Introduction to crystal elasticity and crystal plasticity Prof Swarup Bag Mechanical Engineering Department Indian Institute of Technology Guwahati Week-07 Lecture-16

So when you try to discuss the constitutive model for single crystal, so we have the idea that Schmid law predict the elastic and perfectly plastic behavior of a crystal. So here actually defines the yielding occurs over a slip plane, one specific slip direction and it corresponds through a specific slip system for the different crystals and at the same time there maybe the possibility of the several slip system may active at a time, but purposefully when you try to analyze the plastic deformation of the single crystal structure we generally focus on the plastic deformation behavior on the single slip system.

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•	The Schmid Law predicts the elastic-perfectly plastic
	behavior of a crystal - Yield will begin on a slip system when the shear stress on this system reaches a critical value (CRSS), independent of the tensile stress or any other normal stress on the lattice plane
•	In fact, there is a smooth transition from elastic to plastic behavior that can be described by a power-law behavior
•	The shear strain rate on each slip system is estimated by constitutive relation. By assuming this kinetics of plastic flow (rate-sensitive), we avoid the non-uniqueness of the set of active slip systems typically present in rate- insensitive models.

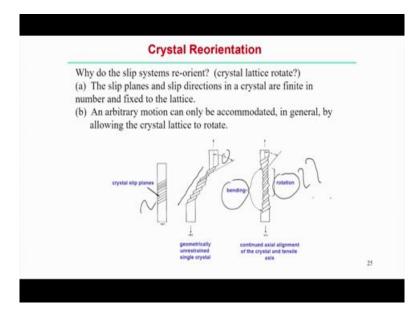
So here yield begins or we consider there is a yielding starts when specific it overcomes the critically resolved shear stress for a specific slip system for a crystal structure. But this critically resolved shear stress is independent of the shear stress value or any other normal stress on the lattice plane. In fact this mechanism when you try to explain the slip for a specific crystals, of a single crystal structure, so there is a transition from the elastic to and plastic zone it is not in a smooth way. So it can also be possible to explain, the transition, smooth transition from elastic to plastic deformation and that can be better explained by the power law behavior. And we have observed that when you try to explain the plastic

deformation in continuum plasticity mechanism in that case, so we describe the deformation of the material in terms of the of plastic deformation material using the power load relation.

So actually represents that normally the complete plastic deformation zone by neglecting the elastic deformation component. So that is the typical of correlation between the stress and strain that follow the power law relation can be explained for the smooth transition from the elastic to plastic behavior. Another significant point here when you try to analyze the deformation behavior, probably the rate of the strain is more important on the slip system and that can be explained by the constitute relation, so by assuming the kinetics of plastic flow which is rate sensitive we can avoid the non uniqueness of the stet of active slip system and that is typically present in the rate insensitive model.

So there is a significant thing, two things one is that whether there is a deformation rate sensitive or whether deformation is the insensitive, that typically we explain in plastic deformation over a continuum scale, we express the relation between stress and strain either by strain hardening coefficient n sigma equal to K Epsilon to the power n. Or if there is a strain rate sensitivity index, we consider then we explain the relation between the strain, stress and strain rate. So similar kind of philosophy can be used here to explain the plastic deformation of the single crystal structure.

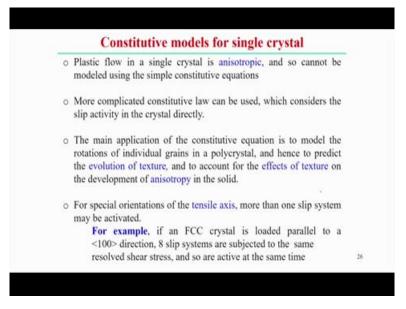
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Let us see how the plastic deformation happens, so once there is a so many slip system active at a time so that questions of the crystal reorientation actually comes into the picture, but why do slip system reorient and why the crystal lattice we try to understand this two phenomena here but if we just focus on the figures here see the crystal slip system here and so many slip system, probably it is representing in the several parallel planes and if there is a axial stress value and at the axis initially and the deformation behavior maybe looks like this so there is a with respect to one plane of the atoms or with respect to one several planes, there is a relative displacement between them and these kinds of displacement, specially for the single crystal structure we can found out that if there is no geometric constant condition the single crystal deformation or single crystal behaves like this and over a several slip planes.

