and assuming Poisson's ratio $\nu = 1/3$.

$$\Delta G_S \approx 4\mu\delta^2 V \qquad (3.39)$$

μ: shear modulus of the matrix, δ: unconstrained misfit,
V: volume of the unconstrained hole in the matrix.

- If the precipitate and inclusion have different elastic moduli, the elastic strain energy is no longer shape-independent, but is a minimum for a sphere if the inclusion is hard and a disc if the inclusion is soft.

81

Now, in case of a spherical inclusions which is the case here also the distortion is purely hider static. Why? Because there is no directional dependence of the distortions it is uniform and all directions. So, therefore, we can actually get it lattice parameter of the new phase as related to epsilon by this parameter remember epsilon is nothing but a misfit strain; the strain because of the change of these atomic sizes. If the elastic modulus of the matrix and the inclusions are same which is not normal in the case it can be same in specific cases and we are assume the poissons ration for the metals are basically one by third 1 by 3 than this strain is basically 2 by 2 2 by third delta is what is known as misfit.

So, therefore, misfit and misfits strain can be related the moment we know the elastic modulus of the matrix and these precipitates as same. So, when the precipitate as a very thin this what will happen? The in situ misfit is no longer equal in all direction we call is a this therefore, there will be there will be some precipitates will be semi coherent sums will be incoherent as a instead is a large perpendicular do the disc very large perpendicular to the disc this is the disc. So, therefore, perpendicular to that is very large and is very small parallel to the disc. So, if it is this is the disc this is the direction it is very large. And this is the direction this is the direction parallel sorry this is the direction parallel is very low.

So, therefore, if I draw it again this is the perpendicular direction was very large and this is the parallel direction which is normally low, that is what you see here. You know this this distortion along these lines or low than along these lines. That is what it says that is what actually dictates the precipitates steps to be is the this. Therefore, we have to take into consideration these misfit strains, if you want to really know the exact steps. Well one can actually calculate; what is the delta g value in case of these misfits. And it is it is very clear the matrix is elastically isotropic these all very big assumptions and therefore, precipitation the matrix a equal elastic modulus then we can actually a assume poisson ratio to be 1 by 3 then delta g s becomes 4 sigma epsilon delta square v where basically this sorry the mu.

Mu is nothing but a shear modulus of the matrix and delta I have already defines a misfit and volume is where is the volume of within matrix un constant whole in the matrix. So, we can add up these things into this equation this. And actually the minimize the whole equations and get these steps to the precipitates; obviously, we will construction we will not do that because we will construction does not take care the misfit strains, but one can actually do much better you know well.

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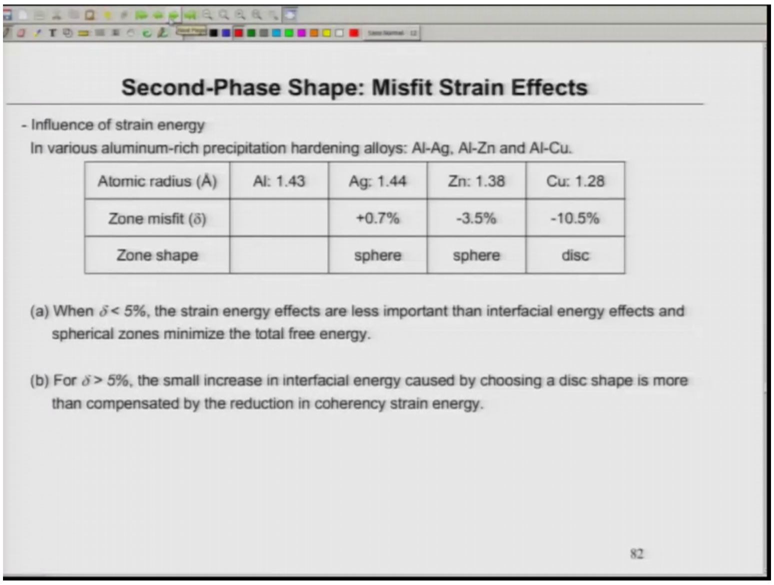

Second-Phase Shape: Misfit Strain Effects

- Influence of strain energy

In various aluminum-rich precipitation hardening alloys: Al-Ag, Al-Zn and Al-Cu.

Atomic radius (Å)	Al: 1.43	Ag: 1.44	Zn: 1.38	Cu: 1.28
Zone misfit (δ)		+0.7%	-3.5%	-10.5%
Zone shape		sphere	sphere	disc

(a) When $\delta < 5\%$, the strain energy effects are less important than interfacial energy effects and spherical zones minimize the total free energy.

(b) For $\delta > 5\%$, the small increase in interfacial energy caused by choosing a disc shape is more than compensated by the reduction in coherency strain energy.

As you see here misfits strain effects very large if I consider suppose aluminum has a size of 1.43 Armstrong as a atomic size and silver as 1.44 therefore, the misfits 0 zone means fit actually has a 0.7 percent this is very small, but it is positive.

A zinc on the other hand it is a minus 13.5 copper is all very large is almost you know 10 percent minus and therefore, the steps will be spherical in case of aluminum silver it will be also spherical in zinc, but this because it is can be created can be accommodated 3 0.5 percent is not very large, but the moment is become copper is very large it will be a disaffected. So, whenever the delta is less than 5 strain energy effects are less important than interfacial energy. And therefore, spherical zones forms, but when is more than 5 than only interfacial energies has to be augmented with or added with these strain energy effects and calculate the these effects.

Let me stop here. And therefore, you see that these interfaces do play very important role. And in the next class I will show you simple thermodynamic analysis, how we can actually use this concepts to explained different phenomena in the in the phase transformations.