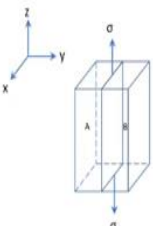


Mechanical Behaviour of Materials
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Lecture - 27
Introduction to Plastic Deformation - VI

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Plastic flow in polycrystals



- Figure showing tensile deformation of a bicrystal.
- The crystals A and B are of the same material but oriented differently with respect to the tensile axis.
- Dilational and shear strains must be matched along the interface (the xz plane) between the crystals.
- This constraint increases the flow stress of a bicrystal in comparison to that of a single crystal.

- Each crystal can be considered to have six strain components; three tensile ($\epsilon_x, \epsilon_y, \epsilon_z$) and three shear ($\gamma_{xy}, \gamma_{yz}, \gamma_{zx}$) components.
- With the coordinates of the schematic bicrystal, the following conditions must be satisfied at the grain boundary in order to provide material continuity across it:

$$\begin{aligned} \epsilon_x^A &= \epsilon_x^B \\ \epsilon_y^A &= \epsilon_y^B \\ \gamma_{xz}^A &= \gamma_{xz}^B \end{aligned}$$

where the superscripts A and B designate the individual crystals of the bicrystal.

- Since one grain has a higher value of $\cos \phi \cos \lambda$ than the other, the constraints described by above Eqs. restrict the deformation of this more favorably oriented grain and result in a higher yield stress (and a greater work-hardening response) of the bicrystal.

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Hello I am Professor S. Sankaran in the Department of Metallurgical and Materials Engineering. So, how do we appreciate this how do we explain this how to visualize this restrain or constraint. Let us now consider a bicrystal A and B there are only two crystal joined together and this is the coordinate of this diagram and then this bicrystal being subjected to tensile load tensile deformation of a bicrystal. So, the crystals A and B are of same material but oriented differently with respect to tensile axis.

So let us assume this dilational and shear strains must be matched along the interface that is xz plane between the crystals. So, we were talking about grain boundary displacement match. So, we are now considering this a bicrystal so this xz plane is an interface. So, here dilational and shear strains must be matched, so how do we visualize this? This constraint increases the flow stress of a bicrystal in comparison to that of the single crystal so that is quite obvious if the single crystal is being deformed.

Then this constraint the additional constraint would not have arisen each crystal can be considered to have a six strain components, three tensile that is ϵ_x , ϵ_y and ϵ_z and three shear γ_{xy} , γ_{xz} , γ_{yz} components. So, we understand all these shear component, strain component we

have sufficient background for that. So, with the coordinates of the schematic of bicrystal the following conditions must be satisfied at the grain boundary in order to provide material continuity across it.

So what are those conditions? The

$$\varepsilon_x^A = \varepsilon_x^B$$

$$\varepsilon_z^A = \varepsilon_z^B$$

$$\gamma_{xz}^A = \gamma_{xz}^B$$

so that is the compatibility condition, where the superscripts A and B designate the individual crystals of the bicrystal. What is the problem here now? Since one grain has a higher value of $\cos\Phi$ and $\cos\lambda$ what is this?

This is nothing but schmid factor than the other the constraints described by the above equation the restrict of the deformation of this more favourably oriented grain and results in a higher yield stress and a greater work hardening response of de bicrystal. So it is now very clear now, even though it is just two crystals joined together their orientation with respect to the tensile axis which is given by a parameter schmid factor.

Whichever the grain will have highest schmid factor will undergo the slip first as compared to the other. So, that is going to cause more strain or more stress, higher yield stress to sustain the plastic deformation or it will exhibit a greater work hardening response. So, this is one nice example to appreciate what is this grain boundary constraint.

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Plastic flow in polycrystals

In a polycrystalline aggregate, the grain boundary constraints are more restrictive than those for a bicrystal and, thus, the level of the stress-strain curve for a polycrystal is correspondingly higher

- Room-temperature tensile (force/stress)-strain curves of single crystals, bicrystals, and polycrystals of (a) niobium and (b) NaCl.

- The higher stress levels and lower ductilities of polycrystals compared to single crystals are due to the restraints that adjacent crystals in a polycrystal place on the deformation of each other.
- The level of the flow stress of a bicrystal depends on the relative misorientation of the two crystals.

