Nanostructures and Nano materials:
Characterization and Properties

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Lecture - 42
Deformation Behavior of Nanomaterials

In this lecture, we learn about the deformation behaviour of nano materials, in this world we always worry about nanotechnology. It means, we need to synthesise nano materials into some useful shapes. So, that is the reason we need to know exactly what will happen once we start deforming a material and make it into some useful shapes.

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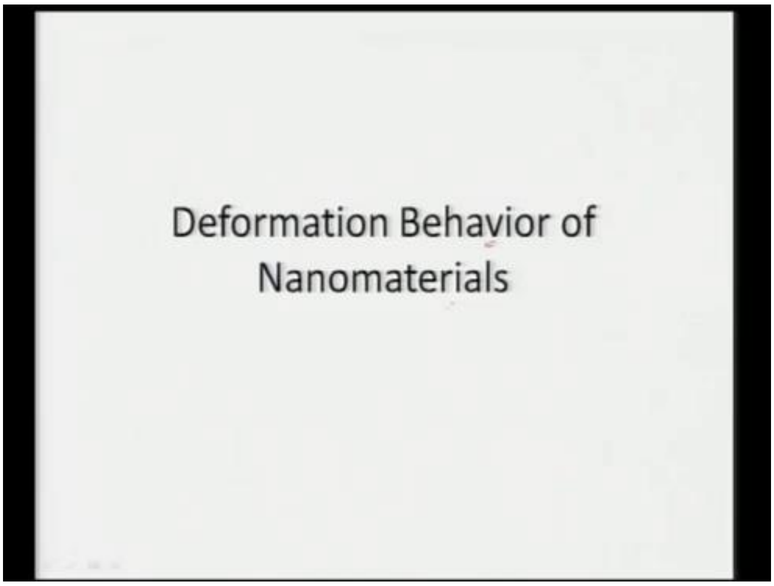

Deformation Behavior of Nanomaterials

So, that is why the deformation behaviour of nano materials it is a very key component in devising nanotechnology. So, we need to learn what is the science? What is the mechanism through which nano materials can respond to certain mechanical stress? Also, there had been very, very contrasting theories related to nano materials because it is very difficult to exactly pin point what is happening in that scale. Again, depending from material to material say from a very ductile copper to ceramic materials, the method of deformation can be very, very different.

And again, with wearing grain sizes generally, a material will not a uniform grain size it might have a variation of grain sizes starting from nano materials to say micro meters.

So, the overall deformation mechanism in nano grains is very, very different than that of micro grains. And also, the interplay between nano and micro can also lead to very much difference in the mechanical property response.

So, that is why people generally researches they find very contrasting properties in terms of the way nano materials behave. So, there is a consistency in terms of developing a material with a consistent grain size and then having seen what is exactly happening at that particular scale is very, very important. So, there are couple of theories which have basically come across.

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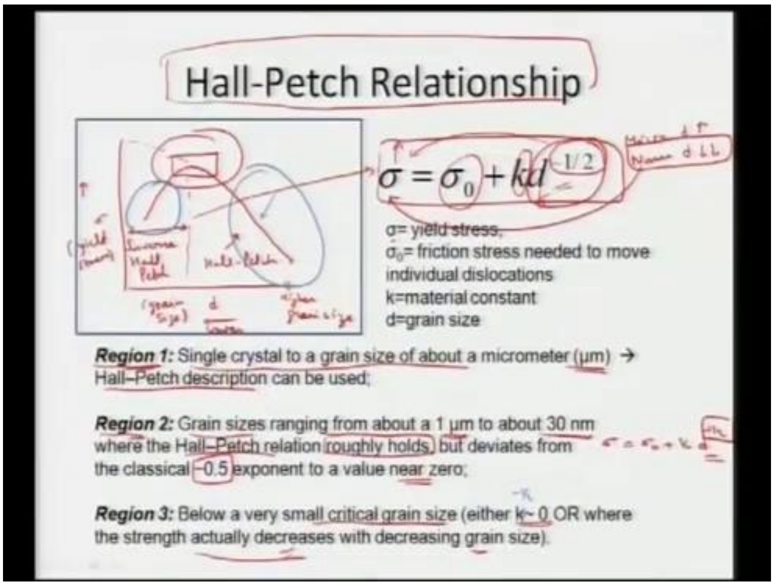

Hall-Petch Relationship

$$\sigma = \sigma_0 + kd^{-1/2}$$

σ= yield stress,
σ_0= friction stress needed to move individual dislocations
k=material constant
d=grain size

Region 1: Single crystal to a grain size of about a micrometer (μm) → Hall–Petch description can be used;

Region 2: Grain sizes ranging from about a 1 μm to about 30 nm where the Hall–Petch relation roughly holds but deviates from the classical −0.5 exponent to a value near zero;

Region 3: Below a very small critical grain size (either k~ 0 OR where the strength actually decreases with decreasing grain size).

So, starting from the very well-known Hall-Petch relationship and the Hall-Petch relationship is given by sigma equal to sigma naught k d power minus 1 by 2 or k under root d. Where, sigma is a yield stress, sigma naught is the friction stress needed to move the individual dislocations, k is a material constant and d is the grain size. So, we can see the yield stress will start increasing, as we have lower and lower grain size. So, that is the basic method of basic relationship between the yield stress and the grain size of the material.

So, we can definitely find that micro when we have micro grains, we have d which is pretty high and then when we have nano grains when d is pretty low. Then we can see when we have nano grains our ultimate yield stress will very, very high. So, that is why people now, start towards manufacturing bulk nano structured materials. Again, in this relationship though it is a continuous relationship, we can see that that once we have sigma and we have grain size.

So, we can see the grains as we have this side is nothing but higher grain size. So, as so we can see as we go for a lower grain size our yield stress starts increasing, but after certain point what happens is, that it starts decreasing at certain point as well. So, according to this relationship Hall-Petch relationship, the stress should keep increasing as we go along. So, this should keep increasing with respect to decreasing grain size, this is a grain size along this side along x axis, along y axis we have the yield stress.

So, this should keep increasing as we lower the grain size, but after certain point we start decrease in the yield stress and this region is called inverse Hall-Petch and this is the Hall-Petch relationship. This also is a reason of concern as we go along I will talk about it. So, this Hall-Petch relationship talk about that sigma equal to sigma naught k d power minus 1 by 2. So, as we start decreasing the grain size we should see a increase in the yeild stress.

There are 3 regions, which are of concern to us right now, we can see that region one. Region one is the it is a region, where we have well as behaviour of Hall-Petches descriptions. So, the Hall-Petch relation is maintained in reason one that is for single crystals to a grain size of about a micrometre. So, when we have grain size pretty high from a single crystal approximately say 1 micrometre, the Hall-Petch relationship is very much valid. That it means, that the sigma is really dependent on the d power minus 1 by 2, so as we start decreasing the grain size we will see an increase in the yield stress.

In region two what is happening is starting from 1 micrometre to say approximately around 30 Nano meters. So, for the grain size which are ranging from around 1 micrometre to about 30 Nanometre Hall-Petch relationship is approximately or roughly holding it, but again it debits from the classical exponents. So, in this case our exponent of sigma equal to sigma naught plus k d power minus 1 by 2. So, this exponent instead of minus 0.5 it comes out to be approximately near 0.

So, that is that is one more possible explanation that because we will come to that later, but what we can see here is that as we are reducing the grain size, we are seeing that exponent is now coming to approximately 0. So, that is what we can see there is slope is approximately along this side. Again if we go much below than that so below a small critical grain size. So, we can again see that our k itself, the constant itself can be 0 or where the strength actually decreases.

So, what is happening is our k is also going to 0 and also our strength is actually decreasing as we decrease the grain size. So, we are talking about this region, so this region in this case we can see that there is a decrease in the yield stress as we are lowering the grain size. In this region we have very, very well maintenance of the Hall-Petch relationship. So, in this case we do not worry much about it because it is well following the Hall-Petch relationship. And then the second region, where we have grain say between 1 micro meter 30 nano metres. The overall exponent of minus 0.5 is basically coming going to approximately 0.

And third case, also we can see the slope itself also is going to 0 it is not k I guess it is slope, the slope is from minus 1.5 it is not going to same, but it is going to 0 itself in the third case as well. So, we can see the Hall-Petch relationship can be described into 3 regions, one region where we have well maintenance of validation of Hall-Petch relation. Then second case the k, the exponent is approximately 0 and the third case we have again decreasing value of yield stress as we further lower the grain size. And that limit is approximately around 15 to 30 nano metre and it can depend from material to material.