And of course there is a angle x0, is the angle between the slip direction and the normal tension axis. Now it is possible to put the constant, that actually happens in the practically because it is slip planes acting in such way and if we put the constant here then continued xl alignment of the crystal looks like the third figure here and here if we see when you try to make the constant deformation or try to make a slip behavior over a constant geometrical constant is there then to arrange that slip planes it is subjected to that some kind of bending as well as the rotation. So that means the slip planes and slip direction in a crystal or finite in number and fix to the lattice point but an arbitrary motion can be accommodated in general by allowing the crystal lattice to rotate and that can be better explained if there is any geometrically constant is there or not. If there is a geometrically constant then definitely crystal planes will subject to some amount of the rotation and with respect to the each and every slip plane when there is a sequentially active the different slip plane with respect to one slip plane to another they will try to reorient with respect to each other. So this is the philosophy of plastic deformation for a single crystal structure when there is a several slip plane actives.

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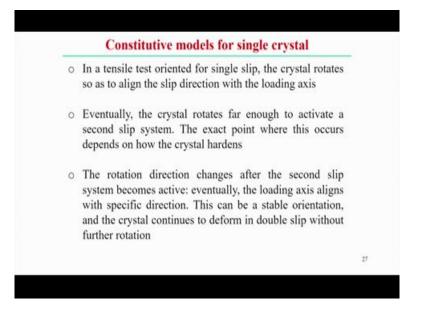
Now how to form the constitutive models for a single crystal structure so here the target is to analyze the constitute model but we have explained esp in the continuum plasticity model, so here similar kidn of things we can explain that plastic flow in the single crystal is anisotropy, so cannot be modeled using the simple constitutive equation. So this plastic anisotropy behavior, it is very difficult or not easy straight forward to mode, because in this case more complicated or constitutive law can be used which consider the slip activity in the crystal directive. Let us see what we can accommodate or we can explain this constitute model in case of single crystal structure.

The main application of the constitutive equation is to model the rotation of the individual grain in polycrystal and hence to predict the evaluation of the texture, and to account for the effects of texture on the development of anisotropy in the solid state, main reason for the anisotropy in the crystal structure that actually comes from the texture formation. So if we try to incorporate the effect of the texture probably in that case we can include the effect of the anisotropy in a plasticity model of the single crystal structure.

Let's us look into that example for a special orientation of the tensile axis. More than one slip system maybe activated, that we have already explain that at least at the ideal condition at least five slip system will be active to maintain the compatability condition in the deformation of a single crystal structure. So for example if an FCC crystal is loaded parallel to 100 direction that is any 1 of the axis of unit cell, 8 slip system are subjected to the same amount of the resolved shear stress and so are active at the same time. so this is just the

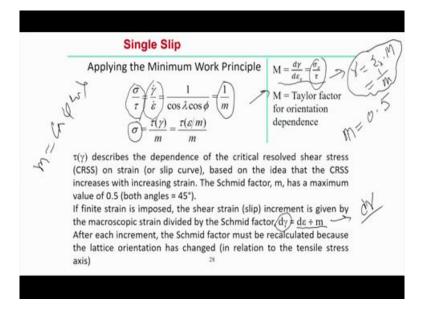
typical example that several slip system may active depending on the which direction the load is acting.

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In a tensile test oriented for single slip, the crystal rotates so as to align the slip direction with the loading axis. So if the tensile test oriented according to a single slip the crystal also rotates to alight the slip direction according to the loading axis. At the same time the crystal rotates for enough for enough to activate a second slip system, the exact point where this occurs depends how the crystal actually becomes harder or how the crystal hardens. The rotation direction changes after the second slip system becomes active and eventually the loading axis align with some specific direction, this can be a stable orientation and the crystal continuous to deform in double slip without further rotation. So actually all these points signifies that with the application of the load how the slip plane actually reorient with respect to first slip plane and the second slip plane and how they can configure in such way that it is accommodated by amount of the rotation.

