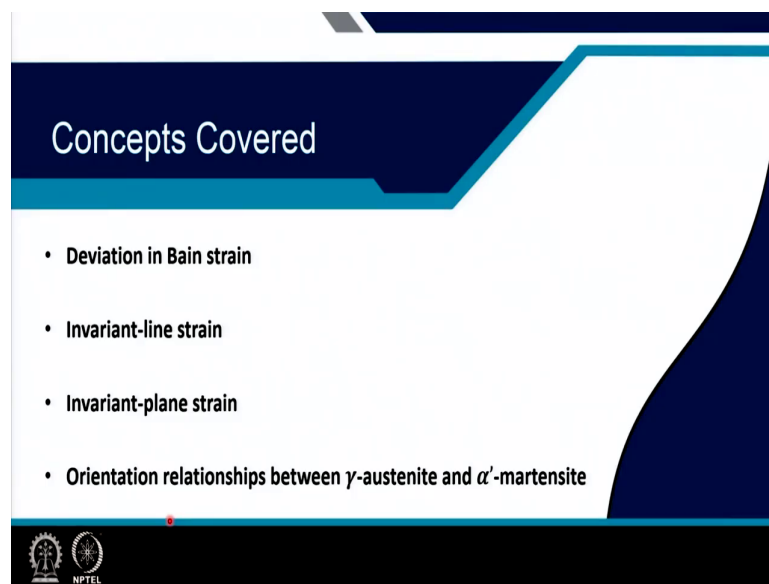


Texture in Materials
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Module - 08
Texture evolution during phase-transformation
Lecture - 42
Orientation Relationships between FCC and BCC/BCT

Good afternoon everyone, and today we will be continuing with our module 8, which is Texture evolution during phase-transformation and this is lecture number 42 and we will be discussing in this lecture about Orientation relationship between FCC and BCC or BCT crystal structure in relationship specifically of steel.

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So, the concepts that will be covered in this lecture is deviation in Bain strain. We learned Bain strain in the previous lecture and then what is invariant line strain and invariant plane strain, why it is necessary to have an line invariant or a plane invariant during phase transformation. Then the fourth one is orientation relationship between gamma austenite and alpha prime martensite other than the Bain transformations that we know.

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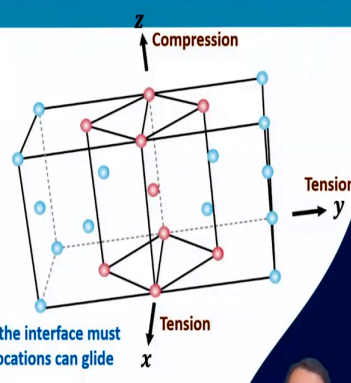
Deviation in Bain strain

During γ - Austenite (FCC) to α' - Martensite (BCC or BCT) transformation, the $\gamma - \alpha'$ interface must be able to move freely without diffusion.
→ This requires stress free fully coherent interface

The $\gamma - \alpha'$ transformation involves strain → stress free fully coherent interface is not possible

In order to enable the $\gamma - \alpha'$ interface to move freely, the interface must be at least semi-coherent such that the interfacial dislocations can glide freely through the interface as the interface moves

As this is diffusion free transformation without thermal activation
→ climb or cross-slip will not suffice.



So, now we have as we have learned in the previous lecture the Bain strain, we have seen that there is a negative strain in the z direction and positive strain in the x and the y direction of the BCC or BCT martensite which is forming. So, while this transformation takes place from the gamma austenite to alpha prime martensite, the interface between the gamma austenite and the alpha prime martensite should be such that it should be able to move freely without any diffusion processes occurring.

So, in order to move this interface freely, the interface has to be fully coherent right. Now, gamma to alpha prime transformation involves strain as I explained earlier and the stress free fully coherent interface may then be impossible right because of the presence of this strain, which occurs while gamma transform into alpha prime.

So, in order to enable the gamma to alpha prime transformation or to enable the gamma to alpha prime interface to move freely, the interface must be at least semi coherent such that the interfacial dislocation can glide freely through the interface as the interface is moving right.