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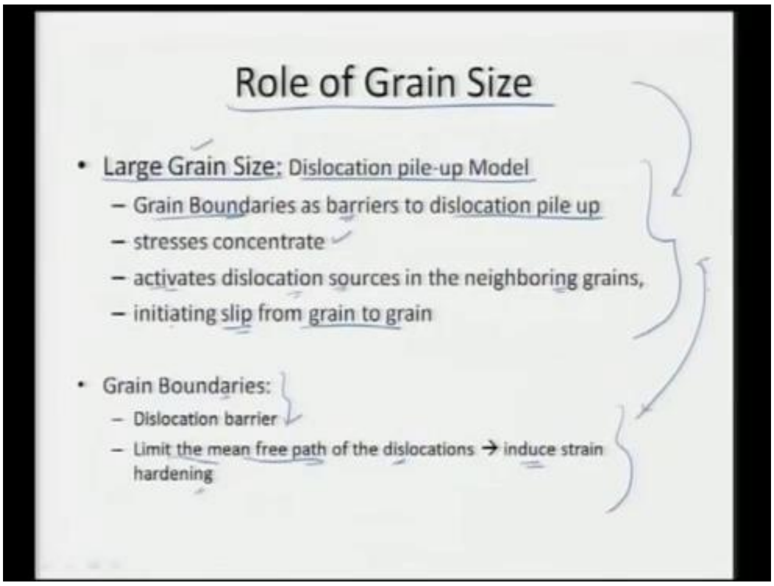

Role of Grain Size

- Large Grain Size: Dislocation pile-up Model
  - Grain Boundaries as barriers to dislocation pile up
  - stresses concentrate
  - activates dislocation sources in the neighboring grains,
  - initiating slip from grain to grain
- Grain Boundaries:
  - Dislocation barrier
  - Limit the mean free path of the dislocations → induce strain hardening

So, what is the role of grain size so there are basically, two models which describe the role of grain size. So, we can see once we have a large range grain size, it incorporates the dislocation pile up model. It means, its associates dislocation it means, pile up occurs due to presence of grain boundary and grain boundary act as a barrier from where, dislocation pile up is accommodated.

And that in turn, will activate the dislocation sources in the nearby grains. So, once we have a grain boundary it is acting as barrier to dislocation pile up. Therefore, what will happen it will start inducing some stress concentrations and that will activate the dislocations sources in the nearby grains? So, in that case it will start initiating slip from grain to grain so once grain will start slipping, it will again lead to the deformation of the grain at much higher stress level

Dislocation pile up theory is applicable to nonmaterial provided that there cannot be high number of dislocations within a grain. And what they will do is, they will limit the mean free path for the dislocation. So, as soon as we have more and more grain boundaries it will start decreasing the distance between the dislocations. And that basically, will induce strain hardening because now, we have more number of dislocations per unit area.

So, we can see there are two different approaches for large grain size, it will act as a barrier to dislocation pile up and that will induce some dislocation sources in the nearby grains. And that will initiate he slip from grain to grain, but at much higher stress level. And secondly, it from the grain boundaries which act also act as a dislocation barrier and they will limit the mean free path of dislocation in turn it will also induce strain hardening. So, that is the way the role of grain size has been defined by two contrasting cases.

So, that is again leading to the some stress, some additional stress that is being generated because of the presence of grain boundaries. So, we can see in a nano crystalline material we have more number of grain boundaries or a very, very high grain boundary area. So, that in turn will generate that will initiate much more of dislocation sources in a nearby grains as well. Even if it is acting as a dislocation pile up, so it will also induce some stresses. It will limit the mean free path of a dislocation and it will again require much more higher stress to pass along the to cover the obstacle of grain. So, in turn will have will observe much strain hardening in this case.

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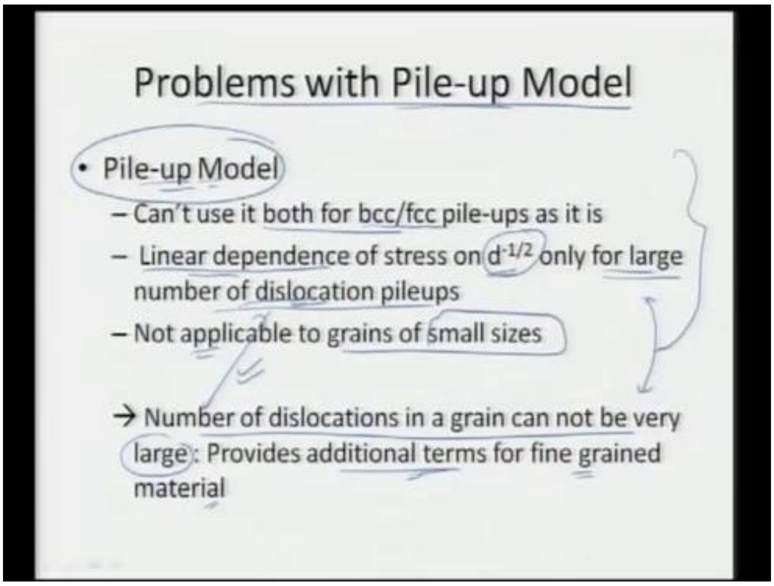

Problems with Pile-up Model

- Pile-up Model
  - Can't use it both for bcc/fcc pile-ups as it is
  - Linear dependence of stress on $d^{-1/2}$ only for large number of dislocation pileups
  - Not applicable to grains of small sizes

→ Number of dislocations in a grain can not be very large : Provides additional terms for fine grained material

But again, there are some problems with the pile up models, so dislocation pile up though it has been said that dislocation start to pile up near the grain boundary. To initiate the stress or they in hence the strain hardening, but again the pile up model we cannot use as it is for both BCC as well as FCC because one more thing is that it is being told that, there is a linear dependence of stress of d power minus 1 by 2, but it is only for large number of dislocation pile ups.

So, what happens is that this model is valid only for grain size approximated 1 micrometre. So, what will happen once the grain sizes much below 1 micrometre, we do not have enough number of dislocations pile up which can occur in a material? So, this pile up model does not become applicable to grains which are of smaller sizes or much lesser than 1 micrometre, but still we see increase in the yield stress which is responsible for enhanced strength of nano crystalline material.

So, this pile up model though we keep saying the grain models are acting as resistors or as a pinning agents for dislocation pile up, but that does not hold true for nano crystalline material. Because first of all this pile up model though it is much well accepted it cannot be utilized for both FCC and BCC type of pile ups as it is. And secondly, there is a linear dependence of stress on deeper minus 1 by 2, but only for large number of dislocation pile ups.

So, as we go about reducing the grain size what will happen we will have only very few dislocations that can occur in a nano crystalline material. So, they do not become applicable to grains of much smaller size, because what is happening here is number of dislocations in a grain size cannot be very large. And the overall assumption here is that we have a large number of dislocations pile ups. So, these two are very, very contrary in nature for nano crystalline as well as micro crystalline. To this pile up model basically cannot really describe what is happening at the nano crystalline regime.

So, we always require some additional terms for the fine grain materials. So, that is why we can see that what is applicable for a forth grain material does not hold true for a fine grain material as well. So, we need to incorporate some additional terms which can take care of this strengthening in the nano crystalline regime. So, these are again the limitations of this pile up model. So, though we are saying that the grains are being responsible for inducing the strain hardening, by either inducing the dislocation nucleation sites in the other grain or initiating nucleation of dislocation sources at other grains or by inducing the pile up by occurring as a barrier to the dislocation.

So, the overall mean free path of dislocations will reduce and that will induce strain hardening, but that requires that the number of dislocations are pretty high. And though that can occur in micro crystalline material that may not hold to for nano crystalline material because in a nano grain we might have very limited region to that may allow say 1 or 2 or 3 or 10’s of dislocations and not more. So, in that turn we require some additional terms to describe a very fine grain material.