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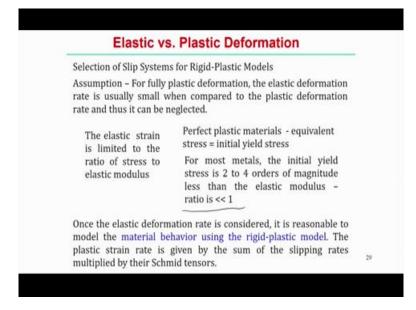
So by taking into all this fact probably it is better to explain that how the models can work, now for a single slip if we consider the single slip system applied the minimum work principal probably we can derive this sigma by normal stress by shear stress in this case equal to in terms of the rate of strain, shear strain rate and the normal strain rate ration and that is represented by 1 by m and m is basically (())(11:46) cos phi cos lambda that is the direction cosine with respect to the define axis in the crystal system. That we have already derived and here we can find out that sigma equal to stress equal to shear stress by m, probably m we can consider the resolve, this is the one factor that depends on the orientation of the axis with the slip direction normal to the slip plane and the tensile axis.

So if we compare that, already we have define that polycrystal is subjected to some amount of the deformation random orientation of the crystal, in that case the Taylor factor for orientation dependents simply estimated by this way so that Taylor factor is basically ratio of the incremental shear strain in terms of the with respect to the incremental normal stress and that is the ratio sigma by tau that is normal stress by shear strain. That is the typical way we estimate the Taylor factor to link between the normal stress and the shear stress component or to link between the increment of the normal strain to the shear strain. And of course this factor takes into effect the orientation dependents and well looking into that similar thing we can find out that probably that in this case the shear stress is the shear stress describe the depends, dependents of the critically resolved shear stress on the strain that means specifically on the slip curve. Based on the idea that the critically resolved shear stress increases with increasing strain, so therefore m can be the maximum Schmid factor m can be the maximum when both the angles become 45 degree that means m the maximum values of m can be 0.5 here. Now this shear strain component can also be explicitly add a function of the ratio, normal strain by m. So here if we see that from the factor of this Taylor factor so here probably we can represent that from here that shear strain is basically the shear stress into , shear stress equal to normal strain into m or shear strain equal to here basically 1 by m.

Now if the finite strain is imposed the shear strain increment is given by the microscopic strain divided by the Schmid factor so probably that microscopic strain can be represented by the Schmid factor where Schmid factor m actually represent the cos phi cos lambda. Now after each increment the Schmid factor must be recalculated because the lattice orientation has change in with respect to the tensile stress axis. So here the point if you try to correlate with the continuum plasticity model where also we have discussed that in the plasticity analysis we generally provide in terms of the incremental mode, specific the incremental mode in the sense the incremental amount of the strain component and what is the corresponding and link in corresponding stress value.

So similarly philosophy can also be used here where the incremental shear strain is basically incremental normal strain by m, so and each times recalculate the m factor m because of the orientation actually change with respect to slip plane or with respect to the tensile stress axis. So once we recalculate all this thing we can accumulate the total amount of the strain and we can use the correlation to link between the stress and strain in terms of or whether it is normal stress or whether it is shear stress component.

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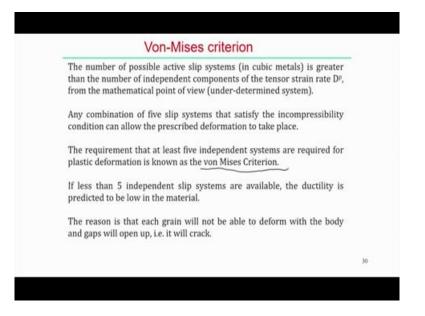


Now we will try to focus on the elastic versus plastic deformation for the analysis of the plastic deformation of the single crystal structure. Selection of the slip system for rigid plastic models that means, rigid plastic models means that the plastic deformation we just analyzing the deformation of the plastic part without the effect of the plastic component. Assumption for fully plastic deformation, the elastic deformation rate is usually small when compared to the plastic deformation rate and that can be neglected that means in case of rigid plastic models probably we can neglect the effect of the elastic components. But the elastic strain is limited to the ration of the stress to the elastic modulus but plastic perfect plastic material is where the equivalent stress is basically with respect to the initial yield stress, but for most of the metals the initial yield stress actually 2 to 4 times of magnitude less than that of the elastic modulus so that we follow the ration is very small as compared to 1.