So, as this is a diffusion free transformation that is without any kind of thermal activation, the dislocations are free to glide. So, it has to glide through the interface so, that the interface moves freely and it does not involve any thermal activation related processes such as you know dislocation, climb or you know the cross slipping of the screw dislocations etcetera.

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INVARIANT-LINE STRAIN To maintain semi-coherency → To maintain interfacial dislocations Glissile

The line vectors of the interfacial dislocations must lie along an invariant line, → That must be a line which joins the γ and α' crystals without any rotation or distortion

This is only satisfied if the Burgers vectors of the interface dislocations does not lie in the interface plane unless the dislocations are screw in character.

If there is any distortion along the dislocation line → Other dislocations are required to accommodate the misfit.

Presence of more than one set of non-parallel dislocations in the interface
→ Intersection of dislocations to form jogs → Sessile dislocations.

So, what is the importance of invariant line strain here? In order to maintain the semi coherency that is to maintain the interfacial dislocation glissile, the line vector you see if we are looking into this structure which shows an edge dislocation here right, and the screw dislocation here, we all know that our dislocation is actually a loop which contains a screw dislocation somewhere here, an edge dislocation somewhere here.

And then it forms a mixed dislocation and then edge screw dislocation and you know the edge dislocation and then again screw dislocation and in between a mixed dislocation. So, dislocation is in a form of a loop which contains a burger vector which is like this right. And this burgers vector in case of the screw dislocation lies parallel to its line vector whereas, the burgers vector this burgers vector is perpendicular to the line vector who at the edge dislocation.

Now, in order to satisfy that this line vector of any interface between the gamma and the alpha prime, that is the line vector corresponding to a certain interfacial dislocation must lie along a line which is known as the invariant line; that means, it must lie in a line which joins the gamma austenite and the alpha prime crystals without any distortion or any rotation, this is only possible if it satisfies that the burgers vector of the interfacial dislocation does not lie in the interfacial plane.

And it can only lie in the interfacial plane when it is a fully screw dislocation. So, if there is any distortion along this dislocation line or this dislocation line vector; that means, interfacial

dislocation line vector, then another dislocations are required to accommodate the misfit and if another dislocation is present or if there are presence of more than one set of nonparallel dislocations in the $\gamma_2 \alpha'$ interface, then this intersection of dislocation will form jogs and make the dislocations sessile.

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It means that for martensitic transformation \rightarrow the deformation which changes the parent- γ into the product- α' must leave one or more lines invariant i.e., undistorted or unrotated.

A deformation which leaves one line invariant is called an 'INVARIANT-LINE STRAIN'.

Bain strain does not satisfy the minimum requirement of martensitic transformation *Bain strain + rigid body rotation brings ab in coincidence with a'b' \rightarrow an Invariant-line Strain*

$[\bar{1}\bar{1}0]\gamma \parallel [100]\alpha'$ $[001]\gamma \parallel [001]\alpha'$

Mathematics of Crystallographic Texture in Martensitic and Related Transformations, H.K.D.H. Bhadeshia, S. Kundu, H. Abreu; Microstructure and Texture in Steels, Springer

So, it means that during the martensitic transformation, the deformation which changes the parent gamma austenite into the product alpha prime martensite must leave at least one-line invariant, which allows the line vector of the dislocation to move through it through the interface from the parent to the product phase without any distortion or any rotation. A deformation which leaves one-line invariant is called an invariant line strain.

So, if we are discussing the Bain strain, we will show you I will show you that the Bain strain does not satisfy the minimum requirement of the martensitic transformation; that means, that with only the Bain strain there is not possible to have any line vector parallel to the line invariant that is a unrotated, undistorted dislocation through the interface from the parent to the product phase is possible.

So, if we look into the z axis of the Bain strain, that we are showing the figure in the previous slides that z axis is the axis where the dislocation sorry the lattice parameter is you know decreasing. So, it has a negative strain whereas, in the x and the y axis the lattice parameter extends when gamma austenite's convert into alpha prime.

