Introduction to crystal elasticity and crystal plasticity
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Hello everybody! Let us start, I think this is the last chapter or last module introduction to crystal elasticity and crystal plasticity.

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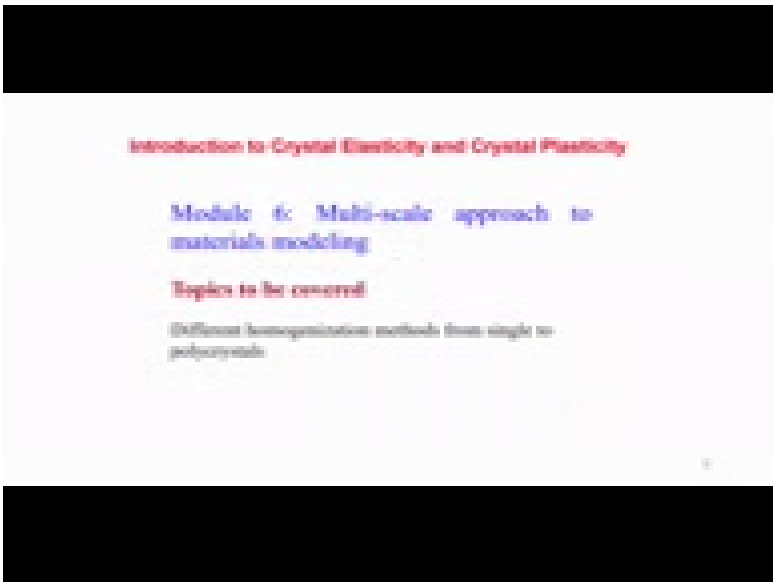

So in this module we will try to focus on the multi scale approach basically the multi-scale modeling approach. So in this chapter or in this module probably I will try to focus on the very introductory level of the multi scale modeling approach and of course it is very specific to material modeling. Although it is a very vast content for multi-scale modeling approach so we will try to focus on selective thing and very basic elementary things related to multi-scale modeling approach to get some idea about the topic. So here the objective is not much going into details of the in depth analysis of the different approaches of the multi-scale modeling, that to understand the subject little bit in easier way. So multi-scale means we understand the modeling approach at different length scale or at different time scales, but problem is that the how to link the different length scale and different time scale and what maybe the consequence of the computational cost to do such different scales of modeling approach at a single time.

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So let us see how we can start with this. So before start on this actually discussion on the multi-scale modeling approach, I will try to acknowledge the following professors, scientist, technicians because this module I have prepared based on their view of this distinguish scientist and the professor and I will try to represent their view on the multi-scale modeling approach.

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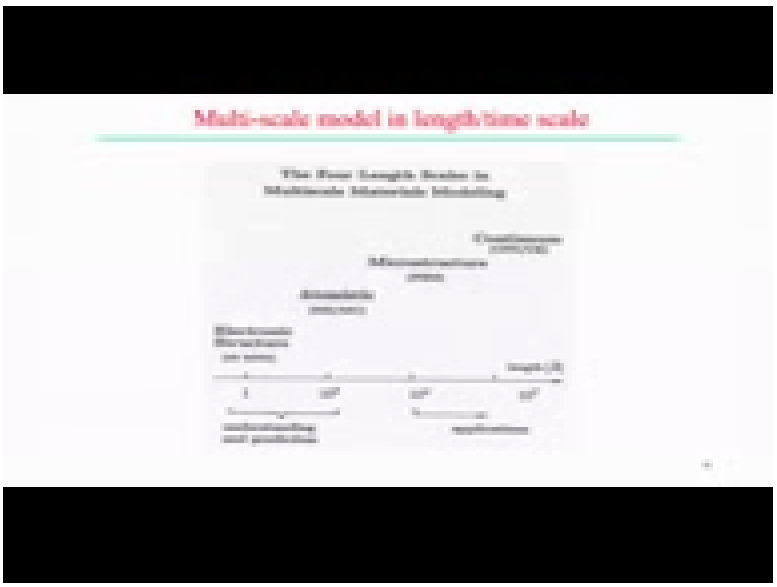

So first if we see that multi-scale modeling approach means how we can conduct the physical model of the process at different time scale or at different length scale. If you see this is the very 4 basic slabs of the multi-scale modeling approach, you see that of course all these cases

the length scale and time scale are different so first we can start with the electronic structure, atomistic structure and then level of the length scale is the microstructure and then finally the continuum model, probably we are very much familiar with the modeling approach using the continuum mechanism and using the continuum scale and here the continuum scale means we understand around order of millimeter range, but if we look in fact the electronic structure the length scale is almost around the level of 10 to the power of minus 10 or 10 to the minus 12 like that. So there is huge difference in the length scale between the electronic structure and continuum scale.

And in between there is a atomistic structure and microstructure they are exist at the different scale and if you see that electronic structure generally we explain that in some kind, using some statistical mechanism or statistical model or we can say the analytical model and we try to understand the electronic structure and then we try to looking into the electronic structure we can predict the atomistic structure using the concept of the molecular dynamics or we use the Monte Carlo simulation to predict the atomistic structure by understand the basic physics of this. But when you approach the next level of the length scale microstructure scale probably we can analyze the microstructure using the finite element method or some kind of constitutive law we use it and we can analyze in some other numerical techniques, also analytical techniques we can use for microstructure, but of course when you next level of this thing continuum we link it with that CFD – Computational fluid dynamics or some other finite volume methods probably we can use or even we can use finite element methods and to analyze the process in the continuum scale.

So it is also important to know that probably it will be the experimental facility or probably the conducting the experiment is relatively costly if we try to do in the lower scale probably electronic structure and atomistic structure, in that scale to conduct the experiment is bit of costly time consuming and uncertainty also and involvement is more but rather if it is possible to conduct the experiment on the continuum scale or probably we can do see, doing the experiment of the microstructure in that scale level it will be relatively low costly. So predicting the experimental results or using the experimental result to the predict the behavior of the materials in the lower scale or probably in the upper scale, that risk to follow the relation or maybe some organized approach is possible and through the multi-scale simulation among the different length scale. Probably it can so upper side, up scaling or it is possible to do the low scale, down scaling also both way it may be possible to develop the some multi-scale approach for the different processes.

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So if we look into that basic approach, in the large multi-scale modeling approach, if we see from the figure that probably if we consider the dynamics of metals and we can start with the length scale in the dislocation phenomena. So dislocation phenomena we can explain the edge dislocation, screw dislocation on the atomistic scale and from that we can predict the dislocation exist in a crystal structure and of course defect and dislocation actually exist due to the due consideration of the we can assume there is a defect exists in this atomistic structure of a specific material and there we can estimate finally the basic elementary in terms of edge and screw dislocation for any kind of single crystal structure.

Now here we can predict the dislocation motion and interaction between the dislocation and then how uhh dislocation energy interaction or probably the exchange of the dislocation energy due to the motion of the dislocation probably that we have explained using the single crystal plasticity that is related to the dislocation dynamics and we can predict the single crystal stress strain relationship whether it is isotropic or anisotropy. But in this case single crystal plasticity is probably if we look into the most of the case if we look into the anisotropy or isotropic behavior plastic behavior of the materials. So looking into the dislocation dynamics probably we can link in the next level the polycrystalline plasticity.

If we see that the polycrystalline plasticity that is the meso scale, the scale is different from the dislocation dynamics and compared to the polycrystalline plasticity, so looking into the single crystal plasticity by averaging all this things maybe we can predict the plastic rule or we can derive the plasticity model in case of polycrystalline structure. But that scale is even

it is in meso scale. Probably we can polycrystalline stress strain responds us polycrystalline stress strain relations can also be derives on this scale but finally next level scale of analysis is the probably that is the continuum scale, so at the continuum scale probably we can represent the strain between the stress and strain in terms of the using the different plastic law.

So we have discussed the continuum plasticity model also and we derived that this models consider both isotropic behavior and anisotropy behavior in aggregate but this model is valid over the continuum scale that means over the around scale of the millimeter, order of the millimeter range. So in this case we estimated Von Mises yield surface and then we from there we can predict the uhh plastic behavior of the materials. So probably the single crystal plasticity is the key fact to link the atomistic scale and the continuum length scale. But how we can link between these two scales that is the most important in the multi-scale modeling approach.

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Now if we look into that basic idea on the material modeling and how we can use the multi-scale approach in material modeling, so if you see that that (())(10:28) dislocation plasticity the resolution is like that first we can start with the atomistic model the molecular dynamics, it is the specific point where we can fix all the atoms and the length scale is around 10 to the power minus 10 meter and from the atomistic model we predict the defect and then we represent within the materials in terms of the dislocation. But that dislocation we consider as a discrete dislocation. So discrete dislocation theory probably we can use it on this scale and

where the scale range is around of the order of 10 to the power minus 8 meter and looking into the discrete dislocation theory we can predict that the continuously distributed dislocation theory so here we can predict that dislocation pattern as a whole when the length scale in this analysis is probably it is more, so it is around 10 to the power minus 7 meter and then once the next level of the crystal plasticity and we can analyze over the individual grain also uhh or as an aggregate the polycrystalline theory also we can use the plastic law or deformation behavior of the grains but within the grains we can use the information of the nature of the dislocation existence here.

But here in this case the length scale is around 10 to the power minus 5 meter and finally we can analyze the macro scale or maybe using the continuum plasticity law, we can predict the plastic behavior of the material. So in this case there is a different theories exist over the different length scale and finally when you try to uhh estimate the plastic behavior in the macro scale or using the continuum plasticity model probably its behavior is the averaging of the (())(10:28) scale of the analysis. Now if you see the polycrystalline idolization of grains with the distributed defects in terms of dislocation. So in this case we can see that both scale of grain and sub-grain structure there is a this is the probably interaction through the grain boundary and that is also the interaction through the grain boundary but how we can represent the behavior of the dislocation within the structure, in this case we represents the behavior in this scales of the grain and the sub-grain structure.

And of course then when you represent this only grain scale in this case all the (())(13:51) also exist within the grain scale and finally represents the aggregate that is the homogenization description of the materials also occurs in this final case and that is the aggregate behavior of the polycrystals which is the aggregate of the individual behavior of the single crystal structure. So these are the different ways or different window of the analysis at a different scale and the we have not looked into that probably the how we can link between all this scales.

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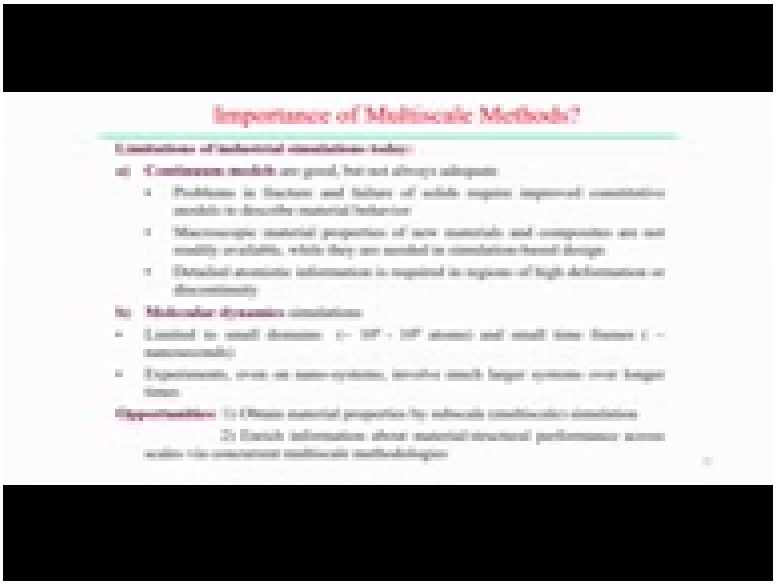

So what is the importance of multi-scale methods but now-a-days the limitation of the industrial simulation is first thing is that of course most of the cases we focus on the continuum model there goes even but they are not always adequate, probably if we consider the problem of the fracture and failure of the solids that actually required till now the improved constitutive model to describe the material behavior. But microscopic material properties of the new material and composites are not readily available but that is very much needed in simulation bases design so that actually of course in this case specifically when the composite if we consider in the new materials, so it is very difficult to predict the behavior of the continuum scale until and unless we can analyze the behavior of the materials in the lower scale.

So detail atomistic information is required in the regions of the high deformation or it exist discontinuity, probably that is more relevant to the composite materials. So that is more restricted use of the continuum model. Now if we on the other side if we look into that molecular dynamic simulation that is also limited to very small domain 10 to the power 6 to 10 to the power 8 atoms probably represents the behavior of the materials as a whole and the small time frame also in the order of the nanosecond time scale we can predict the behavior using the molecular dynamic simulation. But experiment even on the nano system involved much larger system over and at the same time over a large time also required to conduct the experiment. So that are the another limitation of the simulation if we consider the molecular dynamics for a new materials for a new system.