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So in a polycrystalline aggregate, the grain boundary constraints are more restrictive than those for a bicrystal, and thus the level of stress strain curve for a polycrystal is correspondingly higher. So now we expect what kind of stress strain response for a single crystal and polycrystal so we just go through some couple of examples. The room temperature, tensile stress strain curves for single crystal, bicrystals and polycrystals of niobium and sodium chloride is shown here.

So, this is a very nice illustration of experimental results or illustrations what we see here is the niobium single crystal and niobium bicrystals and polycrystal and what you observe is the bicrystal exhibits much higher strength but the polycrystal exhibits significantly higher stress strain response. Of course you see that the strength goes up then the strain values comes down those are all different ideas.

But then here the focus is on the high flow stress arises from the compatibility issues or grain boundary constraints in the polycrystals that is the focus here. So, it clearly shows that idea even in the you know brittle material this is metal and this is a kind of ionic solid. So, it also clearly shows that a single crystal sustained curve though there is no significant work hardening or something.

But if you look at the polycrystal the flow stress is quite steep here as compared to single crystal and bicrystal so that is the illustration here. So, the level of flow stress of a bicrystal depends on the relative misorientation of the two crystals this is very demonstrative.

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Plastic flow in polycrystals

- Each grain in a polycrystal has three shear and tensile components of strain as described above for a bicrystal. However, only five of these are independent, because the dilational strains are related through the constant-volume condition ($\epsilon_x + \epsilon_y + \epsilon_z = 0$) of plastic deformation.
- It can be shown that *five independent slip systems* are required to meet the *boundary compatibility requirements* (these arise from the five independent components of strain).
- That is, the matching of displacements across the boundary necessitates the operation of five independent slip systems, at least in the vicinity of the grain boundaries, in each crystal of the aggregate.
- The term *independent slip systems* needs clarification.
- The number of independent slip systems is related to, but not equal to, the *number of geometrical slip systems*.
- An independent slip system is one for which slip displacements on it can not be duplicated by a combination of displacements on other slip systems.





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So, each grain in a polycrystal has three shear and tensile components of strain as described above for a bicrystal. However out of these six only five of these are independent, because the dilational strains are related through the constant volume condition what is that? That is $\epsilon_x + \epsilon_y + \epsilon_z = 0$ of the plastic deformation. Plastic deformation results in a constant volume. So, this there is a condition there so because of this though we see the six components and the out of six only five of them are independent.

It can be shown that five independent slip systems are required to meet the boundary compatibility requirements these arise from the five independent component of the strain. So, now, we are bringing another terminology or I would say fundamental requirement for plastic flow five independent slip systems are required to meet boundary compatibility requirements how do we understand this?

That is matching of displacement across the boundary necessitates the operation of five independent slip systems at least in the vicinity of the grain boundaries in each crystal of the aggregate very important. So, in order to you know proceed with the deformation without creating a void or cracks the matching of displacement across the boundary is necessary and in order to do that, at least five independent slip systems.

In the each grain at least in the vicinity of the grain boundaries are must that is the idea otherwise the plastic deformation will proceed with some effects. So, now we will concentrate on the term independent slip systems, what is an independent slip systems? The

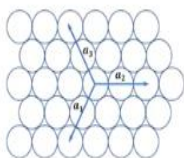
number of independent slip systems related to but not equal to that number of geometrical slip systems.

So when we say that you know the six components three tensile, three shear they are all geometrical slip systems but not necessarily have independent slip systems that is valid for all the crystal systems we can just take some examples to understand this will let us proceed an independent slip system is one for which slip displacements on it cannot be duplicated by a combination of displacements on other slip systems. How do we understand this? We will take some example.

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Plastic flow in polycrystals

- The concept can be illustrated by consideration of basal slip in the hexagonal close packed structure.
- As shown in Fig., there are three geometrically distinct slip systems (the three nonparallel close-packed directions $\bar{a}_1, \bar{a}_2, \bar{a}_3$) within the basal plane in this structure.
- However, an arbitrary displacement in the (positive) $\bar{a}_3$ direction can be duplicated by a combination of equal slip in the (negative) $\bar{a}_1$ and $\bar{a}_2$ directions.
- Thus, the number of independent slip systems for hexagonal basal plane slip is two and not three.



