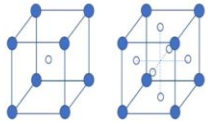


Mechanical Behaviour of Materials
Prof. S. Sankaran
Department of Metallurgical and Materials Engineering
Indian Institute of Science, Madras

Lecture - 21
Introduction to Dislocation IX

(Refer Slide Time: 00:16)



Dislocations in Superlattices



Unit cells of the B2 and L₁₂ superlattices

- Two possible cubic superlattices produced by alloys of composition AB (e.g., CuZn, NiAl) and AB₃ (Cu₃Au, Ni₃Al) are with crystallographic identifications B2 and L₁₂ respectively.
- During nucleation and growth of ordered domains in a disordered crystal, the lattice parameter change is sufficiently small for the atomic planes to remain continuous.
- When the domains meet, the A and B sublattices are either in phase, i.e., in 'step', with each other or out of phase. The later conditions results in an *antiphase boundary* (APB).
- It has characteristic energy because the nearest-neighbour coordination of the superlattice is destroyed: Typical energies are similar to those of stacking faults, i.e., ~10-100 mJ/m²

Introduction to Dislocations, 4th Edition, D. Hull and D.J. Bacon, Butterworth-Heinemann, 2009



Hello, I am Professor S. Sankaran in the Department of Metallurgical and Materials Engineering. Hello everyone let us look at the dislocation super lattices. We have looked at all the dislocation types and energetics and stress fields, motion, dynamics, mechanics everything. So, in that continuation, I just want to cover another aspect of dislocations in superlattice, which is also very important which I wanted to just add to that lecture because I wanted to do it separately because it has some special properties, which is not considered in the conventional dislocation. I would say formulation, so, let us see what is this superlattice dislocations. So, if you look recall all the ordered systems, typical ones are that you know the units are shown here of B2 and L₁₂ superlattices. These are all two possible cubic superlattices produced by alloys of composition AB for example copper zinc and nickel aluminium and AB₃ for example Cu₃Au and Ni₃Al are with crystallographic identifications B2 and L₁₂ respectively. So, how they are forming during nucleation and growth of ordered domains in a disordered crystal, the lattice parameter changes sufficiently small for atomic planes to remain continuous. So, how this is identified then, when the domains meet the A and B sublattices are either in phase, that is in step with other or out of phase.

The later conditions results in antiphase boundary APB, popularly known as APB. It has characteristic energy because the nearest neighbour coordination of the superlattices destroyed. Typical energies are similar to those of stacking faults that is approximately 10 to 100 milli joules meter square. So, what do you have to understand this it is almost similar to the stacking fault energy or surface energy we have been looking at all these things related to dislocation. So, similar ideas are applied here, you can just follow this.

(Refer Slide Time: 02:59)

Slip and Dislocations in Ordered Structures

- (a) A two-dimensional schematic of an ordered AB crystal. A and B atoms are preferred near neighbours.
- (b) Slip by a unit distance, b along the slip plane produces undesirable atomic bonding across the plane
- (c) Slip by the movement of superlattice dislocation (with Burgers vector $= 2b$) does not produce undesirable bonding
- (d) because of the elastic repulsion between the individual dislocations in the superdislocations, it splits.
- Propagation of the superdislocation as a unit is not accompanied by the formation of "poor" bonds across the interface, yet the elastic strain energy ($\cong 2Gb^2$) of the superdislocation is greater than that of two widely separated single dislocations ($\cong Gb^2$)
- As a result of their elastic repulsion, the individual dislocations are separated and improper bonding across the slip plane occurs between them
- In analogy with partial dislocations, the equilibrium separation of the unit dislocations depends on the value of the anti-phase boundary energy

• In crystals such as Cu_3Au , with A_3B stoichiometry and possessing the fcc cubic structure, the superlattice dislocation is composed of two unit $(a/2)[110]$ dislocations.

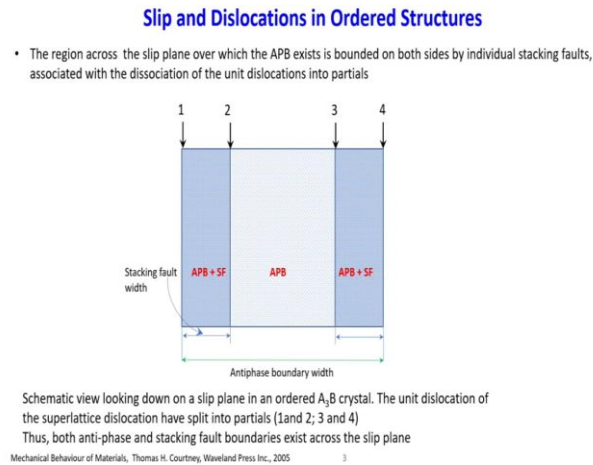
Mechanical Behaviour of Materials, Thomas H. Courtney, Waveland Press Inc., 2005