So once the elastic deformation rate is consider it is reasonable to model the material behavior using the rigid plastic model, the plastic strain rate is given by the some of the slipping rate multiplied by the Schmid tensor. So it is basically that the first thing is that when you try to focus on the rigid plastic model then we can neglect the elastic component, but till we can estimate the rate of elastic deformation and we can compare with the plastic deformation so probably in this case the rate of elastic deformation is very small as compared to the plastic so that we maintain the ratio which is very much less than that of 1. But when you try to estimate the amount of the total plastic increment of total plastic strain in this case probably we can sum it up what is happening for over the different slip system and that

accordingly we can estimate the rate by looking into that what is the Schmid factor for all these cases.

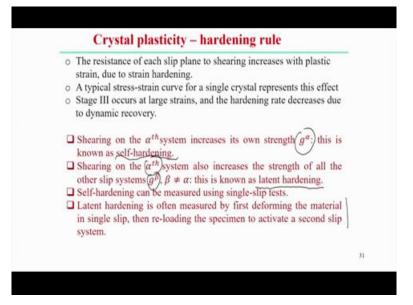
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Now here also we can implement the Von Mises yield criteria in the plasticity model. The number of possible active slip system probably in cubic metals is greater than the number of independent components of the tensor strain rate that is represented by Dp from the mathematical point of view. But any combination of the five slip system that satisfy the incompressibility condition can allow the prescribed deformation to take place. So that we have discussed that what is the requirement of the at least five slip system is active at a time so that is can maintain the incompressibility condition. The requirement at least 5 independent slip system are required for plastic deformation is know as Von Mises criterion here.

But if less than 5 independent slip systems are available the ductility is predicted to be low in the material. The reason is that each grain will not be able to deform with the body and gas will open up that means it will crack. So basically the compatibility condition is a main issue based on that we can decide at least five independent slip system can be active at a time, if it is less than five independent slip system available probably the ductility predicted to be very low in that material because in this prediction it is less than the it will violate the compatibility condition, that actually creates the crack formation during the deformation.

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Now we will try to look into the hardening rule in case of the crystal plasticity model. So here the resistance of each slip plane to shearing increases with plastic deformation and that is the effect of the due to strain hardening effect. A typical stress strain curve for a single crystal structure we have already discussed and we observe that at stage 3 the deformation, the large strain the hardening rate actually decreases and that happens due to the dynamic recovery. So these are the typical observation for the deformation stress curve in case of single crystal structure, now how to use the hardening rule in case of single crystal plasticity model.

So first thing is that we consider the shearing on the alpha th system increases its own strength probably that is define by g alpha and this is known as self hardening. Self hardening in the sense the increment of the strength level due to a specified slip system or due to a specified shearing operation on a slip system. But at the same time this slip system can also affect the deformation behavior of the other slip system, so that means in the second case the shearing on the specified slip system alpha slip system also increases the strength of the all other slip system and that is represented by G beta, so therefore but beta not equal to alpha and this type of hardening is known as the latent hardening.

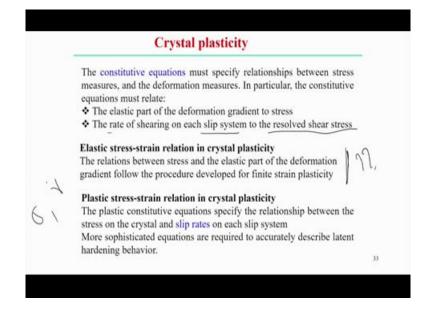
Therefore self hardening can be measured using single slip test but latent hardening is often measured by the first deforming the material into single slip then reloading the specimen to activate the other slip system or maybe to active the second slip system. So these are the way to measure the hardening effect whether it is self hardening or whether we can measure the latent hardening. So basically the self hardening, the increment of the stress level and strength level for a specific slip system direct effect on that or secondly the increment of the strength level for a specific slip system that will affect the other slip system for a specific deformation behavior of a single crystal structure. So once we can measure the self hardening and latent hardening probably we can use to form some equation to predict the hardening behavior of a single crystal structure.