But opportunities obtain material properties probably by subscale multi-scale simulation that can also be done, enrich information about the material structural performance across scale that can be done by concurrent multi-scale methodology. So that is the other ways probably we can look into this aspect to explore the multi-scale method or multi-scale modeling approach in material science.

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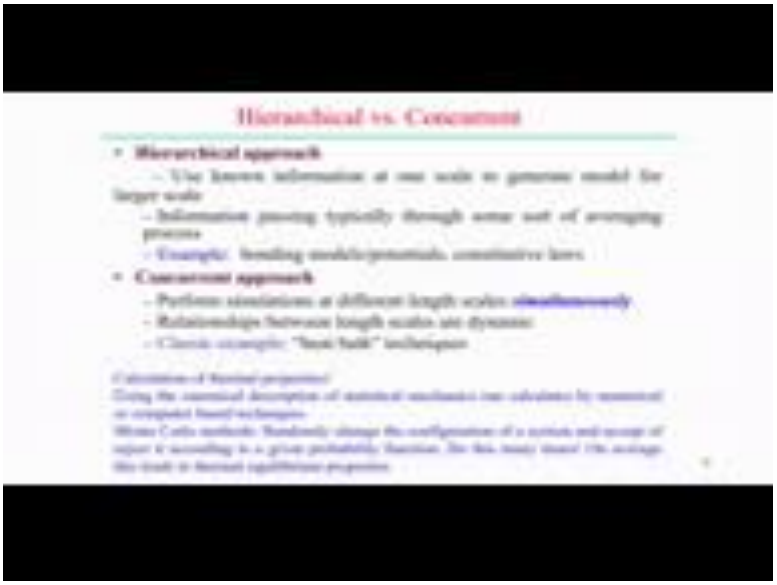

So to do that, that means to analyze the multi-scale modeling approach probably we need to understand that what are the approaches that we generally follow in case of multi-scale modeling, one is the hierarchical approach, another is the concurrent approach. So hierarchical approach we use the node information at one scale to generate model for the larger scale so information passing typically through some sort of the averaging process from lower scale to the next level of the scale. Example bonding models, potential and very other things are constitutive laws probably use in case of hierarchical approach. But concurrent approach in the perform generally simulation at different length scale simultaneously, so relationship between the length scale are dynamic.

One typical example of the concurrent approach is the specifically heat bath technique. Let us see what is heat bath technique, heat bath technique probably used for the calculation of the thermal properties, using the Canonical description of the statistical mechanics one calculates by the numerical or computer based techniques, so one such example of this thing Monte Carlo methods that randomly change the configuration of the system and accept or reject it according to the probability function. If we do for iterative process on a average this list were

the thermal equilibrium property, so this is typical heat bath technique that actually follow the concurrent approach to predict the thermal properties.

But in this case we need a perform simulation at a different scale and most of the cases we need to some iterative approach to trial and error kind of things. But main difficulties of concurrent approach is that the length scale represent between the length scale are dynamics to maintain the dynamic behavior at the interface is really difficult to multi-scale modeling approach, so most of the methods now probably it is more easier to go to the hierarchical approach where the information in the lower scale can be used to predict the behavior of the upper scale.

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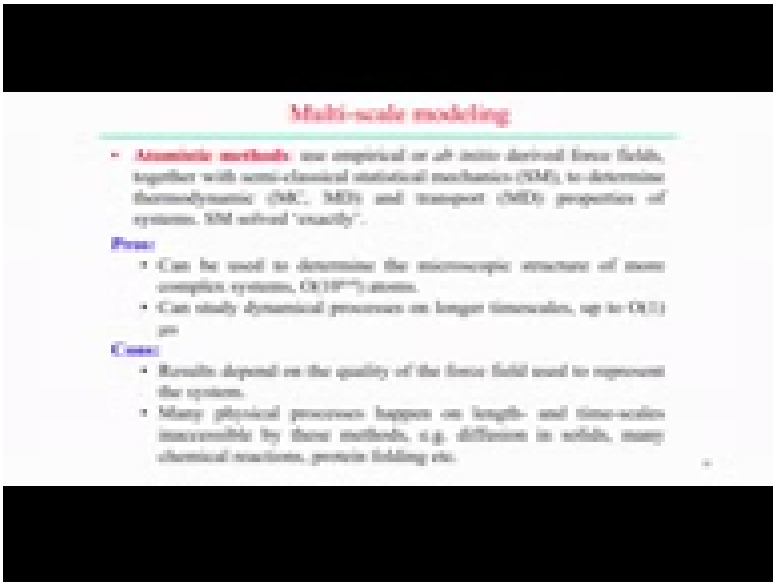

So these are the typical approaches in multi-scale modeling, let us start with the atomistic method. In this case we use the empirical relation and from the very beginning derived the force fields together with semi-classical statistical mechanics to determine the thermodynamics and transport properties of the system. But the statistical mechanics solve actually exactly so of course the atomistic methods use the empirical derive force field but it says it can solve the exactly the data or what maybe the advantages and one sided and other sided of the atomistic method. One is the it can be used to determine the microscopic structure of more complex system probably the order of the 10 to the power of 4 to 6 atoms of this that constitute to one system and using that system the microscopic structure of the system can also be calculated.

But this model can also be dynamical process, consider the dynamical process probably up to longer time scale up to order of one micro second but other side if we look the atomistic methods but results (())(21:02) depends on the quality of the force field used to represent the system. So it is system dependent, many physical process happens on the length at time scale inaccessible probably by this method. For example the diffusion in solid many chemical reaction, chromatic folding, this type of physical process probably difficult to access using this atomistic methods, that is the other sides of the atomistic methods.

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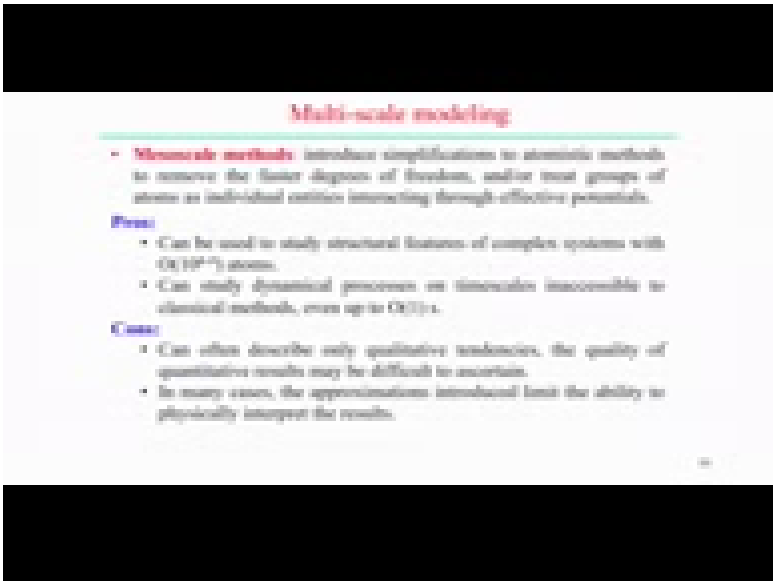

Now if we look into that Mesoscale methods that actually introduce simplification to the atomistic method to remove the first degree of freedom and consider group of atoms as individual entities interacting through the effective potentials. That means the cluster of very group of atoms represents one properties on state and that can be considered in the Mesoscale methods, so probably this mesoscale method is the one is the higher scale approach, higher scale in the sense that scale length is bigger here as compared to the atomistic scale. So the advantage probably can be used to the study structural features of the complex system, so in this case the cluster of atoms or group of atoms can be consider of the order of 10 to the power 8 to 9 atoms to represent the system but dynamical process on the time scale inaccessible to classical methods even up to the one second, so probably we can use the larger time scale using the mesoscale methods.

But this advantage or other side, darker side of the methods is that is open despite only the qualitative tendencies, the quality of quantitative results maybe difficult to a certain

sometimes, in many cases the approximation introduces limit the ability to the physical interpret the results. So these are two disadvantage probably if we consider the mesoscale method.

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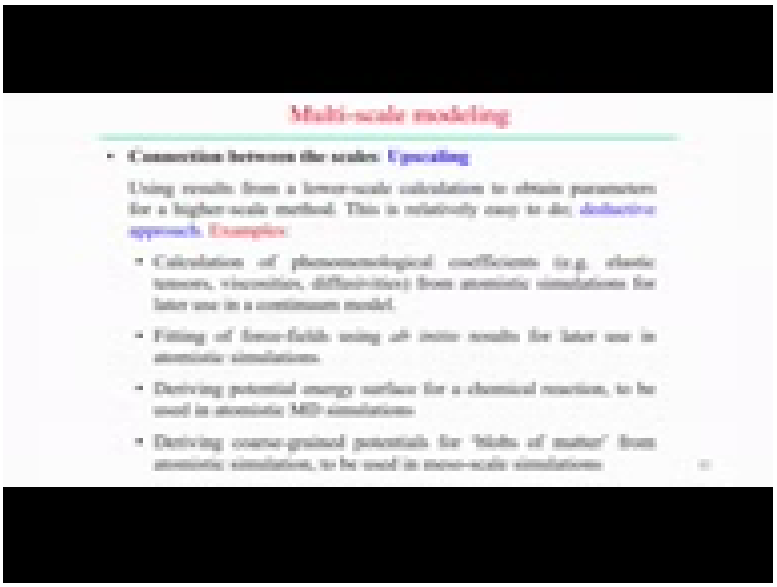

Now continuum methods, in this case we assume that matter is continuous and treat the properties of the system as field quantity, numerically solved the balance, equilibrium equation (())(23:21) with the phenomenological equation to predict the properties of the system. So this is the basic method of the continuum, basic philosophy of the continuum methods, but in principal it can handle system of any macrosize and dynamic process relatively longer time scale. So longer time scale as well as the longer length scale it can handle the problem and it is possible to solve numerically balance equation, we generally solve the numerically equation governing equation we solve it on this scale, but difficulty is that required input for example elastic tension, diffusion coefficient equation of the straight from experiment or that can be derived from the lower scale methods which sometime is difficult to obtain but cannot explain result that depend on the electronic or the molecular level of the details.

So of course continuum method having advantage is one scale probably cannot capture the behavior of the system in the molecular level in details or the electronic structure in details so in that case we need to consider the lower scale methods probably in the atomistic scale model we need to consider.

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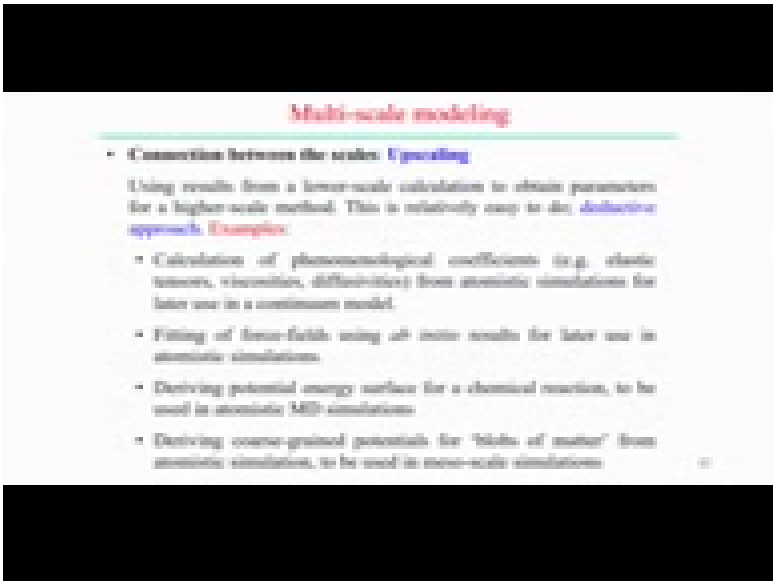

Now of course there are the different scales of analysis and each and every scales having their limitations or their advantages in the different way. But most important or significant things in the multi-scale modeling is the how we can connect at the different length scale, so probably one approach and that is called normally called up scaling methods, so in this case using result from a lower scale calculation to obtain the parameter from the higher scale method, this is relatively easy to do and it is generally called the deductive approach. Maybe you can look into the example of the what is the up scaling method, one thing is that calculation of the phenomenological coefficient for example the elastic tension, viscosity, diffusivities, from the atomistic simulation for later use in a continuum model. So this one we generally we use in case of up scaling this is the one example of the up scaling methods.