Suppose if you look at the slip under dislocations and there is a nice schematic or to I would say that it is very much simplified the schematic in order to understand this little complex or confusing reactions here there are two dimensional schematic of an ordered AB crystal A and B atoms are preferred near neighbours. So, what does it mean it means for A the nearest neighbour is B for a B the nearest neighbour is A. So, that is this AB crystal type suppose, if the slip plane is designated here slips by a unit distance B like a normal lattice along the slip planes produces undesirable atomic bonding across the plane. So, you are seeing this crystal in A which is going to produce the slip with the magnitude of B here, that is a distance and then it creates a standard slip but there is a difference between an ordinary crystal in order crystal here is by just by slip it produces an undesirable bonds. What is undesirable bond here? because we said that then the preferred neighbours are A and B atoms but here it is BB AA BB AA like that. So, the whole across the slip plane so, this is undesirable atomic bonding across the slip plane. So, what? so, slip by the moment of a superlattice dislocation with a burgers vector $2b$ does not produce undesirable bonding suppose if you look at a schematic here.

A 2D lattice, where you see that two edge dislocations are placed side by side when this kind of dislocation passes through this lattice then it does not produce undesirable bonds how? because one slip produces undesirable bond then another dislocation which follows will put the lattice back into the order but what do you or what is the difference between a normal burgers vector and this? A normal burger vectors will be having the magnitude like b here it is too. So, it is said $2b$ burger vectors are no longer b in ordered crystal it is rather $2b$ because of the elastic repulsion between the individual dislocations in the superdislocations it splits. You see, we have the background to understand this the elastic repulsive force between the two edge dislocation will try to keep them away in the partial like a unit dislocation will split into short length partial and then that the partial will recombine and move or it will just wipe separated and then remain stable it is completely based upon the stacking fault energy similarly, here to keep this even though you know, it can move as a pair here the elastic strain energy associated with this is much higher than the normal unit dislocation. So, what happens it splits. So, it splits like this which is shown in the fourth figure (d) here. So, which is quite interesting like know the super dislocation with burgers vector $2b$, that gets split into two unit dislocations edge dislocations leaving behind the anti-phase boundary domain. So, the 2 you can say that it is two super partials are separated widely in between you have the anti-phase domain band actually. So, propagation of these super dislocations as a unit is not accompanied by the formation of poor bonds across the interface. So, if this kind of; you know a pair moves then there is no problem. But yet the elastic strain energy as I just mentioned, which is $2b^2$ of super dislocation is greater than that of two widely separated single dislocations which is Gb^2 . So, Gb^2 energy of this is $Gb^2 \cdot Gb^2$. So, it is widely separated care which is a normal dislocation, but here it is widely separated from the super dislocation but keeping this anti-phase domain in between. So, as a result of this elastic repulsion, the individual dislocations are separated and the improper bonding across the slip plane occurs between them. So, the improper bonding across the slip and it has got a characteristic energy associated with it that is called anti-phase domain energy that is also we have seen. So, in analogy with the partial dislocations the equilibrium separation of the unit dislocation depends on the value of anti-phase boundary energy. So, it is something like you are stacking fault energy, whether it is going to remain a split shockley partials are becomes a unit dislocation similarly, here the whether it is going to remain as a super dislocation or it is going to split into super partial which is decided by the anti-phase boundary energy and the of course, the repulsive force. In crystals such as Cu_3Au with the A_3B stoichiometry and possessing the fcc cubic structure the superlattice dislocation is composed of two unit ($a/2$)

[110] dislocation. So, it is a similar burgers vector but is it is two units. So, that is what is shown here. So, if you approach the problem like this, it is very easy to understand so that is why I brought this schematic.

(Refer Slide Time: 09:31)

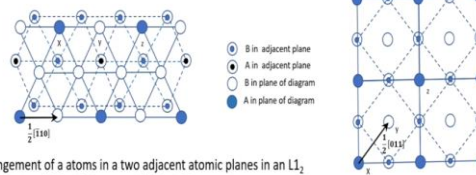


So, now, we can look at the other aspects the region across the slip plane over which the APB exists is bounded on both sides by individual stacking faults associated with the dissociation of the unit dislocations into partials. So, I just showed in the previous schematic where the APB domain is bounded by a two individual unit dislocations. Now we are talking about dissociation of two unit dislocations further into partials. So, that means you have an APB domain and then both sides the unit dislocations are decomposed into two Shockley partials. So, you are going to have a situation where an APB domain in between and then by both sides they are bounded by the APB plus stacking fault. I mean super partials can be there a stacking fault can be there along with the APB on both sides. So, the total width is now considered as anti-phase boundary width.