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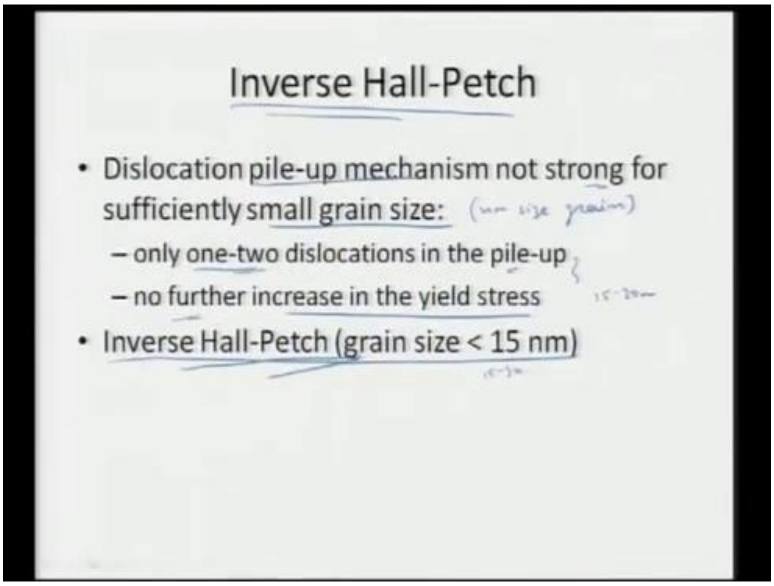

Inverse Hall-Petch

- Dislocation pile-up mechanism not strong for sufficiently small grain size: (nm size grains)
  - only one-two dislocations in the pile-up
  - no further increase in the yield stress 15-30nm
- Inverse Hall-Petch (grain size < 15 nm) 15-30

And also, what is so what is being observed in (Refer Time: 12:52) of that is the dislocation pile up mechanism is not so strong for very fine grain size or a nano metre size grains. So, in turn we will see only 1 2 or maybe 5's of dislocation in the pile up. So, ideally we should not see any further increase in the yield stress. And also, for grain size which are very less than say 10, 15 to 30 nanometre, we will see a inverse Hall-Petch relationship. It means, the overall strength reduces as we increase reduce the grain size.

So, that is again one more finding of this inverse Hall-Petch relationship that the average thing is kind of scattered. So, there are no grains available for inducing the dislocation. And so thereby, we can see an inverse Hall-Petch relationship with grain size less than 15 to 30 nanometre or so because now, there are only 1 or 2 dislocation which can basically pile up. And much below that even one dislocation may find very hard to go into there. And there no further increase in the yield stress or eventually the yield stress basically, decreases as we reduce the grain size that thing is been given as a inverse Hall-Petch relationship.

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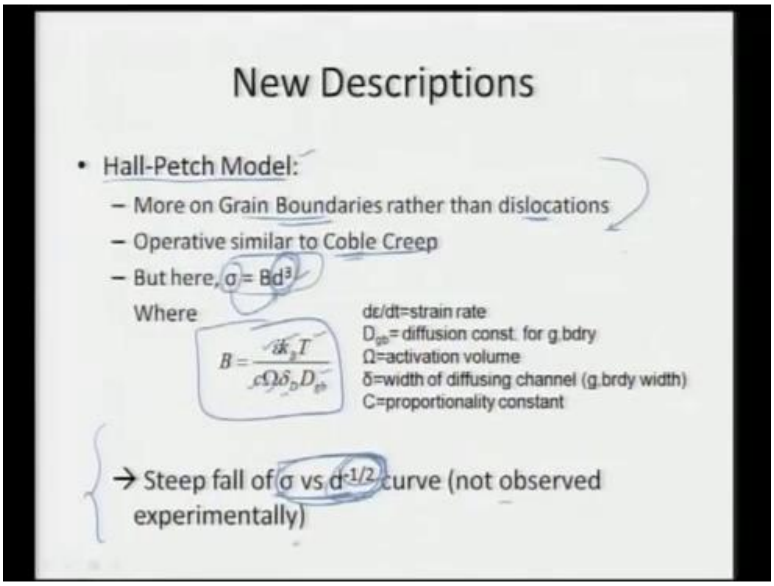

New Descriptions

- Hall-Petch Model:
  - More on Grain Boundaries rather than dislocations
  - Operative similar to Coble Creep
  - But here, $\sigma = Bd^3$

  Where

$$B = \frac{\dot{\varepsilon} k_B T}{c\Omega\delta_D D_{gb}}$$

dε/dt=strain rate
D_{gb}= diffusion const. for g.bdry
Ω=activation volume
δ=width of diffusing channel (g.brdy width)
C=proportionality constant

→ Steep fall of σ vs $d^{-1/2}$ curve (not observed experimentally)

So, essentially new descriptions are required to basically, model what is happening at the because of grain boundary. So, Hall-Petch model is now being said that it is acting more on the grain boundary rather than all dislocation. So, once we talk about dislocations we say about dislocation pile up or generating new sources of dislocation, but right now we can say that Hall-Petch model is more on grain boundary rather than the dislocations.

And it is found that the overall, operation of this one is very similar to that of Coble Creep, but in this case, what is the case is the overall stress is proportional to the D q. So, what is happening here is, so we also say that there is some stress which is responsible for the deformation of this material with respect to D q. So, what we can see here is that oral constant that B, is not dependent on strain rate, Boltzmann constant, absolute temperature.

C is the proportionality constant, omega is the activation volume, delta D is the width of the diffusing channel of the grain boundary and D g b is the diffusion constant for grain boundary. So, we can see the slip can also occur along the grain boundaries and that is responsible for the overall stress. That is being induced by the material for its further deformation. So, but in this case what we are seeing here is, that the sigma has a dependence of D q. So, the stiff fall of sigma versus d minus 1 by 2 is not observed experimentally.

So, that is what we can say here is so for very, very fine grain sizes the overall sigma versus d power minus 1 by 2 curve it is not exactly being observed experimentally. So, again it further needs that though we can incorporate this Coble Creep into the model. It requires some more modification for encompassing the decrease that occurs below certain grain size.

And also, the relationship of deeper minus 1 by 2 only in the micro crystalline regime and then approximately a constraint value of this exponent, along certain grains size limits. So, that is to incorporate that this was a earlier model which basically came into existence by comparing the Coble Creep or the grain boundary diffusion along for encompassing this deformation.

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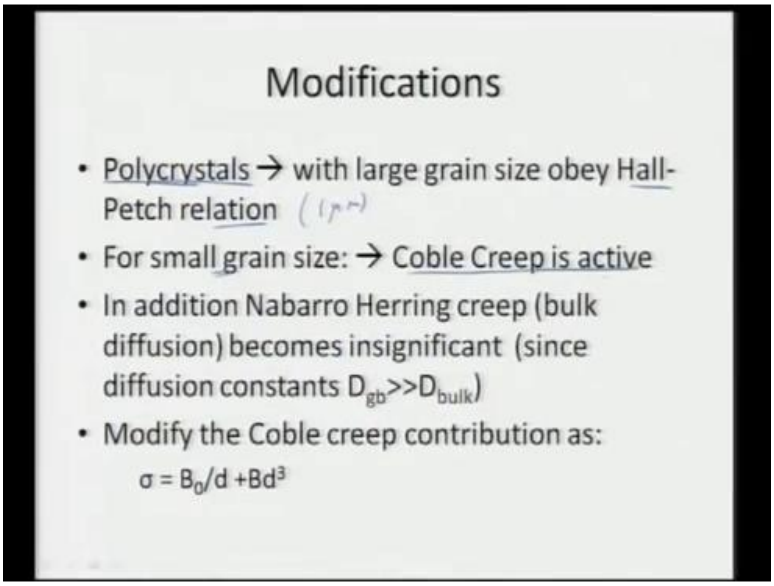

Modifications

- Polycrystals → with large grain size obey Hall-Petch relation (1 μm)
- For small grain size: → Coble Creep is active
- In addition Nabarro Herring creep (bulk diffusion) becomes insignificant (since diffusion constants $D_{gb} >> D_{bulk}$)
- Modify the Coble creep contribution as:
  $\sigma = B_0/d + Bd^3$

So, again we can see that the poly crystals with very large grain size, they will obey Hall-Petch relationship when the grain size is approximately till 1 micrometre, but what is happening is for very smaller grain size, much smaller than 1 micrometre this Coble Creep is active.