- The basal plane in a hexagonal close-packed crystal; the three nonparallel slip directions are noted.
- Although there are three geometrically distinct slip systems, only two are independent in that an arbitrary displacement along the $\bar{a}_3$ slip direction can be duplicated by a suitable combination of slip in the $\bar{a}_1$ and $\bar{a}_2$ directions.



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The concept can be illustrated by considering a basal slip in a hexagonal close packed structure. So, let us take this hexagonal close packed structures where three geometrically distinct slip systems three non-parallel close packed directions $\bar{a}_1, \bar{a}_2, \bar{a}_3$ within the basal plane in this structure so, these three geometrically distinct slip systems are taken. However, an arbitrary displacement in the positive $\bar{a}_3$ direction can be duplicated by a combination of equal slip in the negative $\bar{a}_1$ and $\bar{a}_2$ directions. So, what does it mean?

Suppose if I travel from this point centre along this a_3 vector by 2 units, 1, 2 I am traveling this and then this is my end point. I can also arrive at this point by travelling the negative you know directions of a_2 and a_1 how do I do that? So, if I choose to travel from this end and this direction is negative of a_1 so 1, 2 I am reaching here if I use a_2 that is this and this direction is negative.

So, from here I will go 1, 2 so, I can get see this is what it is shown it cannot be now I am duplicating a_3 by combination of a_1 and a_2 so this is not considered independent. Thus the number of independent slip systems for hexagonal basal plane slip is two and not three. So, this is a nice example to understand this.

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Plastic flow in polycrystals

- The higher flow stresses of polycrystals are also due to geometrical considerations relating to the differing orientations of the individual crystals of the aggregate with respect to the tensile axis.
- Each crystal has its own *characteristic value of the Schmid factor* ($1/m$) and those with the lowest tend to deform last in a tensile test.
- It is reasonable that the tensile yield strength (σ_y) relates to τ_{CRSS} by geometrical relations existing between τ and σ . Thus, in analogy to Eq. , we can write

$$\sigma_y = \bar{m} \tau_{CRSS}$$

where $\bar{m}$ is a suitable average for the polycrystal.

- Many of the dislocations accumulated during plastic flow result from multiplication processes.
- Since dislocation encounters leading to multiplication are "chance" encounters, dislocations accumulated by such processes are called statistically stored dislocations; their corresponding density is designated ρ_s .
- Some plastic deformation is accompanied by internal plastic strain gradients.
- When such gradients are present, *geometrically necessary dislocations (GNDs)* are accumulated in addition to the statistically formed ones.



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The higher flow stresses of polycrystals are also due to geometrical consideration relating to the differing orientations of the individual crystals of aggregate with respect to tensile axis. Each crystal has its own characteristic value of the schmid factor and those with the lowest tend to deform last in a tensile test the highest will deform first, the lowest will deform last that this schmid factor this is one straight forward thumb rule.

So, it is reasonable that the tensile yield strength σ_y relates to τ_{CRSS} by geometrical relation existing between τ and σ . And thus in analogy of the above equation we can write

$$\sigma_y = \bar{m} \tau_{CRSS}$$

the equation which is considered here is the schmid law where $\bar{m}$ is a suitable average for the polycrystal. Many of the dislocations accumulated during plastic flow result from the multiplication process.

Since the dislocation encounters leading to multiplication or chance encounters the dislocation accumulated by such process are called statistically stored dislocations. So, now we are now classifying the kind of dislocation we get generated during plastic deformation before even I go to this description, I just want to add few more points to this schmid factor idea.

So, we say that the highest slip system are the grains in a polycrystal the grain which exhibits highest schmid factor that means that grain is most favourably oriented for this slip, that is the physical mean but that is not alone the factor, how the you know the other grains are going to facilitate for example, you assume that the highest schmid factor grain starts deforming first in a polycrystalline microstructure and as the deformation proceeds if there is no guarantee that the grain which started deforming.

In the first will continue to deform till the end in the same manner, at least the same rate or I would say that this the accumulation of the strain inside that individual grain it is not going to be the same rate till the fracture or the end of this plastic deformation. So, what is that I am trying to say though we say that the grain which has the highest schmid factor will start yielding first, but as the deformation proceeds you do not know what will happen to that strain some other they may start deforming much faster than the grain as the deformation proceeds.