So, so what is this? What shown here?, the schematic on a slip plane in an ordered A_3B crystal the unit dislocation of superlattices dislocation have split into partials. So, the super dislocation has slipped into partials (1, and 2; 3 and 4). Thus both anti-phase and stacking fault boundaries exists across the slipway. So, this is one way of looking at it, what the previous schematic showed, which is shown the other format.

(Refer Slide Time: 11:21)

Dislocations in Superlattices



Arrangement of atoms in two adjacent atomic planes in an $L1_2$ superlattice: (a) (111) planes and (b) {100} planes

- APBs also arise in the core of dislocations in ordered alloys and this is of considerable technological significance because of their influence on the high temperature mechanical properties of these materials.
- As the temperature is increased the CRSS actually increases, an effect known as the *yield stress anomaly*. If the order-disorder transition temperature for the alloy is high enough, the yield stress reaches a peak. (800 – 1000K, Ni_3Al)
- In ordered state, $\frac{1}{2}\langle 110 \rangle$ vectors are not lattice translation vectors and so gliding dislocations leave behind a surface of disorder (APB).
- The perfect dislocation moving on either the {111} or {100} planes of $L1_2$ superlattice consists of two $\frac{1}{2}\langle 110 \rangle$ superpartial dislocations joined by an APB. This superdislocation has a Burgers vector $\langle 110 \rangle$, which is a lattice translation vector.
- The spacing in equilibrium is given by a balance between the elastic repulsive force between the two super partials and the opposing force due to APB energy.

Introduction to Dislocations, 4th Edition, D. Hull and D.J. Bacon, Butterworth-Heinemann, 2009

4



To take into all the possible combinations of faults and boundaries. Now, we will look at the same idea in the atomistic level. So, what is that I am trying to show here; here it is arrangement of atoms in the two adjacent atomic planes in an $L1_2$ superlattice. So, here you are seeing that a completely filled circle, open circle and then open circle inside the black dot and the open circle inside the blue dot.

So, these are all A the first one is A in the plane of the diagram B in the plane of diagram and this one A in adjacent plane and B in adjacent plane. So, you can now clearly see that so, this is BA, BA, BA like that, so AB AB, AB BA something like that. So, this is one and two layers adjacent that is the, the dotted line shows the layer which is below the solid line 1. So, what are these indicate?

They are (111) type of planes. Similarly, you have 100 type of planes of $L1_2$ to superlattice that is nothing but every fcc type of lattice. What are the? What are the points to be noted? Anti-phase boundaries are also arise in the core of dislocations in ordered alloys and this is of considerable technological significance because of their influence on the high temperature mechanical properties of these materials.

So, this is very important that is why, I just wanted to discuss now itself so, that later we can just simply refer these dislocation activities and then move on with the property and mechanical tests and so on. As the temperature is increased the CRSS actually increases and effect known as the yield stress anomaly. See, what you have to recall here is we are going to discuss about the critical resolved shear stress. That is required for the slip to take place. In a normal FCC lattice CRSS is independent of temperature, but in this superlattice it is dependent on temperature as the temperature increases, the CRSS actually increases, that is

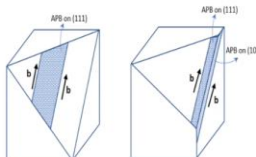
why it is called yield stress anomaly. If the order disorder transition temperature for the alloy is high enough the yield stress reaches a peak. So, you have to have this condition you can have this ordered superlattice or the alloy which contains this kind of atomic structure but they are order disorder transition temperatures should be high then we can exploit this situation to obtain a high yield stress as the I would say normally, above room temperature, I would say or any higher temperature below this transition temperature. For example, what we are looking at is the nickel base super alloy where Ni_3Al is the gamma prime phase in the gamma matrix. So, their transition temperature is in the order of 800 to 1000 Kelvin and then they exhibit this kind of hardening for in the application of turbine blades and so on. So, it is very important applications. So, this is one classical example where, it this particular idea is completely exploited for the technological advancement. In ordered state $1/2 \langle 110 \rangle$ vectors are not lattice translation vectors and so gliding dislocation leave behind a surface of disorder APB. So, in a normal FCC the lattice translation vector is $1/2 \langle 110 \rangle$. But in order the FCC $1/2 \langle 110 \rangle$ is not a lattice translation vector that is why if you just move this atom by this magnitude. Then it leaves behind the disorder that is anti-phase boundary. The perfect dislocation moving on either the $\{111\}$ or $\{100\}$ planes of $L1_2$ superlattice consists of two $1/2 \langle 110 \rangle$ superpartial dislocations joined by an APB. This is exactly we have just demonstrated in the previous slide. This super dislocation has a burgers vector $\langle 110 \rangle$ which is a lattice translation vector. So, now you have to remember this super dislocation can glide on both $\{111\}$ as well as $\{100\}$ please remember that. The spacing in equilibrium is given by the balance between elastic repulsive force between the two super partials and the opposing force due to APB energy.