Let us say the situation is something like this, if we focus on the pointer you see this is the z axis and this corresponds to the lattice of the gamma austenite and after the transformation let us say this red is the lattice parameter corresponding to the alpha prime.

So, in case of x and the y direction, the $1\bar{1}0$ of the gamma austenite becomes parallel to 100 of the alpha prime whereas, in the y direction the 110 of the gamma austenite this 1 becomes parallel to the 010 of the alpha prime. So, there is a slight increase in the lattice parameter from 110 of gamma to 010 of alpha prime which is being denoted here.

Now, if we are looking. So, such a way that the z axis is now vertical and the y axis is on this side horizontal and the x-axis is coming out of the slide, then the initial lattice is shown by this round circle blue colored circle and we can see that when it gets when it forms alpha prime martensite, then the lattice is now distorted something like this.

So, in this case you see that we are looking along the z axis which is basically 001 of gamma which remains parallel to 001 of alpha prime and we know that the lattice of the alpha prime is slightly distorted and it has a negative strain. So, you can see that there is a this lattice parameter has reduced here whereas, in the x and the y axis you see that the lattice parameter has extended.

So, one can imagine that the circle is an under distorted lattice parameter of the gamma prime and the ellipse and if you look it will look like a doughnut and three dimensionally and it becomes a larger lattice parameter in x and y. So, a positive strain and a negative lattice parameter in the z which is a negative strain. Now, if the interface has a dislocation which is undistorted in case of the gamma prime if it is a b and c d, there after it forms you know sorry not gamma prime gamma austenite.

So, after it forms alpha prime, the dislocation substructure becomes a \bar{b} \bar{c} \bar{d} or a prime b prime c prime d prime. So, there is an angular deviation between the you know the line vector of for the gamma austenite and the line vector of the dislocation interfacial dislocation of the alpha prime and none of them are showing that it is undistorted or unrotated all of them are distorted and rotated.

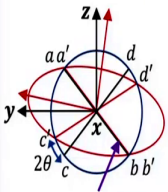
So, none of them are present in a line invariant. So, none of them has an invariant line strain therefore, the Bain strain does not satisfy the minimum requirement of having a invariant line strain. So, but if we give a rigid body rotation after the Bain strain to bring the a prime b

prime in coincident with the previous a, b so, that the interfacial dislocation of the gamma becomes parallel to the interfacial dislocation of you know alpha prime.

And it becomes undistorted and unrotated; that means, it forms an invariant line that is a line where a, b and a dash b dash are parallel between the you know 2 phases gamma and alpha prime in the interface so, that the dislocation can move from you know the parent gamma to the alpha prime without any distortion or rotation. So, the a rigid body rotation can be given this is taken from the work of Bhadeshia and is given in you know Microstructure and Texture in Steel a book published in springer.

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Bain strain + rigid body rotation brings ab in coincidence with $a'b'$ → an Invariant-line Strain



The experimentally observed irrational orientation relationship that differs from Bain strain → Now can be obtained by Bain strain + rigid body rotation

- The Bain orientation relationship does not exist and
- Bain deformation should not form the basis for variant selection

During $\gamma - \alpha'$ transformation → the experimentally observed shape deformation leaves the habit plane undistorted and unrotated → It is an invariant-plane strain