So, it is not just a characteristic schmid factor alone is going to decide the strain accumulation across the gauge length it is a characteristic geometrical constraint each grain experiences during plastic deformation that decides the overall strain accumulation across the gauge length. So, this is one point you have to remember very important point. So, because such a close observations in terms of strain measurements are all just being done now and there are evidences that these kinds of deformation behaviour is happening.

So, it is not just schmid factor there are some other factors at least I would consider to call them as characteristic geometrical constraints during the plastic deformation. Now, we move on to this classification of dislocation what are we saying here? As the deformation proceeds the dislocation density multiplies so, that means the dislocation, dislocation interaction also the probability of the dislocation interacting with other dislocation is also increasing.

So, this is by chance that means, when the dislocation is meeting the other dislocation so frequently because the dislocation density is high. So, this by that process it is also multiplying so it is by chance it is getting generated that is why it is called statistically stored dislocation some plastic deformation is accompanied by internal plastic strain gradients.

Suppose, if the plastic deformation also accompanies or just generates a strain gradient inside the material then what type of dislocation it will generate?

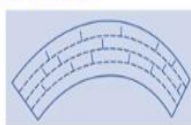
When such as gradients are present geometrically necessary dislocations are accumulated in addition to the statistically formed ones so this is very interesting you have to pay a little more attention to grasp this idea. So, you can ask how this you know, strain gradients are not created in the general plastic deformation that is not the question. The question is how the dislocations are generated, that is the question.

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Geometrically Necessary Dislocations





(a) Plastic bending of a bar of length l and thickness t to a radius of curvature r as in (b) produces a tensile strain on the outer, and a compressive strain on the inner, bar surface. Thus, there are a greater number of atomic planes ($[(l + \delta l)/b]$; b = interatomic spacing) on the outer surface than on the inner one $[(l - \delta l)/b]$. (c) This strain gradient is accommodated by introduction of $2\delta l/b$ geometrically necessary dislocations into the crystal.

- On bending the bar to a radius of curvature r (Fig.) the upper portion of the crystal undergoes tensile deformation; i.e., its length is increased from $l (= r\theta)$ to $l + \delta l (= (r + \frac{t}{2})\theta)$, with δl being positive and of magnitude $t\theta/2$.
- Conversely the inner circumference undergoes compression with a negative length change $t\theta/2$.
- Thus, a strain gradient accompanies the bending, and the magnitude of the strain gradient is the strain difference between the two surfaces ($= 2\delta l/l$) divided by the distance (t) over which the gradient exists, i.e.

$$\text{Strain gradient} = 2 \frac{\delta l}{l} = \frac{\theta}{t} = r^{-1}$$

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So we will see some nice way of illustration suppose you take this single crystal of this dimension measuring length l and the thickness t and it is being subjected to plastic bending like this is what is described here, the plastic bending of the bar of length l and thickness t to a radius of curvature r , this is the radius of curvature r produces a tensile strain on the outer and the compressive strain on the inner surface.

So since it is a bar so inside it is creating a compressive strain and outer it is a tensile strength what are the other quantities we can look at it. So since the length is extended from $l + \delta l$ and here the length is contracted from l to $l - \delta l$ that means, there are greater number of atomic planes that is $(l + \delta l)/b$ where b is inter atomic spacing. So this is theoretically possible when the length is increasing that means, you can greater number of atomic planes on the outer surface than in the inner surface which is nothing but $(l - \delta l)/b$.

This strain gradient is accommodated by introduction of $2\delta l/b$ geometrically necessary dislocation into the crystal. So, that is what is shown here suppose, the increase in the length of the outer surface and the decrease in the length of inner surface that can be accommodated by introduction of the edge dislocation of I mean similar sign here. So this kind of extension of the length is possible by introducing the dislocation like this on the several planes in the crystal.

So we will look at it a little more closely how do we understand this on bending the bar to radius of curvature r the upper portion of the crystal undergoes tensile deformation that its length is increased from l , which is also $r\theta$, you can look at this diagram it is easy to understand $2l + \delta l$ which is also $(r + t/2)\theta$, you see that this is a t and we are saying that we are dividing this upper and inner so it is $t/2$ with the δl being the positive and it has got the magnitude of $t\theta/2$.