So, what is going to decide? whether these two partials are going to remain like this or they are going to just remain and then move that depend upon the, in fact is the ratio of APB energy over the G_b that is elastic force. What is that we are now trying to see from this or understand from this diagram now? Suppose since we have already declared that $1/2 \langle 110 \rangle$ is not the lattice translation vector, but then just to prove that if you just move this layer, the top layer by this magnitude of $1/2[110]$. Then what happens? When you move this, this layer to this position then what happens? Instead of now, you see AB AB AB. Now, if you move like this, then it will become AA BB AA BB like what we have seen in the previous schematic. So, that is what it is creating an APB. On the other hand, very interestingly, if you look at (100) plane and the similar moment of you know the lattice translation vector if you move it, is not lattice translation vector but I am just saying if you move this layer again by $1/2 [011]$ magnitude.

Then what happens here? there is a difference if x goes to y , then that nearest neighbour bonds are not changing in (100), very very important not like in (111), (111) everything changes, it forms an APB but here the nearest neighbour is not changing and the only the second nearest neighbour will change will contribute to the APB energy. So, that is very important. So, that also indirectly says that the displacement from x to y in 100 plane. Do not alter APB or the APB energy in (100) plane is much lower than the (111) plane this is very important point to note. So, that is what we are trying to understand from that.

(Refer Slide Time: 19:33)

Dislocations in Superlattices



(a) Screw superpartial pair with an APB on a {111} plane. (b) Cross-slip onto a {100} plane starting the formation of a Kear-Wilsdorf lock

- The slip system of the ordered structure is apparently stabilized by the dislocation behaviour in the disordered state, for the Burgers vector of the superdislocation is not the shortest lattice vector, which is $\langle 100 \rangle$ in both structures in B2 ordered alloy.
- The requirement that dislocations in superlattices travel in pairs separated by an APB provides the strengthening mechanism. It arises because of a "locking" mechanism that affects the superpartial pair in the screw orientation
- The two $\frac{1}{2}\langle 110 \rangle$ dislocations will be separated by a $\frac{1}{2}\langle 111 \rangle$ APB.
- If one of the superpartials is not dissociated, it can glide on a {100} plane. This cross slip from the {111} plane to the {100} plane may be energetically favourable if the APB energy is lower on {100} than {111} which is the implication of the simple geometrical picture of nearest-neighbour coordination described above.
- Furthermore, depending on the elastic anisotropy of the crystal, the force one partial exerts on the other as a result of its stress field can enhance the stability of this arrangement

Introduction to Dislocations, 4th Edition, D. Hull and D.J. Bacon, Butterworth-Heinemann, 2009 5



So, what are the other important points? The slip system of the ordered structure is apparently stabilized by the dislocation behaviour in the disordered state, for the burgers vector of super dislocation is not the shortest lattice vector which is 100 in both structures in B2 ordered alloy. So, this we have already seen so, what is the shortest lattice vector and translation vector and so on but the requirement that the dislocation in superlattice travel in pairs separated by in APB provides a strengthening mechanism very important. So, what provides the strengthening mechanism? In this alloy or in these kinds of lattices it raises because locking mechanism that affects the super partial pair in the screw orientation. How do we understand this? Let us consider this two schematic, schematic one what you are seeing is that, there are two super partial screws super partial which is just lying on (111) octahedral plane.

And then you have the APB region and then bound by these 2 super partials and they are trying to glide on this on (111). This is what is written here screw super partial pair with APB

on (111) plane and the second one is showing trying to the super partials which is on (111) try to glide on to (100) then what happens this is what we have to see, what happens if one of these super partials is not dissociated it can glide on here (100). So, we have to understand one point here, if you recall in the previous two slides, I keep mentioning that this super partial should remain like this without dissociating further into Shockley partials that is also possible. So, if it is not dissociated and then it can move on (111) plane and then it can also glide on to (100) plane because in L1 2 systems (100) plane is also slip plane, please understand that.