Fitting of the force field using the initial results for later use in atomistic simulation, this is another example we can use the fit the force field from the initial results for the later use in the atomistic simulation. And deriving the potential energy surface for a chemical reaction to be used in the atomistic molecular dynamic simulation. Deriving the course grain potential of the cluster of (())(24:50) of matter, maybe can polycrystal from atomistic simulation to be used in the mesoscale simulation. So up scaling all the up scaling method that always we try to link the lower scale properties behavior in aggregate to link with a higher scale, or if there is a need of the any uhh phenomenological behavior which is required which need to define for the higher scale method that we can generally derive from the lower scale method. That is the basic philosophy of the up scaling method.

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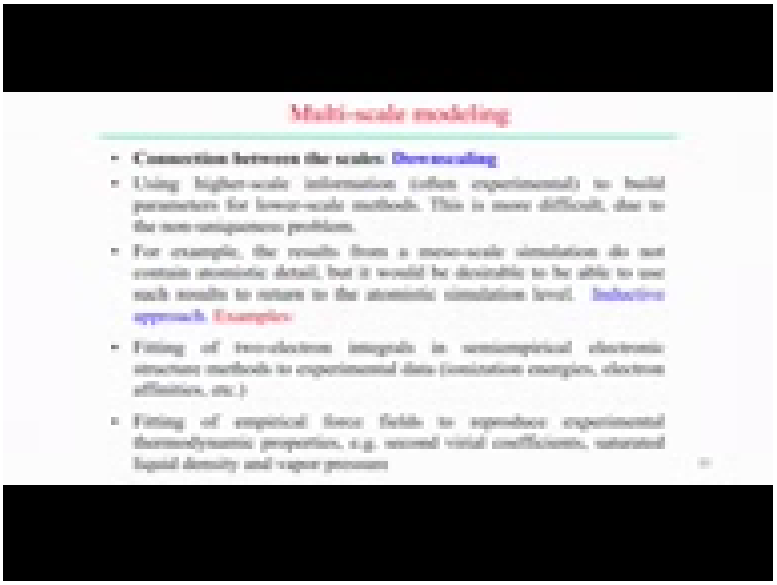

Similarly in down scaling method here the basic philosophy is the using the higher scale information most often it is experimental to build the parameter for the lower scale methods but it is more difficult as compared to the up scaling method because of the non uniqueness of the problem. We can take some examples also, the result from a mesoscale simulation do not contain the atomistic details but it would be desirable to able to use such results to return to the atomistic simulation level, is that is called basically inductive approach. For example fitting of the two electron integral in semi empirical electronic structure methods to experimental data that is called ionization energy electron affinity.

There is a one example of this down scaling method, fitting of the empirical force field to reproduce the experimental thermodynamics properties for example second viral coefficient saturated liquid density and vapor pressure. Probably if we link if we consider although theoretically it is difficult more difficult down scaling approach to link the information from the higher scale to predict the behavior of the lower scale but other way probably if it possible theoretically predict so experimentally it is more easier to conduct the experiment relatively on the higher scale as compared to the lower scale method. So in that way it is advantageous because here we need the information and we can conduct the experiments on the higher scale.

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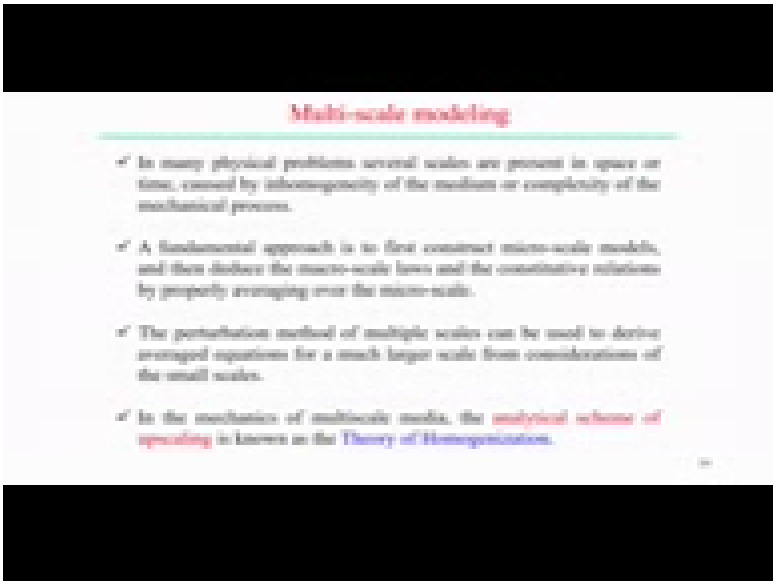

So looking into these two approaches up scaling and down scaling in the multi-scale modeling approach now if we see that in general the multi-scale modeling the few significant points are important here, first point is that in many physical problems several scales are present in space or time probably cause by inhomogeneity of medium or complexity of the mechanical process. So a fundamental approach is to first constitute the multi-scale models and then deduce the multi-scale laws and the constitutive relation by properly averaging over the multi-scale. So that if we look into that multi-scale and the mesoscale model here if we see that basic fundamental approach of the multi-scale modeling linking that average in of the lower scale and that use this information to for the higher scale approach.

The perturbation method of multi-scale can be used to derive the average in equation for a much larger scale from consideration of small scale so in the mechanics of the multi-scale media the analytical scheme of up scaling is generally known as the theory of homogenization. So ultimately the more practical approach in the multi-scale modeling is to consider the probably in the up scaling which is relatively easier.

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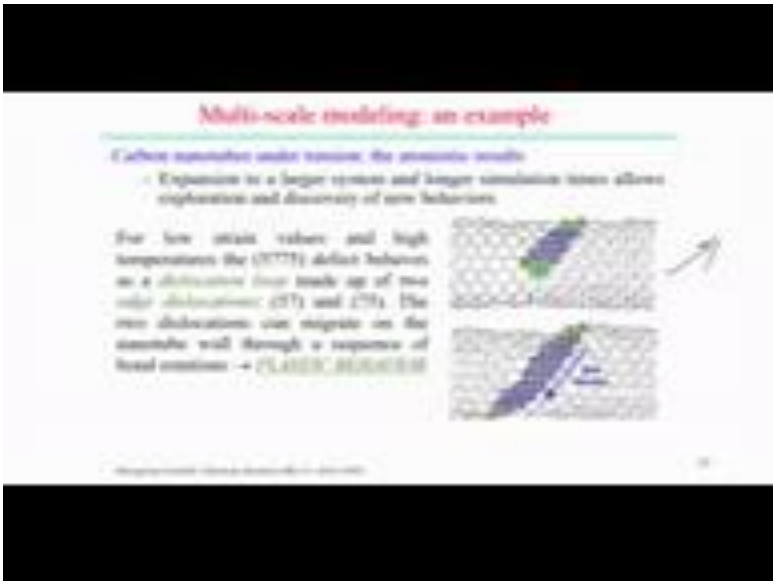

Now if we look into some example probably if you see the multi-scale modeling approach, we will take one example that carbon narratives under tension the atomistic results if we see that the first figure that the expansion to a large system and longer simulation time actually exploration and discovery of the new behavior. So if we allow for longer simulation time probably we can do the simulation based design, we can explore new behaviors. Let us look into this example, at low strain and high temperature, with that condition 5775 defect behavior atomistic structure a dislocation loop. So this 557 and this the 75, these are the this constitutive on dislocation loop made up of the tow edge dislocation that is 57 and 75. Now the two dislocation can migrate on the nanotube wall through a sequence of the bond rotation.

So through a sequence of the bond rotation there is a glide direction so two dislocation can migrate separately to a, if we look into the glide direction so in that direction actually two dislocation uhh migrated here so that type of behavior and that happens due to the sequence of the specific bond rotation in the carbon nanotube. So that type of behavior probably it is due to the plastic behavior of the carbon nanotubes. So this is the observed. So final conclusion from here that with this example we can say that if we longer simulation time if we allow probably we can discover the very new behavior. So that can be modeled and the in specifically when the carbon nanotube is subjected to some kind of tensile force.

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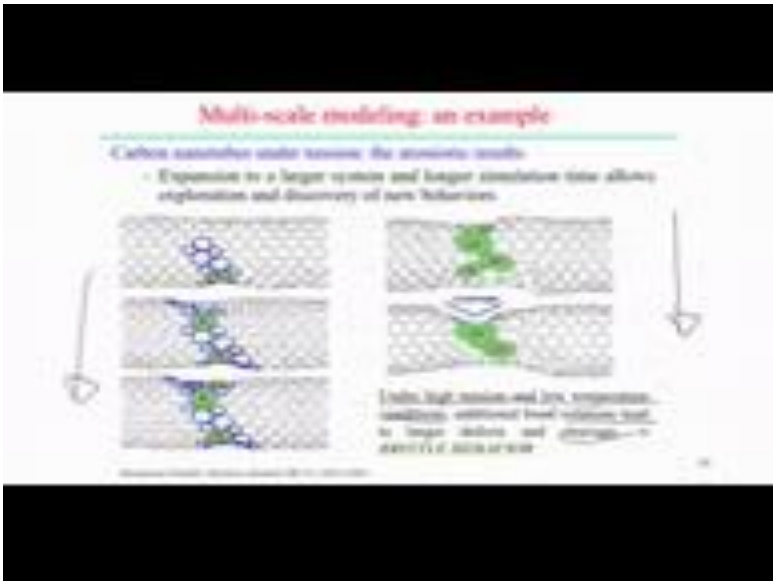

Now if we look into the carbon nanotube under tension the atomistic results but if expansion to a larger system and longer simulation time again if we do this things if we see that under high tension specifically low temperature condition if we see the additional bond rotation finally lead to the larger defect and (())(33:47). So that kind of actually finally leads to the related to the brittle behavior of the carbon nanotubes. So this behavior of the carbon nanotube it is actually the simulation is done for under tension. Now under tension creates the dislocation, it can create the dislocation loop or movement of the dislocation and finally with the if the tension is very high probably we can subjected to (())(34:17) so that is very much obvious through this kind of simulation.

So that simulation having certain importance to predict the behavior of the carbon nanotube which is under tensile force. Now in this case probably if it is a high tension and low temperature this condition is predicts the behavior like the brittle behavior where atomistic structure if in case of the tension, moderate tension probably it can predict the plastic behavior of the carbon nanotubes. So this are the typical example for the simulation based design generally we observe in case of multi-scale approach.

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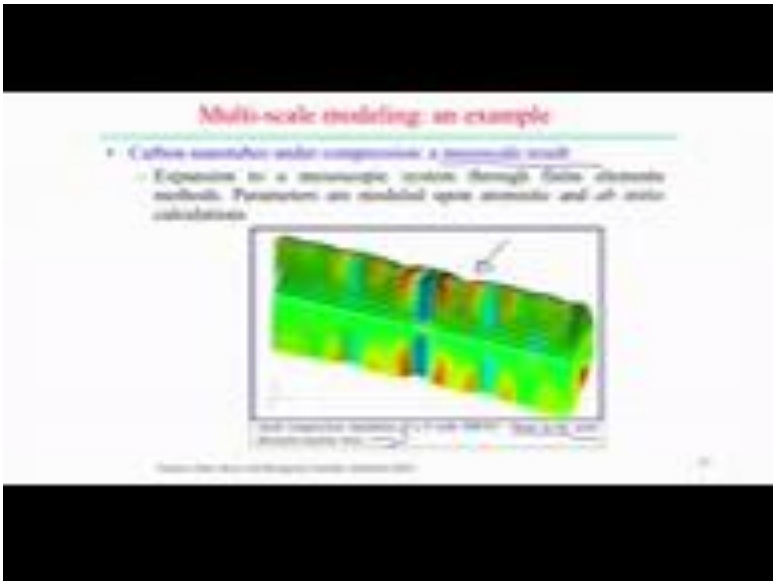

Now this also, the carbon nanotubes under compression but this is a mesoscale result so scale is different here. So expansion to a mescoscopic system through finite element methods, parameters are model of (())(35:17) atomistic but what was the initial calculation. If we see that axial compression simulation of the 9 walls of the carbon nanotube and stress in the axial in the direction we see the simulation that color actually predict the different deformation behavior, deformation behavior corresponding to the different stress level at axial direction. So point is here that simulation can be done in the different scale but here the I think it was in the different scale but here if we conduct the experiment in the mesoscale to predict the different behavior and that can be possible if we consider the different multi-scale approach here.