This would require two non-parallel invariant-lines

Bain strain + rigid body rotation → Cannot produce invariant-plane strain

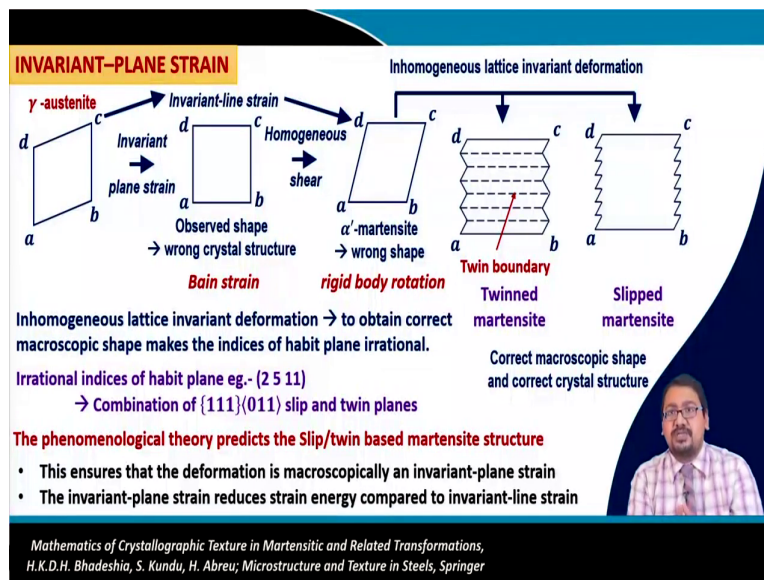
So, what I am saying is that that with a rigid body rotation along with the Bain strain can bring a, b in coincidence with a prime b prime therefore, it becomes an invariant line strain. So, the experimentally observed you know the martensitic transformation if you observe experimentally, it contains an irrational orientation relationship that differs from the Bain strain.

And now this irrational orientation relationship that is a mirror indices of a higher order of the habit plane could be obtained by using a Bain strain plus this rigid body rotation. So, what we understood is, the Bain orientation relationship actually does not exist. So, the Bain deformation as I showed in the previous lecture cannot be used or cannot be the basis to obtain you know various variant selection right.

So, during gamma austenite to alpha prime martensitic transformation, the experimentally observed shape deformation leaves the habit plane you know in a undistorted and unrotated scenario experimentally which is fully actually an invariant plane strain instead of an invariant line strain.

Now, this will require two non parallel invariant line or line invariant strains right. So, Bain strain plus rigid body rotation cannot produce the invariant plane strain, it produces an invariant line strain which makes theoretically the martensitic transformation feasible, but experimentally observed situation is of invariant plane strain because invariant plane strain are thermodynamically more feasible.

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And so, if we look into the invariant plane strain scenario let us take an austenite which looks like this a gamma austenite and if we introduce an invariant plane strain to this. The observed shape change during the process is correct, but the crystal structure that is obtained is different from that of the alpha prime martensite.

Now, this can be considered as a Bain strain. Now in order to you know have an invariant line strain which satisfies the Bain strain plus the rigid body rotation; the rigid body rotation. So, that is an invariant plane strain plus and homogeneous shear if it is given, then the observed crystal structure becomes alpha prime martensite, but the shape formation is uncorrect or different right.

So, in order to avoid this if an inhomogeneous lattice invariant distortion or deformation is given, then either a twin boundary structure something which looks like this or a slip martensitic structure can form and by in this scenario in case of both twin martensite or slip martensite or a combination of this gives not only the correct macroscopic shape change, but also the correct crystal structure.

So, in homogeneous lattice invariant deformation is required to obtain the correct macroscopic shape, which makes the habit plane you know totally irrational and irrational indices often habit plane for example, $2\ 5\ 11$ could exist with a combination of you know $1\ 1\ 1\ 0\ 1\ 1$ type of slip dislocation slip and the twin planes including together.


So, this phenomenological theory predicts the slip twin based martensitic structure formed during the gamma austenite to alpha prime transformation, this ensures that the deformation is macroscopically and invariant plane strain and the invariant plane strain occurs because it ensures a reduced strain energy requirement compared to the formation of an invariant line strain obviously.

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Orientation relationships between γ -austenite and α' -martensite

| | Alternatives | Total number of variants |
|---|--------------|--|
| Kurdjumov-Sachs ($K-S$) | | |
| $\{111\}_\gamma \parallel \{011\}_\alpha$ | 4 | There can be 24 crystallographic variants possible |
| $\langle 011 \rangle_\gamma \parallel \langle 111 \rangle_\alpha$ | 3 | |
| Twinning | 2 | |
| Nishiyama-Wassermann ($N-W$) | | |
| $\{111\}_\gamma \parallel \{011\}_\alpha$ | 4 | 12 |
| $\langle 112 \rangle_\gamma \parallel \langle 111 \rangle_\alpha$ | 3 | |

- The orientation relationship between γ - α' is irrational.
- There is a small angular deviation between original (experimental) irrational orientation and the orientation obtained by $K-S$ or $N-W$.
- As the orientation relationship between γ - α' is irrational, there could be 24 variants instead of 12 for $N-W$.