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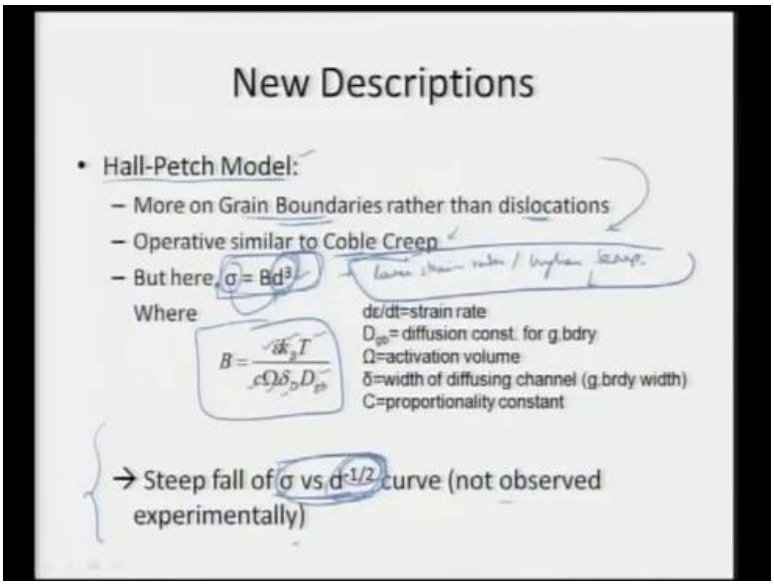

New Descriptions

- Hall-Petch Model:
  - More on Grain Boundaries rather than dislocations
  - Operative similar to Coble Creep
  - But here, σ = Bd³ ← lower strain rate / higher temp.

  Where

  $$B = \frac{k_B T}{c\Omega\delta_D D_{gb}}$$

  dε/dt=strain rate
  D_{gb}= diffusion const. for g.bdry
  Ω=activation volume
  δ=width of diffusing channel (g.brdy width)
  C=proportionality constant

→ Steep fall of σ vs $d^{-1/2}$ curve (not observed experimentally)

That is why we had this earlier term, we had this earlier dependence of this stress on the Coble Creep. So, we can define the stress required for Coble Creep and it can basically, occur at a very low stresses or very low strain rates or even at little higher temperature. So, these are the certain limitations for this one, so we can also see that the deformation can occur easily for nano crystalline materials. For even the temperatures can be much lower as compared to that of a conventional material.

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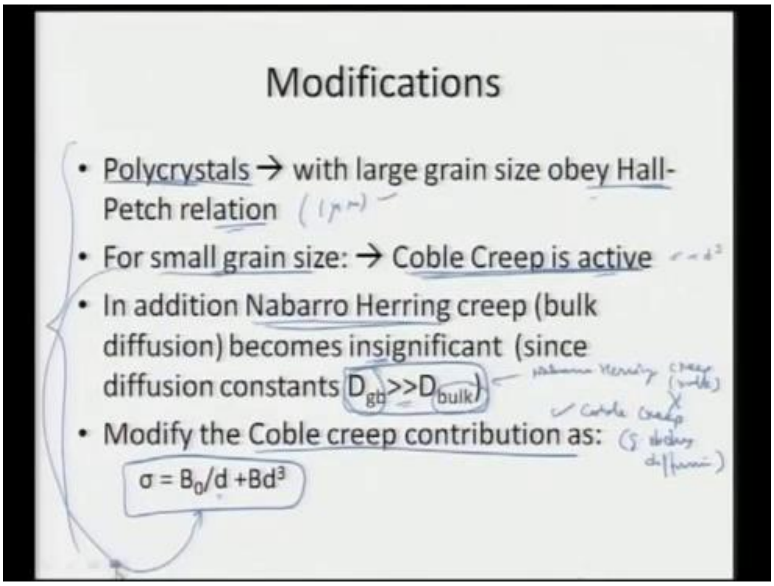

Modifications

- Polycrystals → with large grain size obey Hall-Petch relation (1μm)
- For small grain size: → Coble Creep is active σ ~ d³
- In addition Nabarro Herring creep (bulk diffusion) becomes insignificant (since diffusion constants $D_{gb} \gg D_{bulk}$) ← Nabarro Herring creep (bulk) ✗ ✓ Coble creep
- Modify the Coble creep contribution as: (g bdry diffusion)

  $\sigma = B_0/d + Bd^3$

So, again this can be encompassed so for smaller grain size we can see Coble Creep as pretty much active. That is responsible for the extensive plasticity of this nano crystalline materials so that also need to be considered, but what is the relationship between those two will come to that. Like what is essentially leading to the enhanced stress, yield stress required for the deformation. So, we will see that part.

So, for poly crystals we can see that they are obeying Hall-Petch relationship approximately till 1 micrometre, but for smaller grain size Coble Creep also becomes highly active. It means, the overall dependence of stress on D q is also very, very much also needs to be a considered. Apart, from that what can also happen the bulk diffusion can also occur by a Nabarro Herring Creep, but this Nabarro Herring Creep is basically very insignificant because now our constant for, diffusion constant for grain boundaries very, very higher in comparison to that of the diffusion constant for bulk diffusion.

So, we can see our D g b is very, very higher than D that of bulk. So, we can always ignore this Nabarro Herring Creep that is for the bulk we can always ignore it. And we can always consider the Coble Creep or grain boundary diffusion. So, because in Nano crystalline material we can see that the grain boundary area is also is very, very high. It is diffusion constant also is very, very high in comparison to that of D bulk.

So, we can always ignore this Nabarro Herring Creep, so overall the Coble Creep contribution can modified as sigma is equal B naught, which is a different constant divided by D plus B d q. Now, this is much more seem this is much more similar, to that of what is seen experimentally. So, we can see for where is fine grains we can consider Coble Creep, we can utilise a modified form of the Coble Creep as the stress required for Coble Creep is equal to B naught by D plus B d q.

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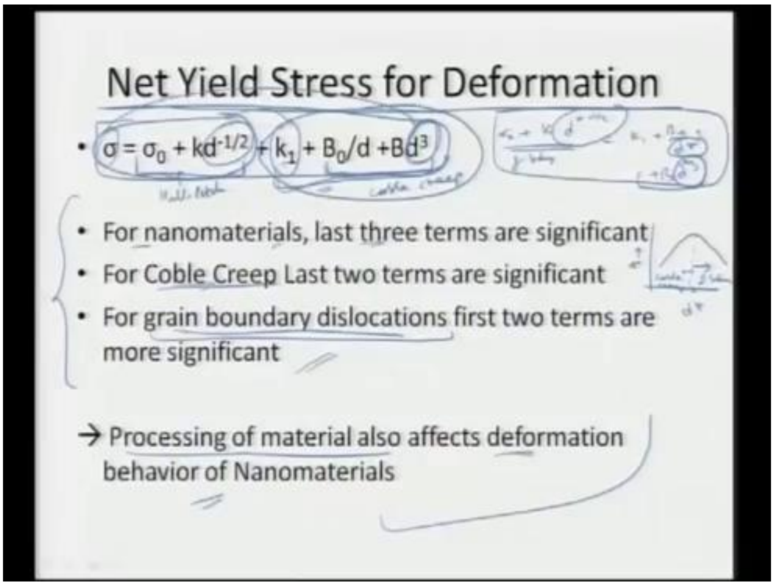

Net Yield Stress for Deformation

- $\sigma = \sigma_0 + kd^{-1/2} + k_1 + B_0/d + Bd^3$

- For nanomaterials, last three terms are significant
- For Coble Creep Last two terms are significant
- For grain boundary dislocations first two terms are more significant

→ Processing of material also affects deformation behavior of Nanomaterials

So, the net yield stress for deformation can come from the contribution both of dislocations the grain boundary dislocations and also for the Coble Creep. So, what we can see is the overall stress which is required is now, dependent on sigma naught plus k d power minus 1 by 2. That is for what is required for that is nothing but the Hall-Petch relationship. And now, there are some additional terms which come into picture because of the Coble Creep and this B naught d everything are nothing but material constant and we can define certain ways of estimating them as well.

So, we can see that this second term becomes very, very much significant we need to incorporate term. So, we can see for nano materials last 3 terms are significant for nano material because now, the Coble Creep also is very, very much dominant. For Coble Creep last 2 terms are predominant, so we can see this k 1 is the constant for a particular material for nano material. For Coble Creep last 2 terms are very much important, for grain boundary dislocations first two terms are very, very much important.

So, what we can see because of dislocation pile up or grain boundary dislocation, we can see that the resistance is coming from the grain boundaries. So, these become very, very much significant, last 2 terms are from the Coble Creep deformation. So, again we can compare these 2 terms and then we can say approximately, we can define a reason where we can see the relative contribution from both of them.

So, we can approximately estimate when the decrement of this stress can occur because in this case we can see that stress is directly proportional to the D q. So, when we have Nano crystalline material the overall dependence of this strain. Basically, now starts reducing as we have finer and finer grain size because stress becomes very much easier when we have certain grain size.

So, initially we had a grain dependence of d power minus 1 by 2, but at certain region we can see that the sigma is not directly proportional to D q, so at certain grain size. So, it means the stress required for deforming a material which is nano crystalline is very, very easy when we have predominance of Coble Creep. So, once we can compare this 2 terms, one term because of the grain boundary dislocation and second thing because of the Creep that is occurring to the Coble Creep, which is predominant because of the grain size again.