So, δl has the magnitude of $t\theta/2$. Conversely the inner circumference undergoes compression with a negative length change of $t\theta/2$ this is positive change, this is negative change. Thus, the strain gradient accompanies the bending and the magnitude of the strain gradient is the strain difference between the two surfaces. So, let us understand this so, strain difference is $1 + \delta l - (1 - \delta l)$ so that will become you know $2\delta l/l$ is the strain.

And this is a difference in the two surfaces and divided by the distance over which the gradient exists that is the gradient exists from the inner surface to the outer surface that is thickness is t . So, we are calculating not just difference, but we are calculating this strain gradient. So, the strain gradient is simply you can visualize this $2\delta l/l$ which is equal to θ/l because you substitute this $t\theta/2$ here so, then you get θ/l which is nothing but r^{-1} .

So, we are defining this $r\theta$ so, it is r^{-1} so strain gradient is r^{-1} so what do you mean by this? What is strain gradient, the rate of change of strain within the volume of the plastic deformation the volume over which the plastic deformation takes place where the rate of change of strain is happening this way. So, that is how you have to understand the strain gradient.

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Geometrically Necessary Dislocations



- The number of crystal planes on the tension surface is the surface length divided by the interatomic spacing b (b is also the Burgers vector magnitude).
- Likewise, the number of atomic planes on the compressed surface is $(l - \delta l)/b$.
- This difference in the number of atomic planes between the surfaces is accommodated by the *introduction of edge dislocations* (all of the same sign) into the crystal, as illustrated in Fig.
- *These are geometrically necessary dislocations.*
- Their number is $2\delta l/b$ and their density ρ_G is this number divided by the crystal surface area, lt . Hence

$$\rho_G = 2 \frac{\delta l}{lt} = (rb)^{-1} = \frac{\text{strain gradient}}{b}$$
- Note that if there were no strain gradient, no geometrical dislocations would be present.
- Moreover, we emphasize that the geometrical dislocations present are in addition to those stored statistically so that the total dislocation density is $(\rho_s + \rho_G)$.

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So now the number of crystal planes on the tension surface is the surface length divided by the interatomic spacing b , b is also the Burgers vectors magnitude sometimes we can take it like that, likewise the number of atomic planes on the compressed surfaces $(l - \delta l)/b$, the difference in the number of atomic planes between the surfaces accommodated by introduction of edge dislocation.

So, you just understand the extra half planes you are introducing all over the place in the outer surface obviously, you know the length will increase. So, this kind of dislocations are called geometrically necessary dislocation see this illustration very nicely fit to the context. So to keep up the geometry to the additional length we are introducing the dislocation into the crystal system. So, that is why it is called the geometrically necessary dislocation.

Their number is $2\delta l/b$ and the density ρ_G is the number divided by the crystal surface lt . So the surface is lt because the length l and width t . Hence,

$$\rho_G = 2 \frac{\delta l}{lbt} = (rb)^{-1} = \frac{\text{strain gradient}}{b}$$

which is nothing but $(rb)^{-1}$ we can also relate that equal to strain gradient/ b please very important point here note that if there were no strain gradient, no geometrical dislocations would be present that is quite obvious.

There is no strain gradient we would not have introduced you know edge dislocation on the top surface if it is a perfect circle I mean a perfect strip of a single crystal there is no strain gradient and strain gradient we have produced by bending it and then doing that we had to

introduce an additional dislocation to accommodate this bending plastic deformation. So this is conceived idea to understand this concept.

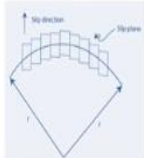
Moreover, we emphasize that geometrical dislocations present are in addition to those stored statistically so, that the total dislocation density is $\rho_s + \rho_G$.

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Geometrically Necessary Dislocations

- The precise density of GNDs depends on the orientation of the slip plane and direction with respect to the bending axis.





The figure illustrates a situation where bending can be accomplished without the introduction of GNDs.

- The single crystal shown here can be bent without the need of introducing geometrical dislocations into it.
- This is because the slip direction is normal to the axis of bending and the slip plane normal is parallel to this axis.
- Thus, the change in shape is accomplished solely by dislocation motion and no plastic strain gradient exists between the sample surfaces.
- Ordinary dislocation glide accommodates the shape change for this situation. Thus, for the general case, the geometrically necessary dislocation density is expressed as
$$\rho_G = \alpha \frac{\text{strain gradient}}{b}$$
where α is a constant of order unity.