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Latent hardening is often qua which specifies the ratio of the the first $r^{\alpha,\beta} = \overset{g^{\beta}}{\overset{g^{\alpha}}{g^{\alpha}}}$ The details of the hardening complex	e strength of the second syste	em to that o

So latent hardening is often quantified by the latent hardening ratio which specific the ratio of the strength of the second system to that of the first system so latent hardening are can be define the strength of the second system, strength of the first system. So this ratio we can use it but it is not necessary for the several slip system, always the ratio should be maintained as a constant. So therefore the details of the hardening behavior of single crystal structure general it is very incomplex in nature so this was just to idea that probably we can use the hardening like continuum plasticity model for a single crystal structure also.

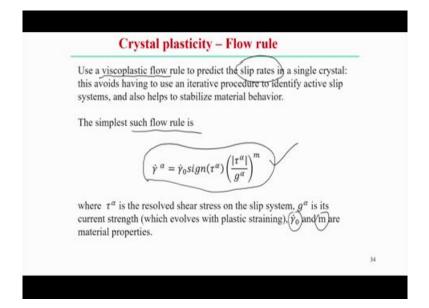
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Now when you as a part of the crystal plasticity theory the constitute equation must specify the relationship between the stress measures and actually deformation measures. So in particular the constitute equation must relate the elastic part of the deformation gradient to the stress and the rate of the shearing on each slip system to the resolved shear stress. So specifically here we are trying to focus on the rate of shearing on each slip system and what is the corresponding to the resolved shear stress. So this constitutive equation will always try to effect this two facts the elastic component as well as the rate dependency of the hardening effect. But if you see the elastic stress strain relation in the crystal plasticity we have already explained, the plasticity in the single crystal structure, the relation between the stress and the elastic part of the deformation gradient actually follow to the constitute develop for finite strain plasticity, so that theory we have explained.

And now plastic stress strain relation in crystal plasticity here it is more significant because the plastic constitutive equation specify the relationship between the stress on the crystal and the slip rate on the slip system. So stress and the slip rate on the slip system, the crystal plasticity try to correlate this two quantity therefore most sophisticated equation is required to accurately describe the latent hardening behavior in this case to probably model the crystal plasticity of single crystal structure.

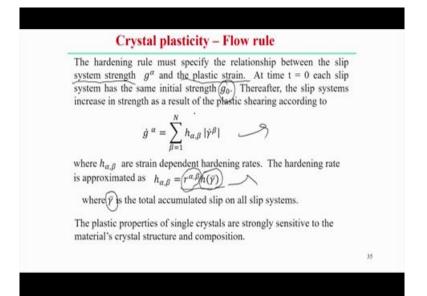
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Now in single crystal structure the flow rule can be decided like that, consider the viscoplastic flow to predict the slip rates in the single crystal structure, so probably we consider the viscoplastic behavior of the material to predict the slip rate in the single crystal structure, so always we try to focus on the slip rate, rate dependent, but avoid having to use an iterative procedure to identify the active slip system, so probably it is difficult to track the individual slip system in terms of the rather than strain rate, so when you try to consider or capture the rate of the slip rate, or maybe in terms of the strain rate, it is more, probably it is more representable then only on the deformation behavior in terms of single strain component.

So this is one of the simplest flow rule generally used and we see in terms of the rate and probably if this rate is significant because we have considered the flow of the material as the viscoplastic flow. So for this viscoplastic flow of the material we can use this relation so where tau actually is the resolved shear stress on the slip system, G is the current strength which evolves with the plastic straining and Gamma 0 dot actually represent and m at the material properties. So m is the not the semi factor here, probably it is the other properties of the material constant, and depends on the properties of the material. So these are the typical flow rule probably we can use in the crystal plasticity model.