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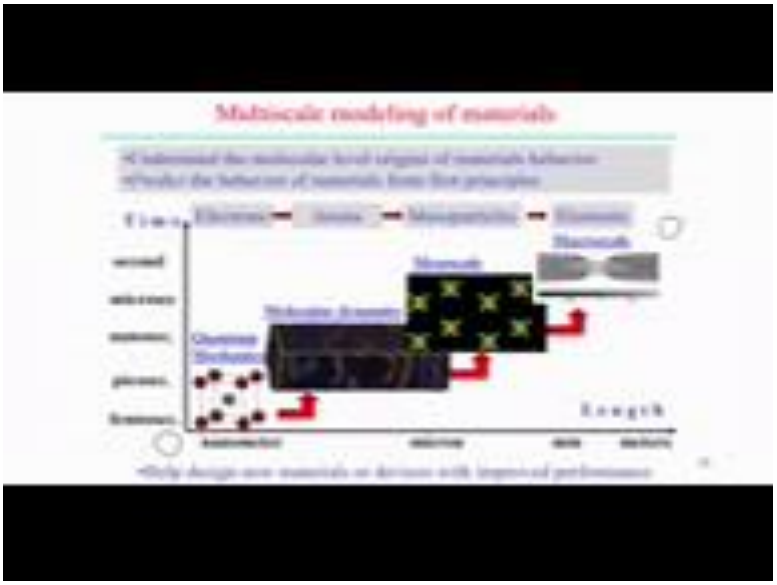

Now in general if you see that multi-scale modeling of the material that always we try to understand the molecular level origin of the material behavior but predict the behavior of the materials from the first principal so if you see also that along the x axis and y axis if you see that the length scale are different, time scale are also different. So in the uhh lower scale femtosecond maybe in the nanometer length scale and the femtosecond time scale that can predict the behavior of the electrons and a whole next level the molecular dynamics the behavior of the atoms atomistic structure a whole then using the behavior of the atoms probably we can, mesoscale, meso particles behavior atomistic structure an aggregate taking the information from the atoms and another next level we can pursue the multi-scale approach, the element so in this case we can consider the length scale millimeter range and the time scale is in the seconds.

So that this time scale or length scale is completely different from this time scale and length scale, there is a huge difference of this thing, but through the multi-scale modeling approach we can link the different scale level taking the information from the lower scale level we can reach up to the upper scale level and all the scale level probably the behavior or the calculation theory the behavior is different. But if we atomistic structure gross if we try to predict multi-scale approach probably we need to link all the different scales, this actually helps to design new materials with improved performances probably if we look into the very lower scale approach that actually helps to design the new materials and device with improved performance, that performance can be measure on the higher scale.

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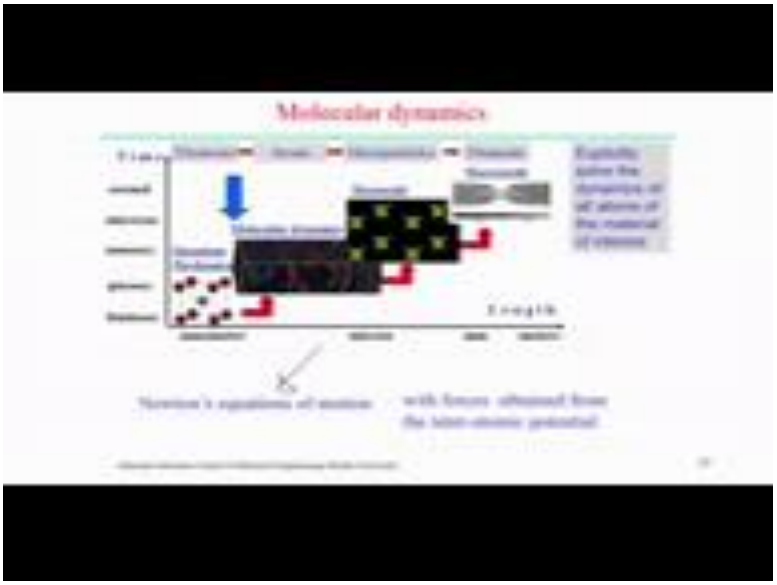

So molecular dynamics if we see that explicitly it solves the dynamics of the all atoms of the materials of interest, so that predict some certain behavior of the molecular dynamics that with the forces we can estimate the theory probably we can look into the force obtain from the inter atomic potential and accordingly we can estimate this thing. What are the same time once it is done the lower scale, simply lower scale means probably we can look into that in microscale if we zoom it, we can reach it ultimately the lower scale the nanometer scale and where the macroscale and we can use the neutrons equation of motion there and we can predict the behavior, but ultimately that behavior can also be linked with the molecular dynamics simulation. That explicitly from the dynamics of the all molecules of the atoms at the low scale.

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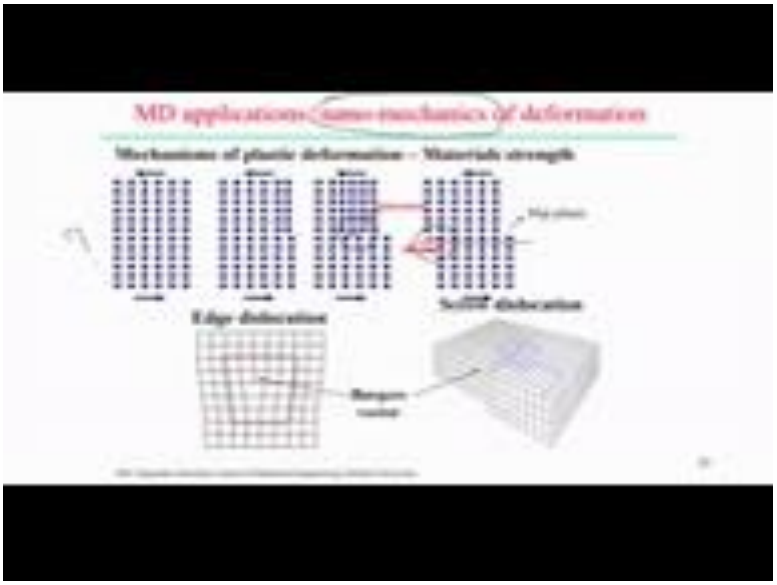

Now this molecular dynamics applications probably if we leave the nanomechanics of the deformation that we have if we start from the very basic thing that the crystal structure metals, we have started actually from the crystal structure from the materials and we start with the very basic model, hard sphere model we represent the crystal at the regular arrangement of the atoms, if there is a disturbance of the regular arrangement of the (())(39:55) then we consider that existence of the defect, it can be point defect, it can be line defect, probably can surface defect atomistic structure well. So that behavior of the representation of the atoms in the crystal structure that was on the nanometer scale. Now from the nanometer scale if we try to understand the mechanics so only to explain this is the regular arrangement of the atoms, now if it is subjected to the shear force like that so over it will create the shear force, it will create the dislocation defect.

In this case it is edge dislocation and it is very idealize case defect existence in terms of dislocation in the crystals so this is the dislocation. Now there is a slip happens over the cluster of the atoms specific on the slip plane and this accounted amount is the consider we can this is the amount of the shear strain in this case average we consider the amount over the slip plane and this phenomena we represented in terms of edge dislocation and the screw dislocation having the difference orientation of the slip plane, slip directions and represent the dislocation in terms of the Burgers vector. But in this mechanics explain on the nanoscale, so that is why it is called the nanomechanics.

And this slip system of the difficult crystal all we have already explained this thing but point is that that explanation all this thing was valid and the nanometer scale that is why it is called nanomechanics. So that mechanics is helpful to finally the (())(41:55) of the dislocation, discrete dislocation dynamics so when the conitnuous dislocation and from there we can predict the mesoscale atomistic structure a grain scale approach mesoscale or maybe atomistic structure a grain scale approach we can reach to the continuum scale. So basically in the materials, the deformation of the metals if we look into the plastic deformation of the metals in the continuum scale and that behavior if we try to zoom then probably we can reach the behavior of the metal on the nanoscale so that is the this are the mechanism in the nanoscale, that we always try to link to predict the polycrystalline and finally the behavior of the materials in the continuum scale by conducting the simple tension testing or shear strain of the piece of a material, in the scale of the millimeter.

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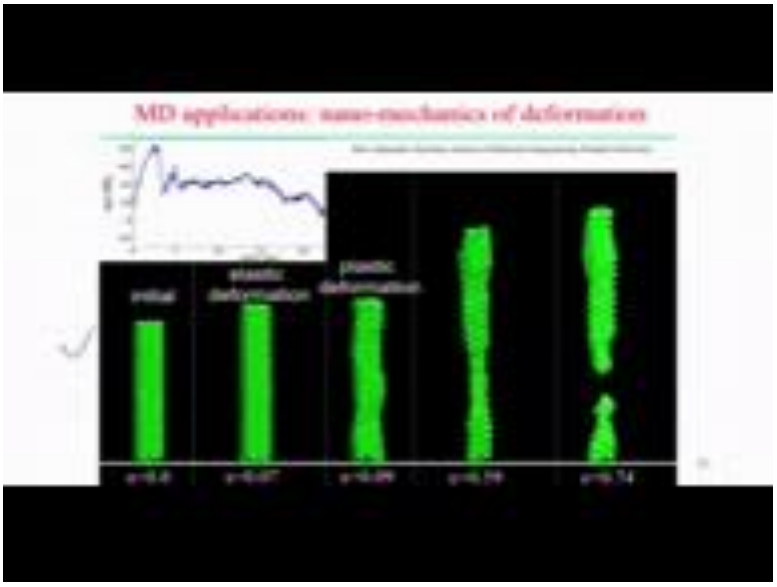

So if we see that molecular dynamics applications specific to analyze the nanomechanics of the deformation, so the lower scale level probably this we are trying to explain the lower scale level, if you see the initial structure was like that the first figure, second figure if you see that are the deformation of the 0.07 there is a elastic deformation happens, now once the elastic stage overcome then the higher strain level, the plastic deformation happens so there is a disturbance of the regular arrangement of the atoms if you see and here if you see the reduction of the section probably in continuum mechanics we generally called atomistic structure a necking and if we see that another scale that is the complete fracture happens separation of the atoms at a very high strain.

So that similar kind of behavior if we observe in the continuum scale also by considering the simple tensile testing, but here if we see that stress versus time that graphical plot it is not very smooth curve, there is a continuously fluctuating nature of the curve if we observe because we measure actually we simulate or whatever through experiment we measure the time scale is picosecond level. So picosecond level the behavior of the molecule or probably if we do the molecular dynamics application so that represented actually not the smooth curve, smooth amount of the stress with respect to time, there is a fluctuation of this time.

But same experiment if we conduct probably in the uhh nano, in the continuum scale or millimeter scale probably that type of fluctuation nature we can eliminate that, fluctuating nature of the stress versus time scale. So this is the typical molecular dynamics applications to explain the nanomechanics of the deformation.

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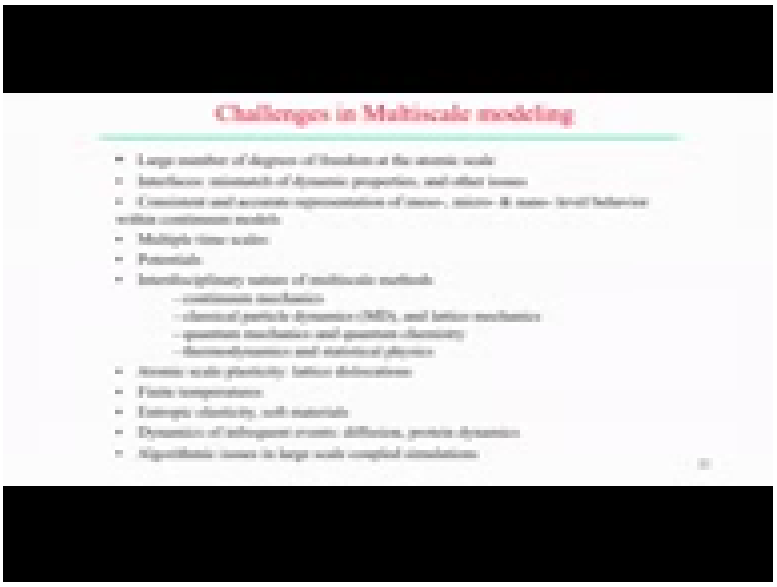

So of course multi-scale modeling is very complex phenomena and there are several challenges also, if we see that the large number of degrees of freedom probably the atomic scale so degrees of freedom is very high the atomic scale to tackle of handle all this degrees of freedom, it is not easy to conduct the simulation and specifically at the low atomistic scale. Second challenge is that interface, so at the interface there is a mismatch of the dynamic properties so at the same time at the interface how we can link the dynamic properties in the automatic scale to the next scale, linking this thing is really difficult in case of multi-scale modeling.