So, that is why the Bain strain comprises not only of a Bain strain with an rigid body rotation. So, the Bain strain simply without a rigid body rotation does not suffice. So, there are various orientation relationship that forms when there is a FCC to BCT or BCC transformation mostly in case of gamma austenite and alpha prime martensite formation. The one of the

important is the Kurdjumov-Sachs relationship and the Kurdjumov-Sachs relationship is considered to be more exact than the Bain relationship.

And it says that the closest packed plane of the gamma austenite phase or the FCC phase remains parallel to the closest packed plane of the alpha prime BCT or BCC phase. So, 111 of gamma remains parallel to 011 of alpha or alpha prime and the closest pack direction of FCC gamma remains parallel to the closest pack direction of the BCT BCC that is alpha prime martensite or alpha ferrite. So, this two things occurs during the phase transformation using the ideal orientation relationship of Kurdjumov Sachs.

Now, to let you know that there are four 111 plane presence in a FCC structure or a FCC crystal structure right. So, there could be four alternative 111's where 111 planes where this phase transformation may take place and every 111 plane contains three 110 directions.

So, for each 111 plane there could be three alternatives of 110 directions where this transformation keeping parallel closely packed direction parallel for gamma to alpha will take place. So, there are three alternatives for that and then for each of these three alternative there is a twinning possibility.

So, it makes the alternative double. So, twinning 2. So, 4 into 3 into 2 makes it 24. So, there are 24 crystallographic variants possible during gamma to alpha prime martensitic transformation using Kurdjumov-Sachs relationship. Now, if we look into another relationship that is the Nishiyama-Wassermann relationship.

The second situation is the Nishiyama-Wassermann relationship, which states that the closest pack plane 111 of FCC that is the gamma austenite remains parallel to the closest pack plane of the alpha or the alpha prime martensite 011 whereas, the here the direction of the gamma austenite is different it is 112 which remains becomes parallel to the 111 of alpha prime that is the closest pack direction of the BCC or BCT phase.

Now, this occurs if you remember that in case of face centered cubic material a dislocation vector that is a dislocation which runs in the 111 plane is along the closest pack direction 110 whereas, during this dislocation glide the dislocation could you know divide itself into two partials.

And these could be 112 type dislocations and unless and until the material cross slips the two partials which have a dislocation line vector 112 type dislocation does not meet it cannot cross slip. In case of phase transformation related phenomena the climb of edge dislocation and cross slipping of screw dislocation is does not matter it does not occur it is not a thermally activated process.

So, in case where the 112 dislocations are more active and it has been found out that mostly maybe in low stacking fault energy materials, the Nishiyama-Wassermann relations suffice more than the Kurdjumov-Sachs relations and in high stacking fault energy material the Kurdjumov-Sachs relation occurs more.

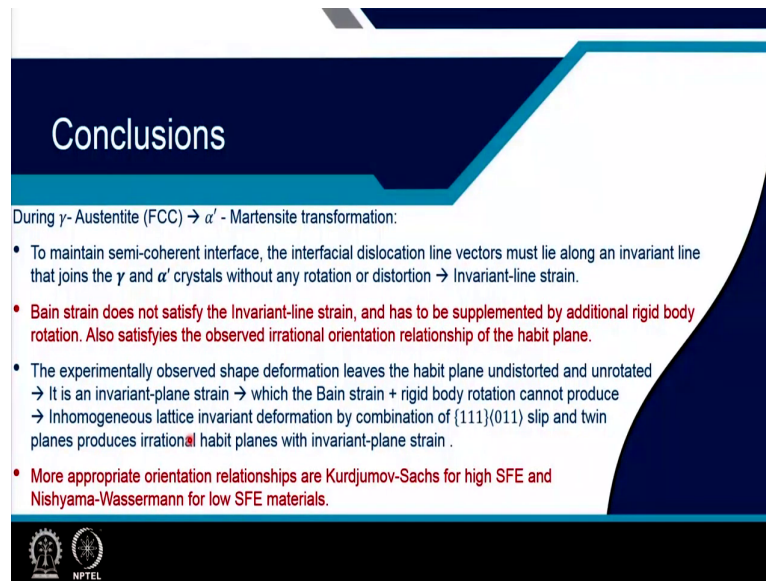
So, as we can see that in case of Nishiyama-Wassermann relation also the alternatives in case of 111 plane of FCC. So, there are four 111 planes of FCC. So, four 111 planes and for each 111 planes there are three possible 112 direction. So, for each of them there are three possible directions.