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Now if we just more in-going into the crystal plasticity model the hardening rule probably must specify the relationship between the slip system strain and the plastic strain, that also it is obvious the system strain to the plastic strain so it would be correlated and that is the better represented by the hardening rule. So at the time t equal to 0 probably each slip system has the same initial strain g0 if we assume that therefore the slip system increase in strength as a result of the plastic shearing according to this equation. So here if you see the h alpha beta at the strain independent hardening rate, and hardening rate is approximated by this curve h equal to r alpha beta and where h is the function of the total accumulated slip on all slip system. So gamma bar is actually the total accumulated slip and for the on slip system and here the hardening rate is approximated this, so basically the hardening ratio and the functional form of this curve, hardening curve with respect to the total accumulated slip on the all slip system.

So there maybe the several possibility of represent this hardening this curve, the hardening rate curve, this several functional form depending upon the deformation behavior of the crystal structure or several (())(30:31) theories are also there. So we can use accordingly this hardening rate curve and we can use the, we can use it in the to the predict the hardening behavior of the single crystal deformation. Therefore the plastic properties of single crystal structure actually strongly sensitive to the material crystal structure as well as the composition. So it is very much dependent crystal structure and the composition, so accordingly we can derive the different types of the curve that represents the relation, that

actually represents the rate of hardening. So I am not going into that details on how we can do that but rather we can focus on a very basic idea, how we can use it.

The theory is built upo	n:
Relations between	e crystal plastic deformation; nacroscopic and microscopic quantities (strain, stress) Hypothesis (Linking or Bridging Assumptions)
Need for a Mean Fie	d Hypothesis to build the theory
At a continuum point:	$\sigma = \langle \sigma^c \rangle$
At an individual crystal:	

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Now we come to the polycrystal plasticity theory, so basic idea on that, the theory actually built on the physics on the single crystal plastic deformation behavior and always we try to represents the relation between the macroscopic to microscopic quantifies in terms of the stress and strain, that is the basic philosophy of the polycrystalline plasticity theory and in this case the mean field hypothesis probably more appropriate so that normally we represent the polycrystalline theory is the averaging behavior of a single crystal structure. Now here need for an mean field hypothesis to build the theory at the continuum point probably represent the aggregate behavior and we represent the stress component as a average of the individual component and if you see there is a link an individual crystal probably having the stress component sigma c and averaging by the several crystal and we can find out this is the average value and that is true for the polycrystalline structure and there are several field theories are also there and using that field theories probably we can link from the single crystal behavior to the polycrystalline plasticity theory. (Refer Slide Time: 32:49)

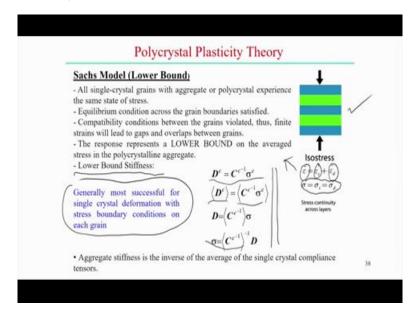
<u>Faylor Model (Upper Bound)</u>	
All single-crystal grains within the aggregi inne state of deformation (strain) Equilibrium condition across the grain bo ceause the vertex stress states required to at each grain vary from grain to grain Compatibility conditions between the grains The response represents an UPPER BOUN ress in the polycrystalline aggregate. Upper Bound Stiffness: Generally most successful for polycrystals with strain boundary conditions on each grain	oundaries violated - ctivate multiple slip s assured.

Now one of the polycrystalline plasticity theory is the Taylor model and that actually decide the upper, sometime it is called the upper bound theory. So in this case what happens, but before looking into that let us look into the right hand side figure, here if you see the structure and probably there is a fiber structure and if you see that if we apply some kind of load, maybe compressive load with the specified direction mentioned in this figure, it actually creates the condition of the isostrain that means same amount of the deformation even there are the two different components or two different materials are there and that condition says the total deformation or maybe total strain remains the same if we consider individual material and this is the condition of the isostrain but this stress or maybe applied load will be sheared by the two different materials, if actually depends on the orientation of that material, so here suppose one is the stress will be divided into two components, sigma x and the sigma d that space is actually applied to the two different individual component of this materials.

Now by looking into this concept we will try to explain the Taylor model to what says that all single crystal grains within the aggregate experience the same state of deformation that means same amount of the strain. But equilibrium approach the grain boundaries violated because the stress state required to active the multiple slip in each grain vary from grain to grain. So in case of polycrystal, if we try to correlate this thing in the polycrystal sample, so in this case, actually since the stress amount is divided so different grains will be subjected to the different amount of the stress because of the strain equilibrium condition across the grain boundary is actually violated.