So, we can see that we can find out certain region at which this term will start decreasing. So, we can see that approximately certain point we have d star, d star means that when we have grain size higher than that, we will see strengthening with the reduction in the grain size. That is we have we have predominance of grain boundary contribution and below that we have contribution from the Coble Creep. So, that is what we can identify that we can have the overall contribution from either from the grain boundary dislocations or it can also come from the Coble Creep.

So, that is how we can distinguish between what is we can also incorporate that term of reduction in the yield strength, yield stress as we are lowering the grain size. Now, though well said about all these three, the main thing is we also need to control the processing of material because that also will affect the deformation behaviour of nano materials. So, once we know what is the overall relationship between those two, we now we can somehow control the material processing and achieve a material for particular deformation for making it in to some useful shapes.

So, that is why we need to see, what is the overall deformation mechanism of this nano crystalline material because now, we know that we have some contribution from the grain boundary because of pile up or generation of new sources of dislocation. And the ease of deformation because of Coble Creep which is predominant for the nano crystalline material. So, we get a Creep can occur at even at very low temperatures. So, that is what combining this two terms we can see overall dependence on d or the grain size. And that dictates that we have certain critical grain size below which we can start seeing decrease in the yield stress.

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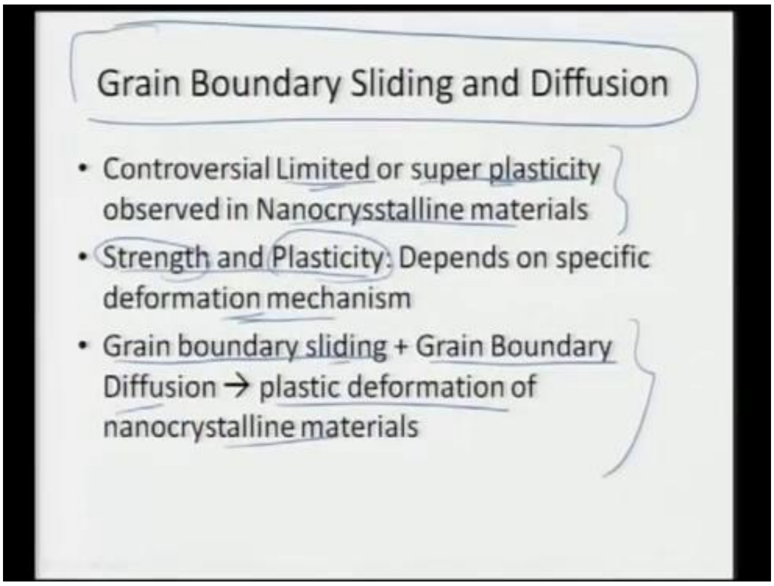

Grain Boundary Sliding and Diffusion

- Controversial Limited or super plasticity observed in Nanocrysstalline materials
- Strength and Plasticity: Depends on specific deformation mechanism
- Grain boundary sliding + Grain Boundary Diffusion → plastic deformation of nanocrystalline materials

So, again there have been so many controversial theories from researchers, that many researchers say that the overall plasticity of the nano crystalline material is very, very low. Whereas, other side is very, very high and again depending on the processing it can induce some defects into the structure. So, again that might lead to change in the plasticity of the materials. So, there had been very controversial theories from regarding the nano crystalline material, which say either they have limited or they have super plastic, plasticity available in nano crystalline materials.

So, that basically is very, very different in different cases because what is happening is strengthen plasticity that depend on the specific deformation mechanism. One needs to know, what is happening exactly what sort of mechanism is predominant when a certain processing is being done or when a certain deformation is being done. So, the overall plasticity which is will result or the strength which will result depends very much on the deformation mechanism, which deformation mechanism is predominant in controlling the deformation.

And thereby, leading to the certain strengthen plasticity. So, there are many theorise which have come about which one is very convincing is that, there is a grain boundary sliding plus grain boundary diffusion. And that leads to the plastic deformation of nano crystalline materials. So, the overall plasticity is achieved to the grain boundary sliding and the grain boundary diffusion. That leads to the plastic deformation of nano crystalline materials.

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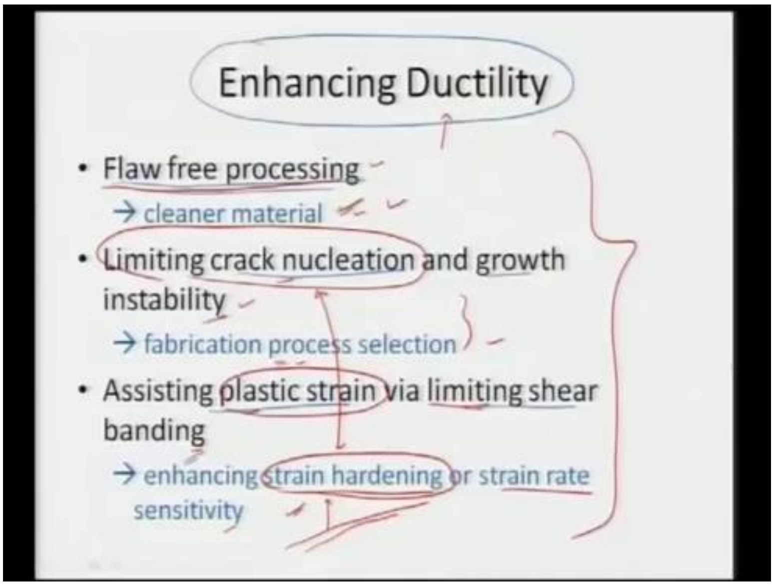

Enhancing Ductility

- Flaw free processing
  - → cleaner material
- Limiting crack nucleation and growth instability
  - → fabrication process selection
- Assisting plastic strain via limiting shear banding
  - → enhancing strain hardening or strain rate sensitivity

So, ductility can be enhanced the overall as we know that strength can be controlled by the Coble and the dislocation part or dislocation coming from, dislocation pile up coming because of grain boundaries, but again apart from that we also want to increase a ductility. So, strength can be controlled by grain size the yield stress, but again the overall ductility can be controlled. Once, we have a flaw free processing that the processing itself does not induce any cracking or any flaw or any inclusion or any impurity into the system. So, we need to have flaw free processing, so that will avoid limiting any generation of crack nucleating points and also it will avoid any growth instability.

Then third part, is that we also need to assist the plastic strain, while limiting the sheer binding once a sheer binding occur it is very catastrophic. So, we need to somehow limit the sheer binding as well. So, for free flaw free processing we can achieve a very cleaner material, so once we have a cleaner material the overall points for crack nucleation they are highly limited. So, flaw free processing will lead to a very cleaner material, so in turn we will have very pure material overall homogeneity of the material is very, very high.

And limiting crack nucleation and growth instability again depends on the kind of strain that we are providing or the fabrication process that you have selected. So, in that case we need to limit the crack nucleation sites. So, that we can avoid any catastrophic failure and growth instability, so we need to avoid any stress concentrator in the material by controlling the processing. And again, once we are assisting the plastic strain it means, we have to in enhance strain hardening or the strain rate sensitivity, so we can somehow limit the sheer binding.

So, we have now three problems through which we can enhance the ductility and three solutions also available, through which we can achieve this enhanced ductility for nano crystalline material. So, we can see for flaw free processing we will get cleaner material by limiting crack nucleation and growth instability, we can choose a particular process which can avoid the crack nucleation and growth instability. And then also, we can enhance the strain hardening or the strainer sensitivity to limit sheer binding. So, thus we can avoid any catastrophic crack propagation or catastrophic failure of the material once we are processing it or once we are synthesising it.

So, that is how we can initiate these 3 parameters of cleaner material particular process selection, but mainly we can see we utilise a limiting crack nucleation. So, we need to limit the crack nucleation and growth. And also assist plastic strain or limit the sheer binding so or maybe strain hardening. So, we can see there are two aspects of limiting crack nucleation and inducing strain hardening into the material. So, by selecting certain protocols we can somehow achieve this, so that we can achieve higher ductility. So, strength can be controlled by grain size and ductility can be achieved by controlling the limit by limiting the crack nucleation or inducing strain hardening.