So, 3 alternatives for 112 gamma to become parallel to 111 alpha. So, a total number of 12 variants is possible because in case of Nishiyama-Wassermann relationship there is no possibility of twinning formation during this phase transformation. However, as said earlier the orientation relationship during a phase transformation and this is an example for gamma austenite and alpha prime and for all other case is to is mostly irrational is always irrational.

So, the habit plane has a combination forms by the combination of slip and twin and have a higher order like for example, as I said 3 7 and 28 say for example, or 25 for example. Now, there is a small angular therefore, there is always a small at least a small angular deviation between the experimentally observed orientation the relationship between the parent and the product phase and the ideal orientation relationship observed from the Kurdjumov-Sachs and Nishiyama-Wassermann relationship.

Therefore, if we are talking about the Nishiyama-Wassermann relationship too because of the deviation from the ideal relationship and because of the formation of an irrational habit plane instead of 12 possible number of variants, there will be 24 number of variants in case of Nishiyama-Wassermann relationship too.


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Conclusions

During γ -Austenite (FCC) \rightarrow α' - Martensite transformation:

- To maintain semi-coherent interface, the interfacial dislocation line vectors must lie along an invariant line that joins the γ and α' crystals without any rotation or distortion \rightarrow Invariant-line strain.
- Bain strain does not satisfy the Invariant-line strain, and has to be supplemented by additional rigid body rotation. Also satisfies the observed irrational orientation relationship of the habit plane.
- The experimentally observed shape deformation leaves the habit plane undistorted and unrotated \rightarrow It is an invariant-plane strain \rightarrow which the Bain strain + rigid body rotation cannot produce \rightarrow Inhomogeneous lattice invariant deformation by combination of $\{111\}\{011\}$ slip and twin planes produces irrational habit planes with invariant-plane strain .
- More appropriate orientation relationships are Kurdjumov-Sachs for high SFE and Nishiyama-Wassermann for low SFE materials.

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So, in this lecture class, we found out that during austenite which is a face centered cubic material to alpha prime which is martensite and is a body centered tetragonal or body centered cubic material transformation. In order to maintain a semi coherent interface the interfacial dislocation line vector must lie along an invariant line that joins the gamma austenite to alpha prime crystal without any distortion or any rotation.

So, theoretically, it should maintain an invariant line strain and Bain strain does not satisfy this invariant line strain and has to be supplemented by an additional rigid body rotation which also satisfies the irrational habit plane formation or the orientation relationship of the habit plane right. The experimentally observed shape deformation shape change leaves the habit plane undistorted the whole plane undistorted and unrotated.

So, it is not an invariant line strain it is actually an invariant plane strain which the Bain strain plus the rigid body rotation actually could not suffice. So, this inhomogeneous lattice invariant deformation by the combination of 111 011 type slip dislocation slip and the twinning, that produces irrational habit plane and invariant plane line is given by this inhomogeneous lattice invariant deformation right.

So, more appropriate orientation relationship could be Kurdjumov-Sachs relationship which is mostly for high stacking fault energy materials and Nishiyama-Wassermann relationship which is for low stacking fault energy material, but both can be observed in various situations and that is it for this lecture today.

Thank you very much.