But compatibility conditions between the grain is assured since the same amount of deformation that means same amount of deformation is associated with the each and every grain. So with this specified model the response actually represents the upper bound on the average stress in the polycrystalline aggregate and we can simply estimate that sigma c cc into dc that means stress in terms of the stiffness, so here this second equation actually indicates the averaging of the single behavior of the single crystal structure and finally we can find out that sigma equal to cc into d so average stiffness is the average of the polycrystal is the average stiffness, is the average of the single crystal stiffness tensor. So this is the basic philosophy to model for the to explain the Taylor model considering the displacement continuum approach the layer.

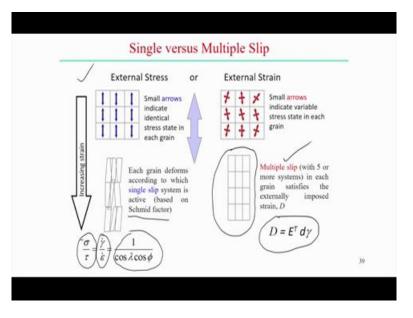
But this theory actually applicable generally most successful for polycrystal with the strain boundary conditions on each grain, actually this Taylor model we have already explained to maintain the computability condition, so better this condition is successfully for polycrystal, but in this case the strain boundary condition on each grain should be mentioned. So this is the one model.



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We can explain the another model that is called Sachs model that is the lower bound theory probably in this case and before looking into that we can look into that right hand side figure, here if you see that isostress condition so probably looking into the orientation of the fiber, in this case if we apply the compressive stress is mentioned in this figure, in that case here the stress remains the same, that is the isostress condition for all the grains, for all the components of this material but the amount of the deformation if you shear between the two components of the material. So that means this is the total strain consist of the two component of the strain. So this concept probably we can implement to explain the Sachs model. We can say that all single crystal grains we can aggregate or polycrystal explain the same state of the stress, so when it is subjected to the same amount of the stress state then definitely it will try to satisfy the equilibrium condition across the grain boundary.

But compatibility conditions between the grains actually violated the finite amount of the strain or different amount of the strain for the different polycrystal, actually leads to the gap and probably or overlaps between the grains. So this responds represents the lower bound on the average stress in the polycrystalline aggregate but if we find out the lower bound stiffness, here if we see from the similar strategy we can find out that average stiffness is the inverse of the average of the single crystal compliance tensor. So this is the average tensor according to the Sachs model and the it is obvious the difference between the Taylor model and Sachs model only in terms of the whether we are isostress deformation model or isostrain model. So this model Sachs model actually generally most successful for the single crystal deformation to explain that but with the stress boundary condition on each grain.



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Now let us look into, physically try to understand the single versus multiple slip, it will be better understood that first case or maybe left hand side we consider the external stress is applied so small arrow indicate the identical stress state in each grain. So all the identical stress state in the each grain and here each grain actually deforms according to which the single slip system is active. So that can be better explain in terms on the Schmid factor, so that stress by shear stress or rate can be represented by this, Schmid factor. So that formula can be used it here when the grain are subjected to external stress and here it is subjected to the philosophy of the single system active on the Schmid factor.

Now if we look into the external strain, that means if it is the external strain remains the same so small arrow variable stress strain but the deformation level remains the same, so here look into this, the deformation level that means the deformation remains the same for all the grains but there is a variation of the stress state so in this case probably the multiple slip which is five or more system in each grain satisfy the externally imposed strain that means when you material is subjected to external strain with the variable stress state then multiple slip system is active and in this case it is necessary to satisfy the externally imposed strain condition and D can be represented by this amount of the elastic deformation case, the Et in terms of the elastic modulus and the amount of the shear strain.

So here we have tried to explain that the different approaches for the single crystal plasticity models but I have not explained in terms of the details of the models, probably there is a several, it can be extended to develop different kind of crystal plasticity model or to explain this phenomena what we have discussed in a crystal plasticity model. So thank you very much for your kind attention.