Third point is that consistent and accurate and representation of the mesoscale, microscale and nanolevel behavior within continuum model so really difficult to represent all the scale level behavior in one scale probably in continuum scale it is difficult to represent all the behavior of the three lower scale. Fourth point is that how to link the different time scale because atomistic model probably in the picosecond or femtosecond level the analysis, but in continuum scale we analyze in the order of the second. So linking the multiple scale is really difficult at then inter disciplinary nature of the multi-scale method for example continuum mechanics how to apply, continuum mechanics, classical particle dynamics, lattice mechanics, quantum mechanics and quantum chemistry and thermodynamics and statistical physics, all inter disciplinary nature of the multi-scale metal linking between this two is uhh difficultly in the multi-scale modeling approach.

Atomics scale plasticity, so plastic behavior predict of the constitutive law in the atomic scale and is the really difficult that actually normally atomic scale plasticity and to link with the lattice dislocation, in the plastic behavior of the lattice dislocation and linking between this two difficult in the multi-scale modeling approach. Probably finite temperature this at the (())(48:11) into plasticity soft material, there are several issues in the multi-scale modeling,. Dynamics of the infrequent event probably which is not very frequent for example diffusion, protein dynamics is the really challenging task in multi-scale modeling approach.

And finally development of the algorithm issues in the large scale and couple simulation in length scale and time scale and to do that development of the algorithm is really challenging task in multi-scale modeling approach.

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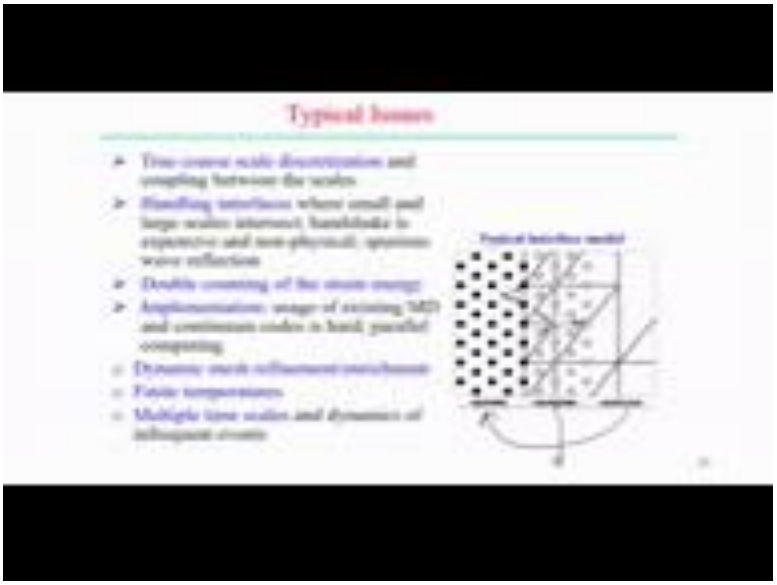

So look into all this problem now typical issues very specific to a problem say the true course scale discretization and coupling between the scales. So if we see the figure, here we are trying to link between the atomistic scale the representation in the lattice point and probably we assuming the each and every lattice point one atom but it is not liked in the continuum model, but how to represents the interface between these two atomistic model to link in the continuum model that is why the discretization in the continuum scale and discretization of the atomistic scale are actually different and because the scales are different so how the link between these two scales that is the one significant issue.

Second point is the how to handle the interface, the small and the large scale intersect therefore is (())(49:44) is expensive and nonphysical spurious way reflection happen also. So probably the technique (())(49:51) is required but how to make the process successful to link the this two different scale at the interface. Sometimes double counting of the strain energy that is the one issue, the implementation, using of the molecular dynamics and continuum score is hard probably we need the huge computational resource, parallel computational method maybe required in this case and other things are that when you try to interface at the link the two scale of the interface probably the dynamic mesh refinement enrichment is more, computationally more expensive and multiple time scale and dynamics of the infrequent event to link of this thing is really difficult and that are the typical issues associated with the multi-scale modeling approach.

So in a nutshell or in general we can say that the difficulties or simply we can say the difficulties of the continuum scale and the atomistic scale the represent discretization of the domain or in this true scales are different and second point is that how hand shaking that means how we can link the two interface that is the second difficulties in the multi-scale modeling approach.

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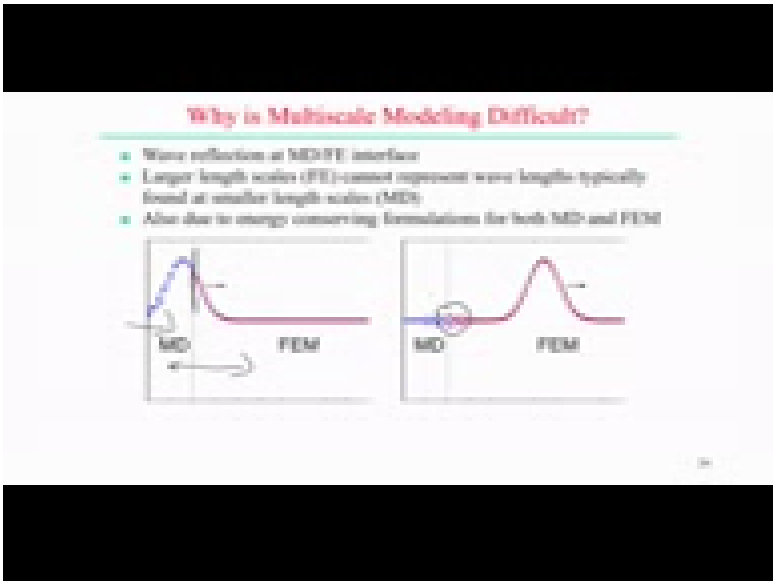

Now why the multi-scale modeling is difficult, let us look into details that probably the f reflection happens from the molecular dynamic simulation and of course this is the molecular dynamic reflection from the molecular dynamic simulation and when you try to link the molecular dynamics and the finite element methods simulation, so at the interface how to represent the dynamic reflection from the molecular dynamics. Next the large length scale cannot represents the wave length scale typically found at the small length scale so that is the another issue or difficulties because large length scale normally we use in the finite (())(52:03) methods, it is not suitable to represent, to capture the wave reflection specifically in the lower scale for example in this case the scale of the molecular dynamics. Also due to energy conserving formula for both molecular dynamics and finite element method is really difficult at the interface conserve the energy when you try to link this two scales between the molecular 1dynamics and finite elements. So this are the typical issues.

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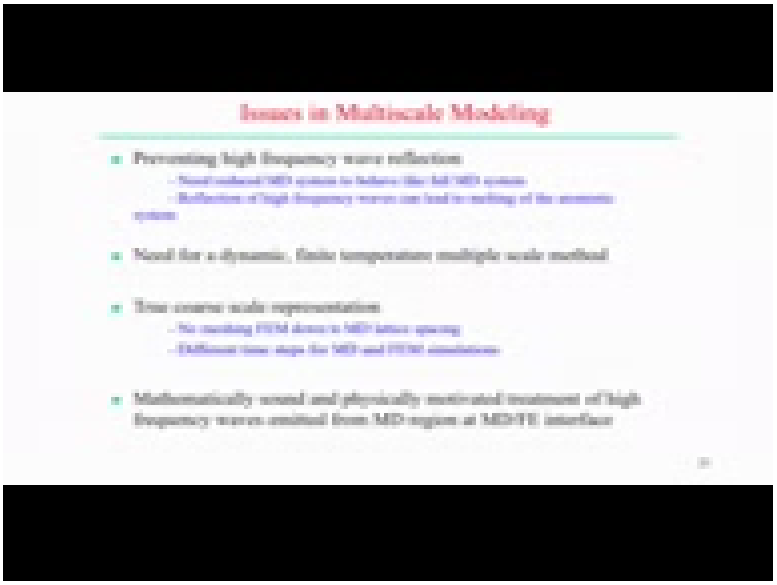

Now other issues probably in general we can say preventing high frequency web reflection need to reduce the molecular dynamic system can be done, to we have like a full molecular dynamic system. Reflection of the high frequency (())(52:57) can lead to the melting of the atomistic system, so that should be very careful to link how we can reduce the molecular dynamic system to link the uhh to be up like in the full molecular dynamic system. At the same time need for a dynamic finite temperature multiple scale method that is definitely needed. True coarse scale representation no messing FEM down to the uhh molecular dynamics lattice spacing.

So it is practically important, it is practically significant that it is not possible to create the mesh in the finite element that actually satisfied to the requirement for the molecular dynamics lattice spacing, so that kind of messing is difficult to do using the finite element. The same time different time steps for the molecular dynamics and the FEM simulation. So time scale for the FEM simulation on the different scales, mesoscale, or the continuum scale of microscale and the molecular dynamic scale are completely different so to match between this two also difficult or linking between this two really difficult in case of multi-scale modeling approach. Mathematically sound and physically motivated treatment of high frequency where (())(54:19) from the molecular dynamic region at the md or fe interface is really need to know.

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So looking into all these challenges in multi-scale modeling, probably now we will look into that macroscale approach to material modeling. Here if we see that material modeling so first thing is that macroscale is the fully homogenize description effect of the both grain and sub-grain, heterogeneity on the material response R are implicitly model by internal state variables. So (())(55:03) sub-grain heterogeneity on the material response are normally model considering the internal state variables. Second point is that by discretizing the explicit representation of the microstructure the approach loses the capability to model the state of the material in terms of the direct mapping between the microstructure and the properties. So probably when we try to idealize the polycrystalline behavior using or heterogeneity behavior in a single crystal and that we try to represent in a single, uhh polycrystalline behavior as an aggregate in that case the individual heterogeneity behavior can be lost in this case and rather than we can use some aggregate behavior on this case.

Typically used to solve the large boundary value problem since the approach used to reduce number of the degrees of freedom to represent the material response at each continuum point, so this is the first idealization, polycrystal idealization, next we represents the finite element method, finite element in the continuum scale. Probably in this case we need a low degree of freedom and we represent the material response at the reach continuum point but mechanical characterization test, mechanical parameter determination that actually play important role and that we can conduct the experiment and we can represent that behavior mechanical test and quick use the test data of the properties and we do the simulation.

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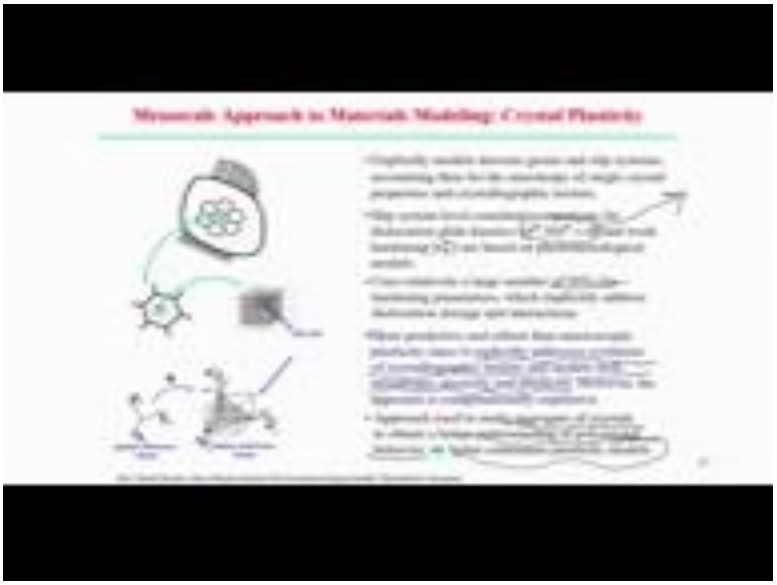

So similarly mesoscale approach to the material modeling related to the crystal plasticity, here if we see that explicitly modeled the discrete grain and the slip system accounting them for the anisotropy for single crystal properties and the crystallographic texture. So slip system level actually constitute the equation of dislocation kinetics, so if we see the slip system we use generally the slip system equation as a rate dependent and the work hardening also based on the phenomenological model we use in the, we can predict the slip system of the polycrystalline structure.

So relatively a large number internal state variables for hardening parameter generally used which implicitly address the dislocation storage and interacted between the dislocation. It is of course more predictive robust that the miscroscopic plasticity since it explicitly address the evolution of the crystallographic texture and models for both anisotropy elasticity and plasticity, however the approach is computationally expensive, of course it is a mesoscale is the more predictive approach to consider the crystallographic texture and models for crystal anisotropy uhh plasticity model, but in this case the approach of course the computationally expensive.

So point is that when you try to reduce the scale of the analysis so it becomes more computationally expensive to capture the behavior of the different length scale or different time scale. Approach used to study the aggregate the crystal to obtain better understanding of polycrystal behavior. So better continuum plasticity models probably need it and that we can enrich the better continuum plasticity model probably by linking into the mesoscale approach

where we explicitly consider the different textural behavior, texture direction and the plasticity law, anisotropy plasticity in the polycrystalline structure so that is more predictive to enrich the models for the continuum plasticity model, so it is also necessary to link the lower scale behavior to become the more predictive behavior for the higher scale.