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So the precise density of GNDs depends on the orientation of the slip plane and the direction with respect to the bending axis. So, this is another important idea about this GNDs let us look at that what is that? The figure illustrates the situation where the bending can be accomplished without the introduction of the GNDs. See, previously we said that additional edge dislocations are inserted to accommodate the plastic deformation that is how the length of the outer surface got increased from l to $l + \delta l$.

But now, we are seeing we can also do this without introducing GNDs how do we understand this? The single crystal shown here can be bent without the need of introducing geometrical dislocation into it. This is because the slip direction is normal to the axis of bending and the slip plane normal is parallel to this axis. So what is this axis? The axis is this, through which we are bending see this is a slip direction and the normal to the slip plane are also parallel to this and slip direction is perpendicular to this axis.

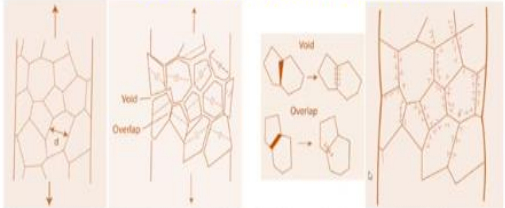
And that is why they each slip plane is you know you can see that each one is a glide plane so it simply glides and then it produces the slip over and there is no gradient. Thus the change in shape is accompanied solely by a dislocation motion and no plastic strain gradient exists

between the sample surfaces. So, that is why it is important to understand that GND density depends upon the orientation of the slip plane and direction with respect to the bending axis or any plastic deformation orientation.

Ordinary dislocation glide accommodates the shape change for this situation thus for a general case the geometrically necessary dislocation density is expressed as $\rho_G = \alpha \cdot (\text{strain gradient}/b)$, where α is a constant of order unity. So this is one way of understanding this strain gradient.

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Geometrically Necessary Dislocations



- An alternative way of viewing the constraints that individual crystals place on each other during polycrystalline deformation is provided in Fig.
- The figure shows that geometrically necessary dislocations can provide compatibility of displacements between adjacent grains.
- Figure shows the deformation that each grain would experience in the absence of constraints, i.e., the strain it would undergo if deformed as a single crystal.
- Without the constraints, either voids or grain "overlap" would ensue, and this does not happen.
- In addition to previously discussed aspects of multiple slip, voids or overlaps among grains can be eliminated by geometrically necessary dislocations that accommodate the strain gradients that exist between individual grains.
- The dislocation arrangements required to produce compatibility are illustrated in Figs.

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How this concept is useful in a general case in a polycrystalline deformation how this concept is useful. So, if you look at this schematic here the image is a polycrystalline microstructure which has been subjected to tensile deformation the average grain diameter is d and what is shown here is you can see that as the deformation proceeds you are able to see that the creation of voids and the overlaps of the strain to the other this situation shown here is you know completely unconstrained deformation.

So that is what we are saying here an alternative way of viewing the constraints that individual crystals place on each other during polycrystalline deformation is provided these four figures. The figure shows that geometrically necessary dislocations can provide compatibility of displacements between adjacent grains. So, what happens is this is without constraint I mean it produces the voids and overlap.

And what can be done here is to avoid this void instead of a void it can be a dislocation spread on the interface. Instead of overlap, it could be a dislocation distribution between them just to accommodate that kind of constraints that is what it is showing. Figure also shows the deformation that each grain would experience in the absence of constraints that is the strain it would undergo, if it deformed as a single crystal that is what is shown here. Without the constraint voids and would ensue and this does not happen in a reality.

So all these voids and overlaps are nicely accommodated through generation of geometrically necessary dislocations. And whatever the ideas we have seen, it nicely supports this concept. And in addition to the previously discussed aspects of multiple slip voids and overlaps among the grains can be eliminated by geometrically necessary dislocation that accommodate the strain gradients that exists between the individual grains and the dislocation arrangements required to produce compatibility are illustrated in this figure.

So what you see here is we have brought this concept of GNDs and also we have now shown how in polycrystalline deformation, how it accommodates the strain gradient and allow the deformations to proceed without forming the voids or overlap other defects and so on. We will stop here and we will continue our discussion in the next lecture. Thank you.