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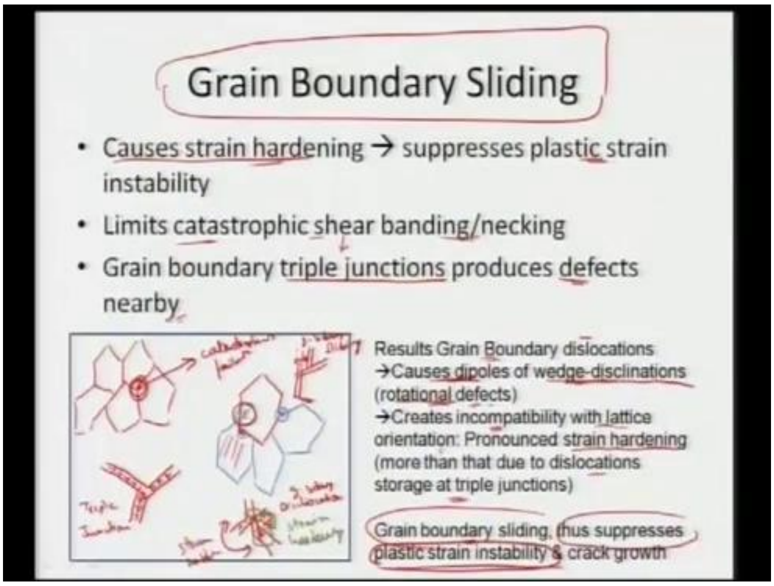

Grain Boundary Sliding

- Causes strain hardening → suppresses plastic strain instability
- Limits catastrophic shear banding/necking
- Grain boundary triple junctions produces defects nearby

Results Grain Boundary dislocations
→Causes dipoles of wedge-disclinations (rotational defects)
→Creates incompatibility with lattice orientation: Pronounced strain hardening (more than that due to dislocations storage at triple junctions)

Grain boundary sliding, thus suppresses plastic strain instability & crack growth

So, again to achieve those things we there are 2 phenomena which we need to control, one thing is the grain boundary sliding. So, we can see that grain boundary sliding what it does is it causes strain hardening. So, once this strain harden, so we can suppress the plastic strain instability. So, we can avoid the formation of sheer binds catastrophic sheer binds. So, we can see that this grain boundary sliding can limit the catastrophic sheer binding or necking that can occur.

So, generally what happens is it can also essentially what it is doing is, it is also inducing some defects near the grain boundaries not at the grain boundary triple junctions, but at near those sides. So, what we can see here is that once we have grains generally, grains are very much hexagonal in nature. And then we see there are some predominant in a regular material, but what happens in nano crystalline materials is now, this reason is now further defected.

It means once, we have this sort of an arrangement, the third grain will now generate from this point now, third grain will not generate from this point it will start generating from some other point. So, what is happening is now, we are avoiding the generation of triple point. Those triple points will be there, but now we can minimise this is the triple point, but in this case the triple point is out here. That should have been here, but know a defect is generated one a nearby point.

So, we can see a nearby point we have generated at a defect and that is now reducing the overall stress concentration that is occurring in the material. And thereby we can reduce the defects exactly at the triple points. So, what is happening here is that we are limiting the triple junctions and we are producing defect in the nearby regions. So, that is what we are able to see here, what it is doing is, it is resulting the grain boundary dislocation. Now, we are resulting a grain boundary dislocation and that is resulting the wedge-disclinations or rotational defects.

So, what is happening here is initially, we should have seen that we should have a grain boundary like this. Ideally, we should have a have a grain boundary triple junction like this, but now what do we have. Now, we have some region which is like this now, in turn what we have done we have now shifted the grain boundary point to certain other region. And what we are seeing, we are seeing is a grain boundary dislocation. And also what is happening it is also creating some sort of a dipole because if wedge-disclinations.

So, we can see that the overall grain boundary dislocation, the dislocation at the grain boundary had certain orientation. Now, what is happening here is the overall disclamation is now, arrived because now we have one sort of dislocation here, second sort of dislocation here. So, we can see there is kind of a polarity that can generate between these two points this is called as wedge-disclinations.

So, we can see there is a kind of wedge-disclinations or rotational defect that can arise because of presence of these two points, which are the defects near the grain boundary. So, what is happening is it is causing a dipole or a wedge-disclinations, which are nothing but rotational defects. Now, once we have rotational defects it creates incompatibility with the lattice orientation. So, lattice will have certain orientation and this wedge will start creating some rotational defect.

So, what is happening here is now, this will cause some pronoun strain hardening and that is much more stronger than that can arise from the pile up of dislocation or dislocations storage at triple junction. So, once we had this dislocation storage at triple junction, this point would have become very much weaker, but now the strains are coming because now we have 2 different points, one here and second one here.

So, this is causing some rotational defect and that is causing strain hardening because of defect which are much near to the grain boundary not exactly at the triple point. And now, it can result the sliding of the grain boundary and thereby, it can suppress the plastic strain instability. Otherwise, what can happen that this point will become, so weaker that it can just lead to catastrophic failure, but in the second case now, we have some rotational component into the picture.

And that will cause some wedge-disclination that will come over wedge-disclination, it will induce some strain hardening and lead to the movement of or sleeping of this grain boundary. So, the grain boundary will slide, so that is what we are seeing that the grain boundary has now slided to some other location. We can see we can see this point the grain boundary has slided from one region to from this point to nearby, region. So, we can see the grain boundary sliding that has occurred into the material.

Now, this is the one which is inducing this plain plastic strain instability, which is suppressing the plain strain instability because of this grain boundary is sliding. So, we can see that the grain boundary sliding is a very essential component to cause strain hardening the material. And it suppresses the plastic strain instability which can lead to catastrophic failure or by producing sheer bends. So, that is what the necking or the sheer bending is now, being avoided and that is being incurred by moving this defect areas away from the triple point.

So, triple point instead of triple point we have a defect region, near the triple junction and that causes kind of a polarity between along those 2 points by causing a dipole or a wedge-disclination. Now, that in turn it is a very strong rotational component and that will lead to formation of some lattice creating some incomparability in the lattice orientation. And that essentially leads to strain hardening because of dislocation at those particular points.

So, we had only triple junction that will be very, very catastrophic because now, we have defect located exactly at one point. Whereas, in the second case we have a rotational component and that will lead to the grain boundary sliding. And that is very much responsible for avoiding the plain, the plastic strain necking or the sheer bending that could have occurred catastrophically.

So, grain boundary sliding will assist the deformation in a very gradual fashion, but also with much more strain hardening. And this strain hardening is very much higher than that it can come about from pile up of dislocation at the triple junction. So, in that case we can achieve very high plasticity via avoiding this sheer binding or necking or avoiding this plastic strain instability in the nano crystalline material. So, that is one more advantage of grain boundary sliding, the dominance of grain boundary sliding in the nano crystalline materials. So, once we have induce some strain hardening because of the grain boundary sliding. Now, this additional stress also has to be now removed gradually.

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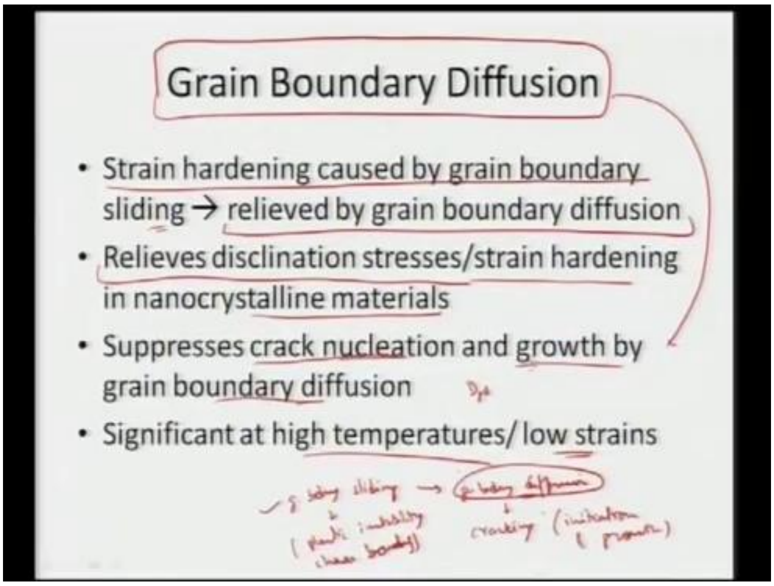

Grain Boundary Diffusion

- Strain hardening caused by grain boundary sliding → relieved by grain boundary diffusion
- Relieves disclination stresses/strain hardening in nanocrystalline materials
- Suppresses crack nucleation and growth by grain boundary diffusion
- Significant at high temperatures/ low strains

So, it can accommodate more and more straining, so that is why we have grain boundary diffusion, which is also we require it to capture. So, that we can relive the stresses that are being generated by the or the strain that are being generated by the strain hardening. So, we can see the strain hardening which is been caused by the grain boundary sliding that has to be removed or release by grain boundary diffusion. So, what is happening is now we have generated those wedge-disclination near the triple junctions or the grain boundary, near the grain triple junctions. So, we need to relive those dislocations which are nothing but the stresses of strain hardening in Nano crystalline material.