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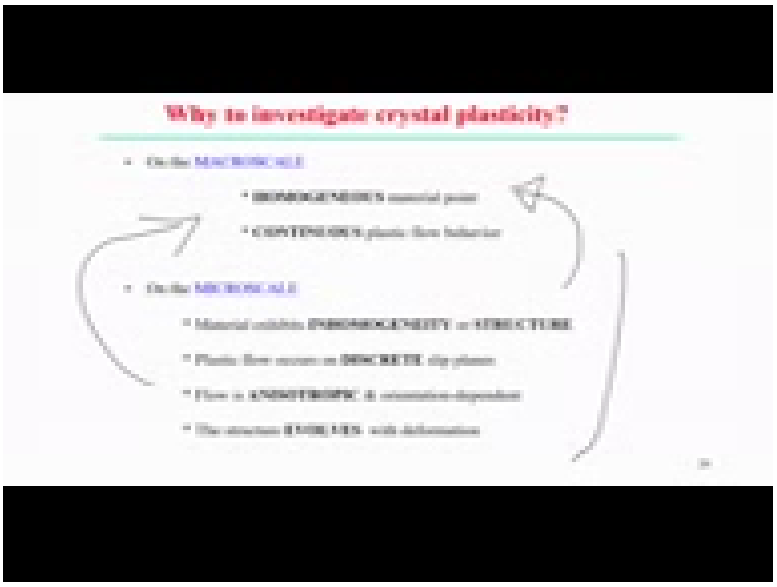

Now way to investigate the crystal plasticity in this case? Probably we see on the microscale, homogenous material point most of them we consider and continuous plastic flow behavior is considered, but if we zoom the scale or if we lower the scale, in the microscale if we look the behavior are different, in this case the material exhibits the inhomogeneity or structure difference is there, plastic flow occurs on the discrete slip planes, flow is anisotropy and orientation dependent of course the structure evolves with the deformation. So all this behavior in the microscale probably we can represents all this behavior in the miscroscale which is inhomogeneity anisotropy, probably we can represent on the miscroscale model which consider the, most of the cases we consider the homogenous material point or view and of course it consider the continuous plastic behavior.

Because we have learnt that if we consider the crystal plasticity and we observe that the plastic deformation of the single crystal may happen of the different orientation, different direction on the specific slip system so it is generally we consider that is the discrete system, discrete deformation system but which is not the case of the microscale application so that is the one way to link the macroscale to the microscale approach in the crystal plasticity model by simply averaging the behavior or we considering the behavior in the different way, for

example is like it is homogenous or heterogeneous or whether it is continuous or discontinuous, so that type of behavior we need to consider when we try to do the modeling approach relative the higher scale specifically in this case the microscale approach.

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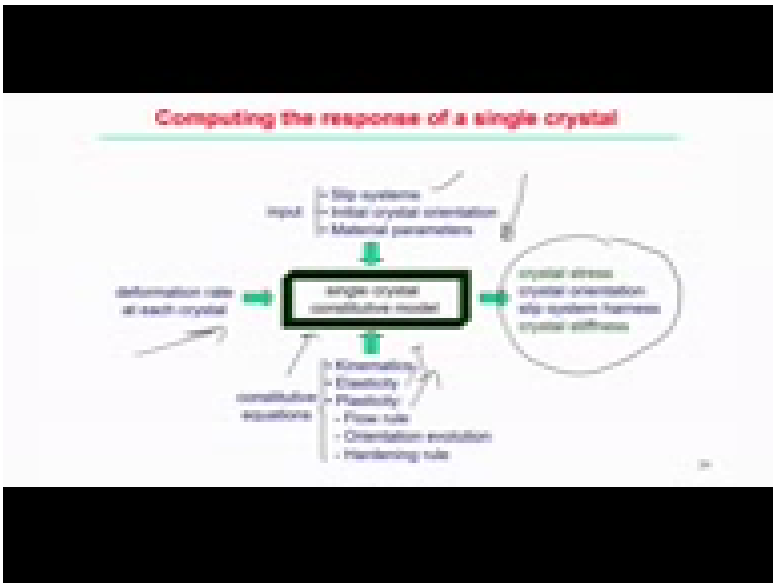

Now what are the several important, how computationally expensive in the single crystal behavior when you try to compute the response of the different stress strain behavior of the single crystal structure, so what are the input in the system, firstly the slip system need to know the slip system what was the initial crystal orientation and the other material parameter need to define this typical input to the system, to make the constitutive model for the single crystal structure. Other is the deformation rate at each crystal that information also needed and what are the kinetics of the deformation behavior. Plasticity and plasticity means plasticity of the single crystal structure in terms of the flow rule, hardening rule, orientation evolution, change of orientation evolution, all the constitutive information actually link and finally we can predict the crystal stress and final prediction of the crystal orientation, slip system hardness and crystal stiffness.

So computationally getting all this information to construct a single crystal constitutive model in terms of the crystal state and crystal orientation and slip system hardness in terms of the crystal stiffness is really expensive, but it is necessary to model for the deformation behavior of the single crystal structure.

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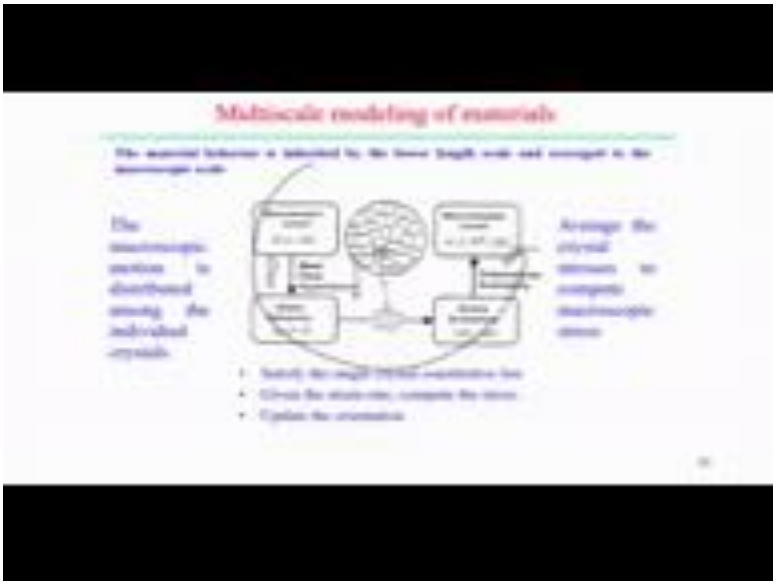

Now sometime or most of the cases the metal behavior inherited by lower strength scale that is the actually behavior of the, if we scale down we can look into the actually behavior, actually physical phenomena associated with the material and if we go up scaling, higher scale probably we are trying to averaging and specific to the macroscopic scale. So in the macroscopic motion is distributed among the individual crystals, so in this case we see the always we try to follow the main field of hypothesis in the macroscopic level and what is the great behavior, different state variable so we need to explain the grain behavior and we averaging this thing and probably produce the (())(64:14) field hypothesis and in this case the finally the orientation averaging and we can predict the macroscopic level at the different state variable. So average the crystal stress to compute the microscopic stress we use this completely system. But we satisfy the single crystal constitute law, given the strain rate actually compute the stress and finally update the orientation, so this is the one scale of approach.

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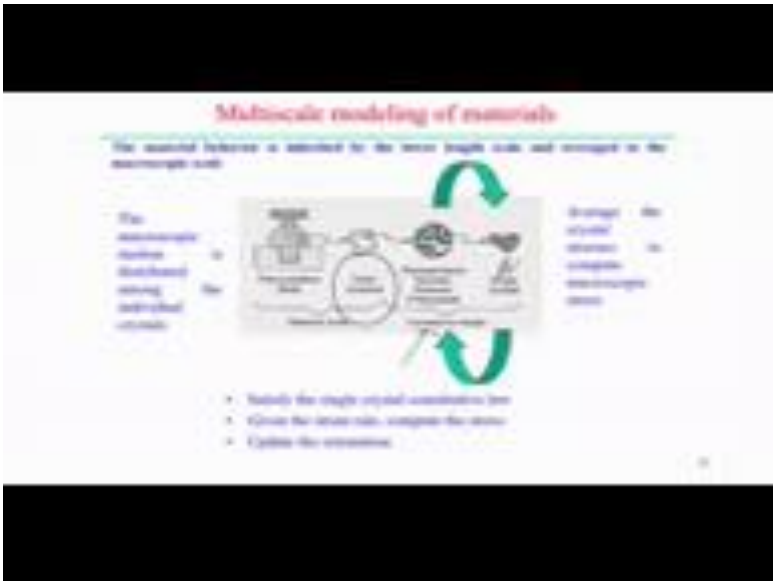

Next scale of approach we see that we generally use the constitutive model in the lower scale single crystal structure and then polycrystalline behavior was (())(64:59) or we focus on the representative material element, that behavior is the representative element actually Bf a whole of this specific material and finally uhh for all this two cases we generally follow the constitutive model but finally we try to use, we try to (())(65:20) larger scale polycrystalline body as a sample material in continuum scale, we consider the finite element simulation and that actually needs the that we use actually (())(65:36) law to predict behavior of the system, but all these cases the different length scale probably we can link into the different length scale and time scale using some multi-scale modeling approach.

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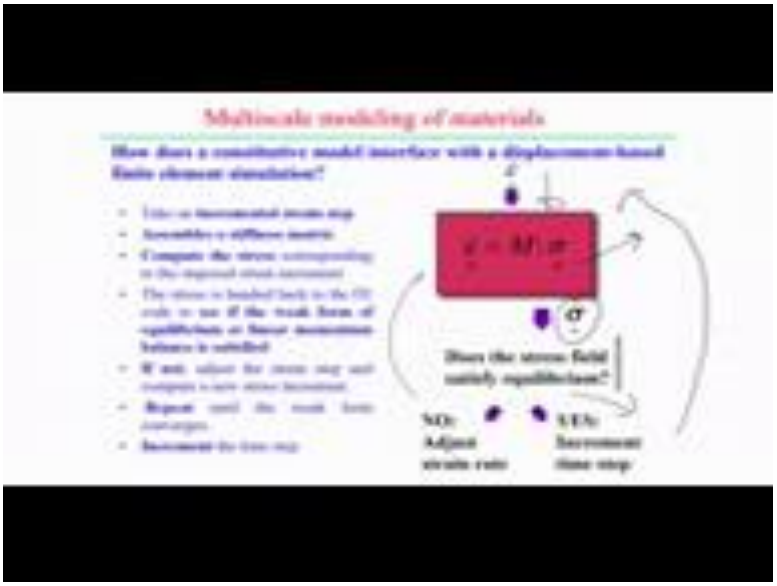

Now question is the constitute model interface with a displacement bases finite level simulation, if we see that if we consider that first we take an increment of the strain step, assemble the stiffness matrix, then we compute the stress corresponding to the (())(66:12) strain increment and stress is handed back to the finite element core to see if there is a quick form of the equilibrium or linear moment equation is satisfied or not. If it is not satisfied then adjust the strain step and compute the new stress increment and repeat until the weak converges, so then once get the converge solution and shift to the increment next time step and shift to the next step.

So incremental strain step, estimate the stress value, output from the system, whether it is satisfying the equilibrium equation or not, if it is yes then we can increment the time step probably next level, if it is no then again we need to adjust the strain rate. So this is the typical approach of constitute model interface with the displacement based finite element simulation.

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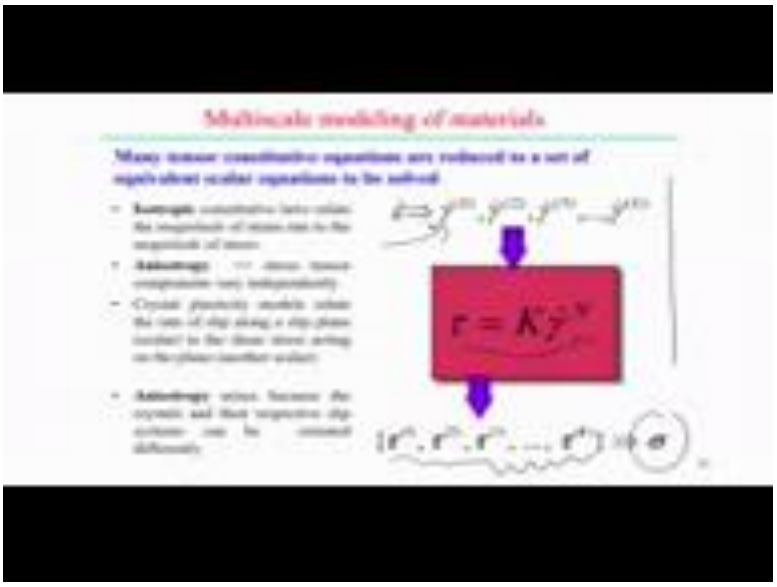

Now the simulation many tension constitutive equation are reduced to a set of equivalent scalar equation to be solved, for example when we try to analyze the continuum plasticity model we assumed that there is a effective stress or equivalent stress value and sometimes we call the Von Mises equivalent stress value and that equivalent stress actually the equivalent form of the representation of the stress strain. So if there is 9 component of the or 6 component of the stress is there that 6 component we can represents one single value that is called the effective stress or the equivalent form of the stress, so that is used to predict the

law in case of plasticity mode. So similar kind of things we can use it or that means some tension we can convert in terms of the scalar quantity and we can use to conduct the or to modify the different law or is use in the constitutive equation.