The cross slip from (111) plane to the (111), (100) plane maybe energetically favourable with the APB energy is lower on (100) than (111) which is the implication of this simple geometrical picture of nearest neighbour coordination described level. So, this is very clear. So, when the glide can go to (100) plane there APB energy is lower. So, that is energetically favourable situation.

That is why it glides but then there is a problem what is the problem? Problem is furthermore depending on the elastic anisotropy of the crystal; the force one partial exerts on the other as a result of its stress field can enhance the stability of this arrangement. So, whether it goes to the next plane there are so many constraints, I am saying that there are so many constraints, it is not going to just glide easily, we are yet to discuss the crucial constraint point what is that?


(Refer Slide Time: 23:15)

Dislocations in Superlattices

- When cross slip of a screw superdislocation onto {100} planes occurs, glide of the remainder of the dislocation on the {111} system is restricted because the *Peierls stress* resisting glide on {100} is much higher than that on {111}.
- Thus, the applied stress has to be increased to maintain plastic flow. The {100} cross-slipped segment is known as a *Kear-Wilsdorf lock*.
- The effect of temperature that results in the yield stress anomaly referred to above probably arises from the case with which a $\frac{1}{2}\langle 110 \rangle$ superpartial can cross slip onto a {100} plane. If it is dissociated into two $\frac{1}{6}\langle 112 \rangle$ Shockley partials on a {111} plane, *it will have to constrict*, and the energy barrier for that can be overcome by thermal activation.
- The result is increased hardening due to cross slip with increasing temperature as seen experimentally



Introduction to Dislocations, 4th Edition, D. Hull and D.J. Bacon, Butterworth-Heinemann, 2009



When the cross slip of a screw super dislocation onto {100} planes occurs, glide of the remainder of the dislocation on the {111} system is restricted because the Peierls stress resisting glide on 100 is much higher than that of {111}. So, this is very interesting, we are

qualified to understand this statement we have now seen what is Peierls stress what is Peierls stress? Peierls stress is a stress to move a dislocation in a perfect crystal we have seen that. So, that is more on $\{100\}$ as compared to $\{111\}$. So, once the dislocation glides on $\{111\}$ plane and even though it goes to $\{100\}$ plane it gets stuck because there is a restriction by the Peierls stress this is one aspect to look at it. What are the other aspects? Thus the applied stress has to be increased to maintain the plastic flow. So, we are talking about plastic deformation here then only the dislocation will move. So, the applied force has to be increased.

So, we are talking about how the dislocation mechanisms cause the increase in the applied load or yield stress we are talking about that. So, the $\{100\}$ cross slip segment is known I mean this kind of locked system which causes the more applied stress. This segment is known as Kear-Wilsdorf lock. What is that I will go back to this image now; this is much more nicely displaying that idea.

So, it is trying to glide to (100) plane but then there is a restriction so it gets locked here, it gets locked here so, this lock is called Kear-Wilsdorf lock, very interesting point. The effect of temperature that results in the yield stress anomaly referred to above probably arises from the case with which a $\frac{1}{2}\langle 110 \rangle$ super partial can cross slip into $\{100\}$ plane. So, this could be the reason this kind of a lock or could be one of the primary reasons for the yield stress anomaly exhibited by these alloys very important point or we can also look at the other way if it is dissociated into two $\frac{1}{6}\langle 112 \rangle$ Shockley partials on a $\{111\}$ plane. It will have the constrict even if you think that we said that if the one of the partial super partial is not dissociated then it can glide even if it is dissociated into further Shockley partials of magnitude $\frac{1}{6}\langle 112 \rangle$, it has to constrict and it has to narrow down by applied load in order to become a unit dislocation then further?

So, these things require energy. So, that is an energy barrier for that can be overcome by the thermal activation. So, that is why the high temperatures provide this thermal activation through which even if it is dissociated, dislocation can combine to a unit dislocation and further glide. This results in increased hardening due to cross slip increasing temperature as seen experimentally. So, this is all experimentally determined all this hardening with a temperature increase in all the experimentally observed so, these are the dislocation core mechanisms which is responsible for I mean this is at least believed to be responsible for the yield stress anomaly. So, it also you know also gives us a nice perspective of dislocation superlattices how it behaves very differently as compared to the normal lattices. Thank you.