So, what it will do is now, once we have those declinations those are also again very high stress points. So, they can also act as a stress razor and they can act as a crack nucleation sides. So, we need to suppress those cracks nucleation and growth by this grain boundary diffusion. So, once we can allow the grain boundary to diffuse then it can encompass those reasons and in turn it will remove those stress or strain nucleating sites.

The strain hardening has been caused by this grain boundary sliding, it also is essential that we release those stresses. Otherwise, they can turn as a nucleating sites for cracking its growth. So, we see that the grain boundary diffusion also is very, very essential component in controlling the deformation that can be incurred by nano crystalline materials. So, what we are seeing is the strain hardening which is been caused by grain boundary sliding that has to be relieved by the grain boundary diffusion.

So, what is happening that what we say earlier was a wedge-disclination that are arising at near the triple junctions? So, we have region which are also defect which are also defected near the triple point. So, we are now releasing the triple points and relieving the defect near those regions. So, in turn that can also act as a stress razor or a stress concentrator. So, we need to also allow to release those stresses or strings from those regions.

So, what we can see is that we can relive those disclination stresses of strain hardening in Nano crystalline materials via grain boundary diffusion. So, what in turn it will do is it will suppress the crack nucleation and growth because of this grain boundary diffusion. So, it will encompass those regions which are defected and now, it can accommodate those it can somehow release those stresses because if grain boundary diffusion. And it allow very equilibrium flow of material around those regions.

So, the overall grain boundary diffusion is also very much critical in controlling the stress or in terms of removing or releasing those stresses or strain hardening in those materials. And that is very significant either at higher temperature or lower strain. So, once we are deforming the material at either higher temperature or lower strains the material gets enough time for relaxing itself. So, that is we can see super plasticity when we have very high temperatures or very low straining rates of deforming the material. So, in this case we can see that the grain boundary sliding, has to be compensated by grain boundary diffusion.

So, in this case what we are trying, we are trying to limit the cracking both initiation and growth and by grain boundary sliding we are limiting the plastic instability or sheer bending. So, we can see there are two components by grain boundary sliding we are trying to control the plastic instability or sheer bending and via grain boundary diffusion. We are trying to release the stresses, which are been caused by strain hardening because of grain boundary sliding. And to achieve this grain boundary diffusion we need to work the material at a very high temperatures or at lower strains. So, that it becomes easier to release those disclination stresses or strain hardening in a nano crystalline materials.

So, both the components grain boundary sliding and grain boundary diffusion are very, very important because once grain boundary sliding is inducing, certain strain hardening into the material that has to be released. So, the material can accommodate much more deformation or much more working on the same material, but this working has to be done at pretty high temperatures or very low strains or low strain rates.

So, in turn what is happening it is reliving the disclination stresses or the wedge-disclination stresses, which are inducing a rotational component and leading to this grain boundary sliding. So, at certain level those stresses have to remove so the more working of the material can be done. To again, without cracking the material or inducing the crack growth. So, in that fashion grain boundary diffusion also becomes very, very important component of that.

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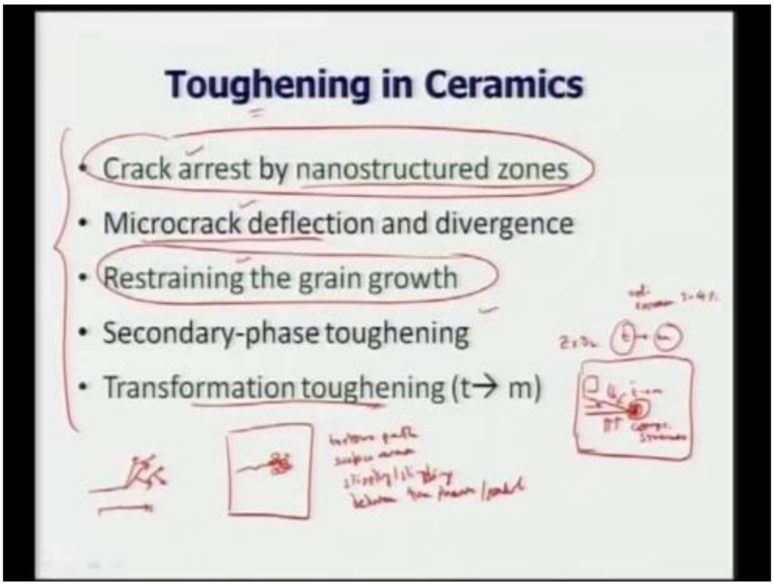

Toughening in Ceramics

- Crack arrest by nanostructured zones
- Microcrack deflection and divergence
- Restraining the grain growth
- Secondary-phase toughening
- Transformation toughening (t→ m)

Now, coming to the final aspect of toughening say in ceramics, we can also toughen the material via inducing some nano structured zones. So, we can see that Nano structured zone can also act as region where we can arrest the crack. So, once we have a Nano crystalline material now, the crack among, the crack is propagating it will have to encompass very tortuous path. Also, the surface area is so high that it can also accommodate some slipping or sliding between the faces or particles.

So, thereby the crack can get arrested at the nano structured zone so once, we have very fine grain structure. The crack once it is propagating it can get arrested at those regions. Also, it can do is micro crack deflection, so once we have a crack propagating and once we start deflecting it change the path of the rack itself. Now, the crack bifurcates and it also requires much higher energy to propagate further because it initially started with a unidirection.

So, it wanted to from left to right, but now once we are deflecting the crack and diverging the crack. Now, crack is propagating in very different directions and in turn it is losing the energy by creation of new surfaces also, we can restrain the grain growth. So, as we see that now once we have a very fine grain size, we can encompass more number of a dislocation that may not hold true for ceramics, but restraining the grain growth now we can allow the grain boundary to act as barrier for further propagation of crack. And in turn, it can assist in the toughening of the ceramic.

Also, we can induce some secondary faces, so like secondary faces can be much tougher like in ceramics we can add some nano structured tubular particles on a non-spherical particles. And that can act as a regions to absorb the shock and also we can achieve transformation toughening in some materials. Like in nano crystalline materials we can see that specifically for zirconia, we can achieve a tetragonal to mono clinic transformation and nano crystalline materials. That might be much more easier for the material to undergo this transformation because we have very limited regimes where, the material has to transform.

So, exactly in front of the crack tape once we have very high stresses the stress transformation can allow tetragonal to monoclinic transformation of zirconia. And in turn, what is happening the shock is being absorbed because of this particular transformation. And now, the crack will experience compressive stresses and then it will lead to the closure of the crack. So, this transformation toughening is occurring by expansion of the volume by say 3 to 4 percent volume expansion and since, crack is now opening up it will start closing down because of the stresses, because of the expansion of the material. So, in turn it will lead to transformation toughening.

So, we can see again toughening in ceramics can be accommodated by nano structured materials via arresting the crack, via deflection of the crack via restraining the crack grain growth or via inducing the secondary phase toughening via inducing Nano crystalline materials such as carbon nano tubes or via transformation toughening. And in nano crystalline material once, we have a nano particle or nano phase which is present ahead to the crack tape. It becomes very easier for the stress to undertake the transformation because these particles nano particles are highly unstable or Meta stable in nature.

So, in that way they can easily transform to the stable phase, which is monoclinic and intend induce volume expansion of approximately 3 to 4 percent and that will eventually lead to the closure of the crack. So, we can see the application of this nano crystalline materials in toughening the ceramics which is a very, very critical component these days because for structural materials the ceramics are very, very highly placed. So, in turn we can utilize nano crystalline materials for inducing toughening in the ceramics which is otherwise of a highly brittle material.

So, this toughening in ceramics can occur via arresting the crack or via deflecting the crack or via restricting the grain growth or via inducing the nano size phases or particles and of the crack tape. Now, because of the instability of this particle they can easily transform to the stable phase, while inducing some compressive stresses. And thereby, closing the crack, so we can see these particular things are possible because of the nano structured materials. And it eases out the toughening which can be achieved in the even in ceramics.