So isotropic constitutive laws relate the magnitude of the strain rate to the magnitude of the stress, so relate the magnitude of the stress to the magnitude of the stress but anisotropy stress strain are component are actually vary independently so crystal plasticity models actually relate the rate of the slip along a slip plane that slip plane we can consider as a scalar quantity to the shear stress acting on the plane, that can also be another scalar quantity, so that shear stress is finally can be constituted with respect to the rate of the shear strain. So anisotropy arises because the crystal and their respective slip system can oriented differently because of that the anisotropy actually exist so that different stress values at the different crystal system can also be equivalent form or in terms of the scalar quantity can be represent as the link with the single stress state or scalar values of the component. So that is another approach that we generally follow in the crystal plasticity model.

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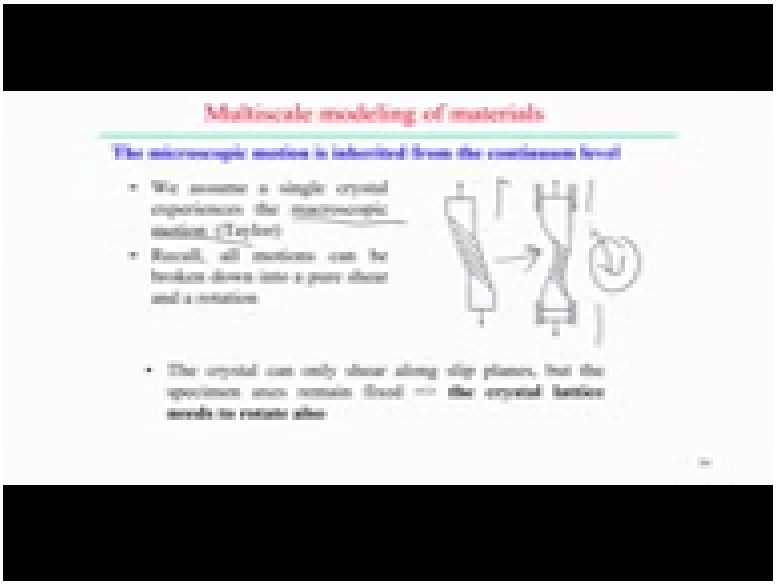

The microscopic motion if you see that inherited from the continuum level if we consider the microscopic motion actually inherited from the continuum model so how we can explain like that, the continuum model in the sense for example simple if we conduct the tension test of a specimen of a sample so we can execute the tensile stress and corresponding stress strain diagram but with the application of the external on the samples what maybe the changes happens in the microscopically, so if you see the microscopically and if we try to explain the

microscopically the single crystal behavior we see that single crystal experience the microscopic motion, how is it like that. Because recall all motions can be broken down into the pure shear and the rotation, we have explain that when it is subjected to, specimen is subjected to tensile loading the several slip system at a at a single time.

So there is a (())(70:43) constant or that is the restriction of this direction of this load and if we make some constant motion of this thing so from the theory of the uhh plastic deformation slip happens in case of single crystal structure you see that it is uhh if we put the constant then there is maybe some slip will happen along with rotation, so the crystal can only shear and the slip plane but the specimen axis remains the fix so crystal lattice also needs to rotate itself so it is subjected to rotation itself, so we can make the conclusion that this microscopic rotation or microscopic motion is inherited from the continuum scale. So we need to consider that, that microscopic motion we actually need to consider when we try to make some constitutive model in the crystal plasticity.

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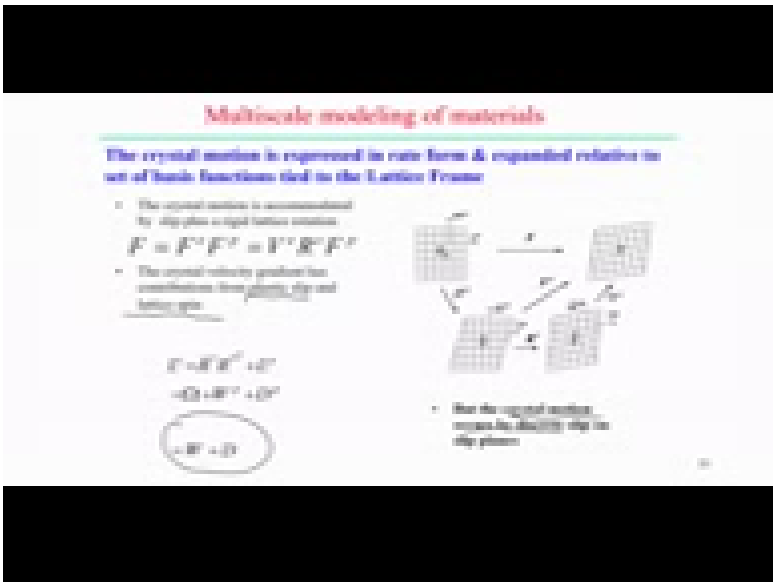

So crystal motion is expressed in the rate form and the (())(71:50) is related to the set of basis function, uhh tied in the lattice frame, so different frame, if you see the crystal motion is accommodated by the slip (())(71:59) a rigid lattice rotation so the crystal velocity gradient has contribution from the plastic slip so both plastic slip atomistic structure well as the lattice pin, so that two components we can consider in this case to explain the uhh motion of the uhh in term of the rate form why because this is the reason sometime we represent the hardening

law in the crystal plasticity in terms of the rate, so both crystal motions occurs and discrete slip plane.

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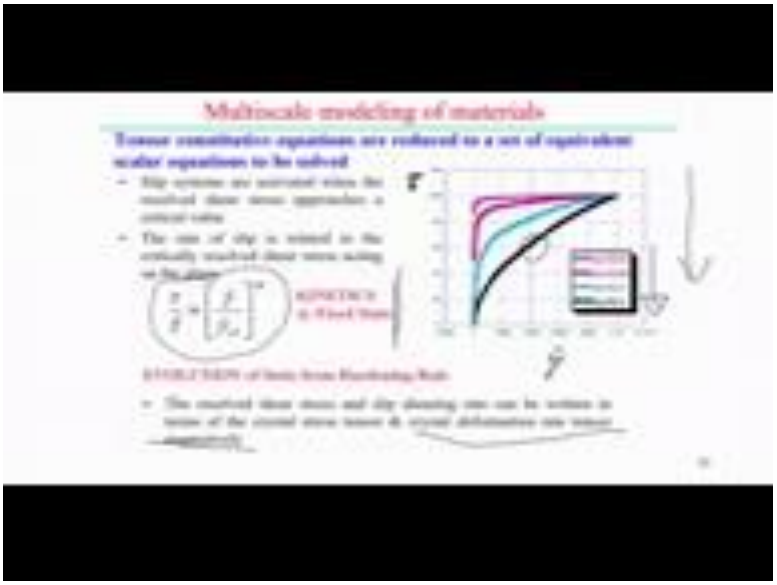

Now tension constitutive equation are reduced to a set of equivalent scalar quantities so we have already explained that, sometimes we represent the stress tension in the form the equivalent form of the equation that is the single scalar quantity so that can be said that slip system are activated when the resolve shear stress approaches the critical value but the rate of the slip is related to the critically resolve shear stress acting on the planes that is the relation between the shear stress and the rate of the shear stress and accordingly we can consider the kinetics and the fix state, so if we see the figure right hand side, different values of the m, the relation between the stress and the strain rate, if you see the constitute relation can vary depending upon the different values of the m.

So with this behavior probably it is possible to evoluation of the state from the hardening rule, the resolved shear stress and the slip shearing rate can be written in terms of the crystal stress tension and the crystal deformation rate tension respectively. So I am not too much tension, mathematical derivation or related to all this phenomena. But ultimately we can form the constitute relation in terms of the shear stress and the rate of the shear strain and accordingly we can evaluate the hardening rule even in the crystal plasticity model.

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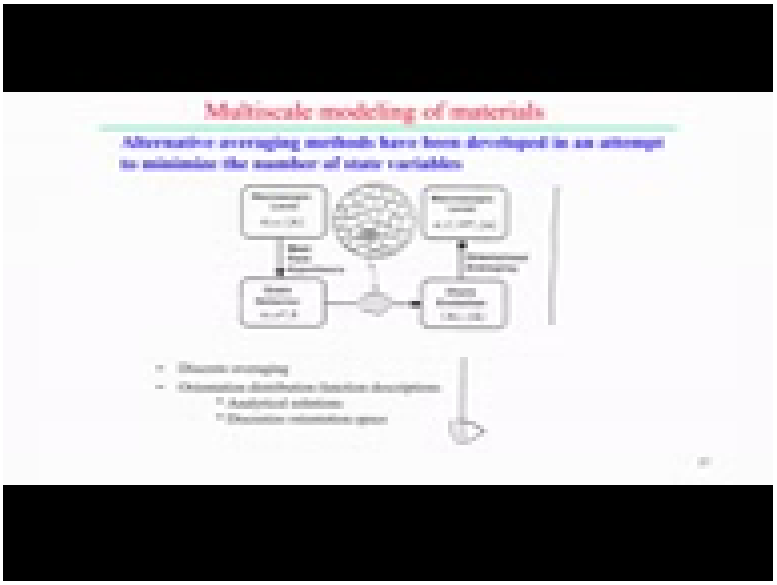

Similarly alternative averaging method (())(74:17) develop in an atom to minimize the number of strain variable, that is also important issue in the microscopic model, that if it is possible to reduce the internal stress variable so that can be done from the discrete averaging of the certain of the properties, so uhh that analytical solution of discretization space these are the uhh that we can derive the function, orientation distribution functions that actually try to description based on the analytical solution or (())(74:52) it is possible to reduce the number of strain variable in the microscopic model.

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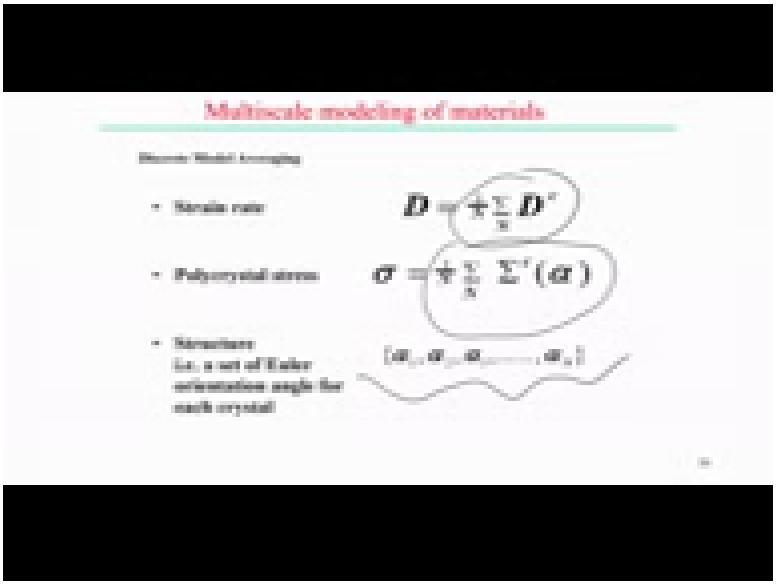

So this is the discrete model averaging strain rate, simply averaging of this thing, polycrystal stress, you can make through averaging and structure in the set of (())(75:10) orientation angles of the each crystal. So that are the typical discrete averaging discrete model averaging the all the state properties.