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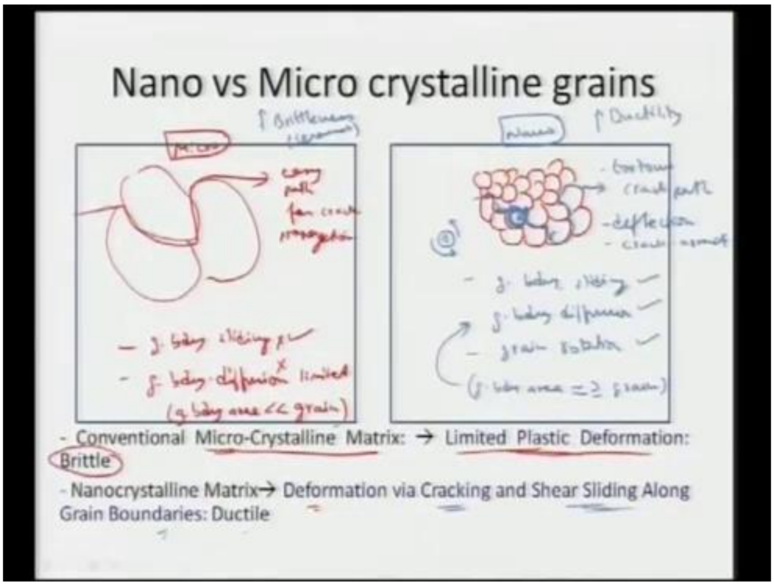

Nano vs Micro crystalline grains

- Conventional Micro-Crystalline Matrix: → Limited Plastic Deformation: Brittle
- Nanocrystalline Matrix→ Deformation via Cracking and Shear Sliding Along Grain Boundaries: Ductile

So, seeing nano versus micro crystalline grains, so in what happens in conventional micro crystalline grains is we can get very limited plastic deformation. So, in nano crystalline materials first of all we can see when a crack has to propagate it can find easy path of easy path for propagation. There is no presence of any grain boundary sliding and grain mode diffusion is also very, very much limited because the grain boundary area is very much lesser than that of the area of bulk.

So, what is happening is in the micro crystalline materials, we have very high grain size, very large grain size. So, we can find very path for crack propagation, grain mode is sliding basically been absent, green mode diffusion also is very limited because the grain boundary area also is very very lesser than that of a grain. So, in conventional micro crystalline materials what we can see we can see very limited plastic deformation and eventually the material is very, very brittle specifically, for ceramics.

Otherwise, what happens in nano crystalline material is deformation via cracking and sheer sliding can also occur along the grain boundary? So, first of all we have Nano crystalline material we can see that for a similar region what we can see the crack path can be very, very tortuous. The coverage also is very much higher for, so once we can see when the crack has basically, being generated it can be very, very tortuous by the time it comes out, so very tortuous crack path.

The crack deflection can also occur very easily because now grain size have very different curvatures. So, deflection of crack path can also occur, it can also get restrained or it can also get arrested, the crack arrest can also occur because now a days covering much more area it is creating many more new surface. So, it can also get absorbed or it can get arrested very easily in a nano crystalline material. Apart, from that it also incurs grain boundary sliding, grain boundary diffusion also the grain rotation can also occur.

If a particle is not tightly bound to nearby it can also basically, act as a free surface and it can rotate itself and in turn it can accommodate additional energy for its rotation. And it can absorb the additional stresses that are incorporated into the material. It can act as a free surface and in turn it can also absorb shock because in this case our grain boundary area is very much higher or comparable to that of grain. So, that phenomena of grain boundary diffusion also becomes very, very much appreciable.

So, what we are seeing is the deformation via cracking and sheer sliding along the grain boundaries. So, sliding can also occur between the grain boundaries that makes the material very, very ductile because we have grain boundary sliding, we have grain diffusion grain rotation can also occur. And also, sheer sliding along grain boundaries that can also occur. So, in turn what is happening in the nano that we are seeing much more high ductility specifically for ceramics?

In this case, we have very high brittleness for ceramics and the ductility can also enhance for metallic materials as well because of all these phenomena like grain mode siding, grain mode diffusion that can also occur very easily in the nano crystalline material. So, this covers the overall paradise of nano versus micro crystalline grain.

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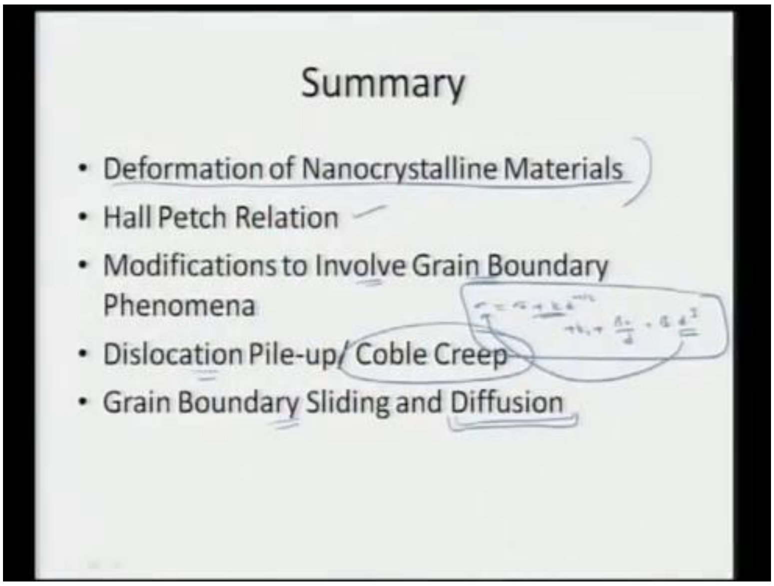

Summary

- Deformation of Nanocrystalline Materials
- Hall Petch Relation
- Modifications to Involve Grain Boundary Phenomena
- Dislocation Pile-up/ Coble Creep
- Grain Boundary Sliding and Diffusion

$\sigma = \sigma_0 + k d^{-1/2}$

$+ k_1 + \frac{A_1}{d} + G d^2$

So, we can see, what is the role of Nano crystalline material in terms of deformation, how it can deform and how it can provide much more toughening to the material both in turns of stresses as well as ductility. So, we can see deformation of nano crystalline material it is being dictated by this Hall-Petch relationship. So, till 1 micrometre we can see a very much validation of Hall-Petch relationship, but starting from 1 2 around 30 Nanometre. We can see that the Hall-Petch relationship the exponent is not exactly minus 0.5, it comes down near to 0.

And, so we see a some horizontal plateau and then apart from that we can also see for grains which are much smaller than 30 Nanometre. Inverse Hall-Petch relationship can also be very, very predominant because in that case, so apart from Hall-Petch what we can see that. Now, what is happening is there is something happening at the grain boundary, so modifications are done involve some grain boundary phenomena like what is happening because of the Coble Creep.

So, there are two things, one thing is dislocation pile up can also occur at very lower grain sizes. So, that those are responsible for region for enhancement of the yield stress with reduction in the grain size, but at certain critical grain size below that we start seeing decrease in the yield stress with decreasing grain size. And that thing is being responsible by the responsible because of that thing is attributed to the Coble Creep.

Now, we need to inculcate many different terms, so we can yield stress is equal to sigma naught plus 3 to the power minus 1 by 2, which is coming out because of the grain boundary or dislocations which are getting piled up plus some constraint. And then we see components of Coble Creep which now, make sure that the smaller the grain size smaller is the yield stress. And those things are responsible for reduction in the yield stress as we reduce the grain sizes.

So, we can see the dislocation pile up and Coble Creep model can also come along. Apart, from that the toughening or the ductility of nano crystalline material is very, very high because of grain boundary sliding. Once, we have nano crystalline material it starts inducing defects near the triple points not exactly the triple points. That leads to wedge-disclination and that induces a kind of a dipole or a rotational component. And in turn it leads to the grain boundary sliding and thereby it the overall deformation can be enhanced because now we don’t have stress concentrated at the triple junctions.

And, but those have to be accommodate by grain boundary diffusion to release those strain hardened regions, we also require grain boundary diffusion that has to occur for encompassing the enhance placidity. Apart, from that we also see the difference between micro and nano crystalline materials because what is happening in micro crystalline material is we have components of an extra energy coming because of the nano faces.

The ease of transformation and say transformation toughening or also the grain boundary sliding, grain ordinary diffusion even the grain boundary rotation can also occur and grain boundary slipping or sheering can also occur. That induces much more toughening or ductility in the nano crystalline material in compare to that of micro crystalline material. And with this basically, with this we complete the overall paradigm of nano difference between nano and the micro components of crystalline materials for the yield stress or the ductility or the overall deformation of this nano crystalline material. So, with this I end my lecture here thank you.