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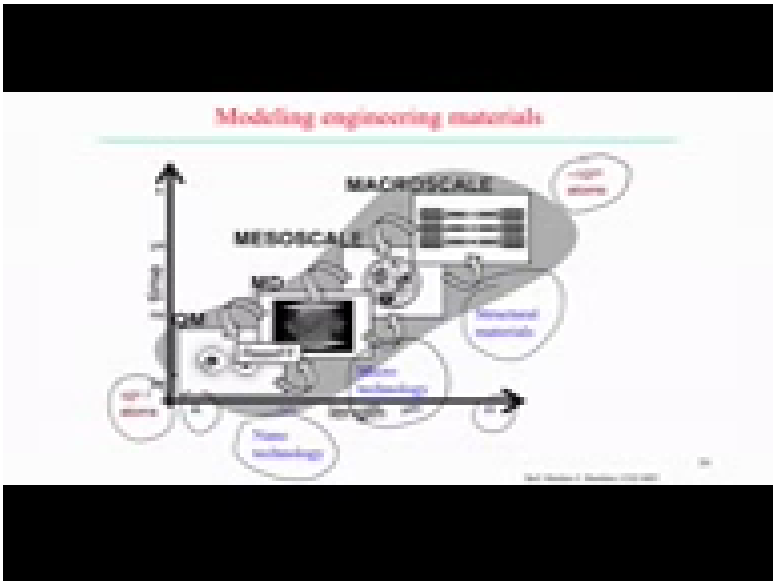

Now we come to the second part of this thing that modeling of the engineering material, what are the different approaches for that, so if we see that modeling engineering materials so there are different scale, we have explained the several times that there is a different length scale and time scale, the quantum mechanics and molecular dynamics, mesoscale and microscale probably these are the 4 or 5 scales can be used to explain the multi-scale modeling approach. Now here if you see the representation of this scale is the, 10 to the power 23 atoms, but probably in this case 10 to the power 0 to 2 atoms in the continuum mechanics that is the representative volume in terms of atoms and if you see the scale is a very 10 to the power minus 13 and here it is the micrometer or meter scale or millimeter scale. Now over the continuum mechanics, molecular dynamics based on the mechanics, physics on that the nano technology can be explained. Then based on the mesoscale application the micro-technology come out and finally microscale approach the structural mechanics or continuum mechanics approach can be explained over the different scales, so scales multi-scale analysis so accordingly there are different levels of the technology has been developed.

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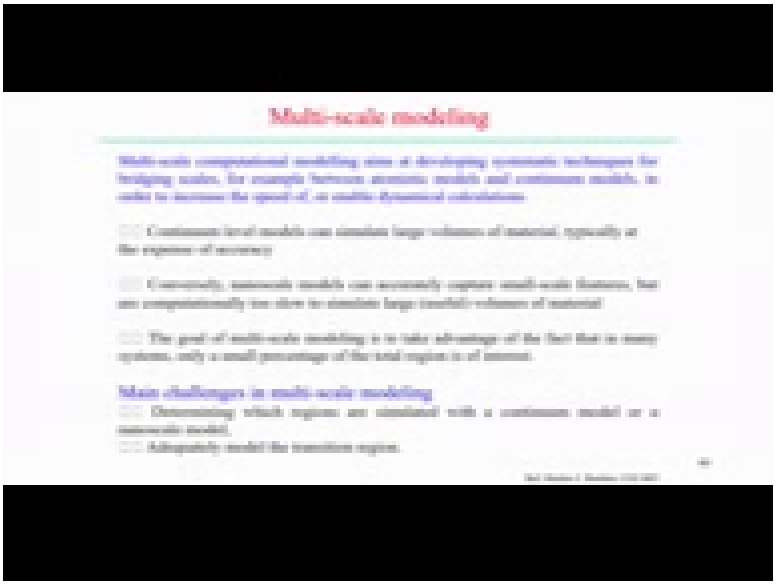

Now the multi-scale modeling approach, the computational modeling generally aims to developing the systematic techniques for bridging the scales, for example between the atomistic model and continuum models in order to increase the speed or enable dynamical calculation that is the basic objective of the multi-scale computational models. Continuum level models of course can simulate large volumes of the materials which is not possible for the molecular dynamics so typically at the expense of the accuracy. Of course when we consider the continuum level of the model the large volume of the material try to focus on the analysis is not possible to capture exactly, the phenomena in the lower scale quantum mechanics of the molecular dynamics. So that is why continuum level models we always do the large volume of the materials and analysis but at the expense of the accuracy.

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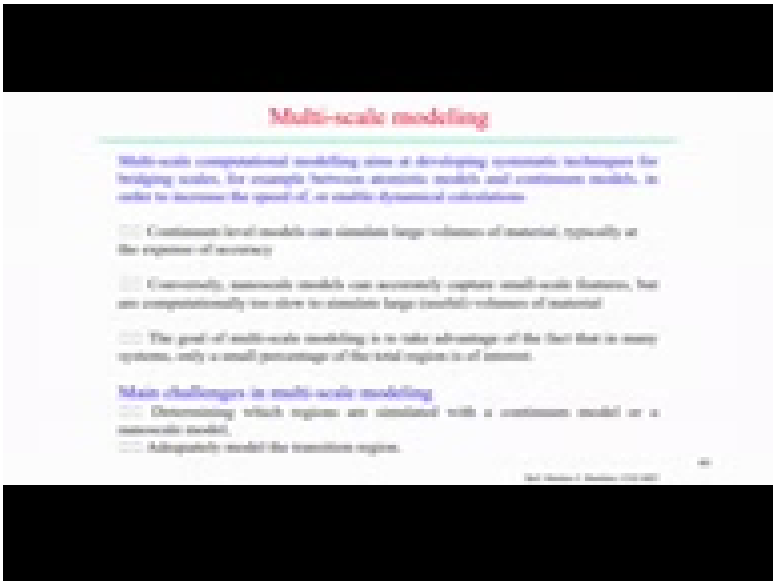

Conversely the nanoscale models can accurately capture the small scale phenomena, small scale features but actually computationally too slow to simulate as compared to the large volumes of the materials. So computationally expensive large volume of the materials is really the main obstacle that when you try to focus, capture the nanoscale phenomena, therefore the goal of the multiscale is to the take the advantage of the fact that in many system only a small percentage of the total region is of interest, so strategically very small component or small part of interest truly we can look link the different scale to capture the features or at the different scale and that is the basic philosophy of the multi-scale modeling approach.

But main challenges multi-scale modeling approach the determining when the regions aren't simulated with the continuum model or the nanoscale model but adequately model the transition region that is the two obstacles related to the multi-scale modeling approach.

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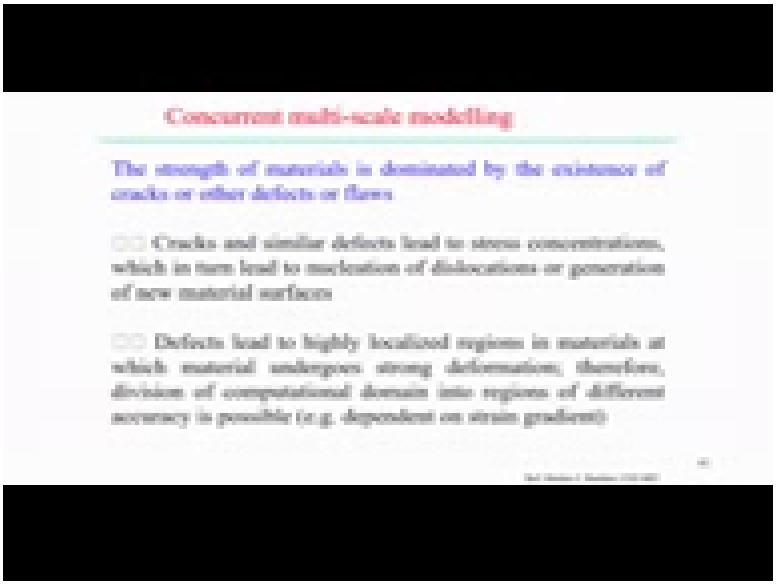

One approach is that explain that concurrent multi-scale modeling approach and hierarchical approach so here we try to look into the concurrent multi-scale modeling approach. One thing is the the strength of the material is actually dominated by the existence of the (())(79:43) or other defect or flows. So probably that concurrent multi-scale modeling approach will try to explain considering the strength of the material or formation of the (())(79:57) during the deformation of the metals. Cracks and similar defects actually lead to the stress concentration which in turn lead to the nucleation of the dislocation or generation of the material surface. So generation of the cracks can be explained like that, there is a nucleation happens so it starts from the nucleation and finally the development of that small crack that after that there is a fracture happens, the samples of the material of interest.

Now defect actually leads to the highly localized region in materials and which (())(80:39) undergoes a strong deformation therefore division of the computation (())(80:44) into different regions of the different accuracy is possible depending upon the strain gradient. So probably we can link the atomistic behavior in the scale of the continuum when you try to fracture, analyze the fracture mechanics and to get that actual information what is the cause of the fracture in the scale of the molecular dynamics or in the scale of the next level of scales.

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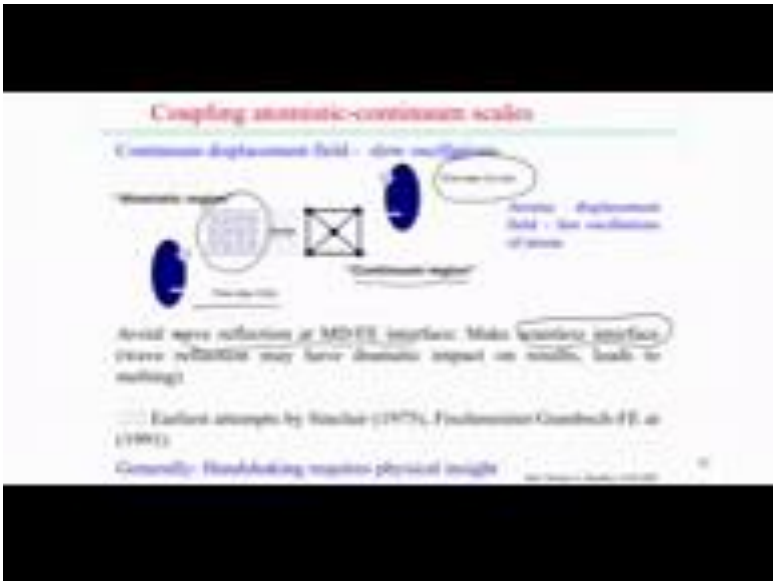

But how we can do that continuum displacement field we see the atomistic region time steps here, this is atomistic region time step here is along the order of femtosecond but in other case continuum region the time step is the order of the greater than milisecond. But atomic displacement field probably related to the first oscillation of the atoms, now how we can link these two scales through the multi-scale modeling approach. Normally we avoid the wave reflection at the interface between the molecular dynamics level and the finite element interface. It is possible to make the seamless interface uhh that because that wave reflection maybe have dramatic impact on the results sometimes leads to the melting. So make seamless probably the one challenge for the multi-scale modeling approach. Several attempts earlier but normally we can follow the hand shaking between these two uhh link, between these two scales of the analysis but for the hand shaking we need the physical insight of the mechanism, of the process.

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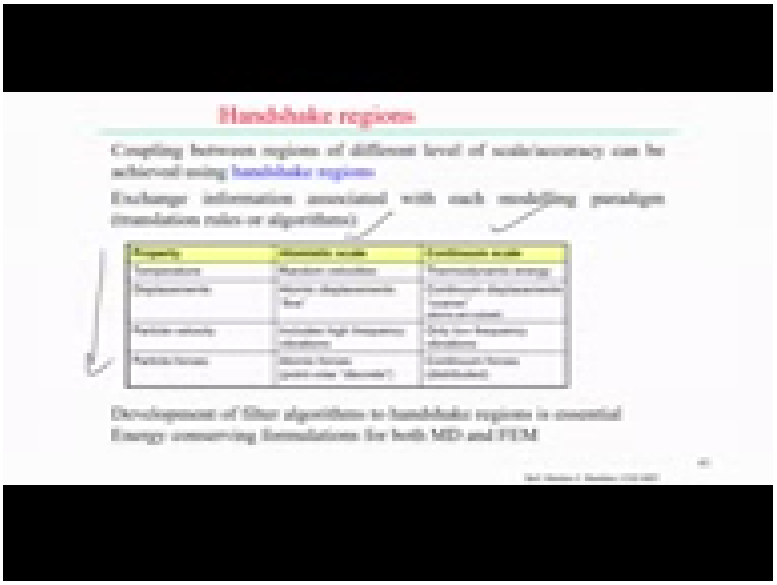

Now handshake region, we can coupling the regions of the different level scale or accuracy can be achieved using the handshake region so or that method, but in this case the exchange information associated with the each modeling is required so here the translation rule or which algorithm is needed, specific algorithm is needed to exchange the information at the handshake region. So what are the typical, if you see the different property and the different scale atomistic scale and continuum scale we see the temperature, atomistic scale the property temperature represented by random velocities but in continuum scale probably more associated with the thermodynamic energy. So the scale of analysis and the two different scale, the property is represented or associated with the different levels.

Displacement the atomistic displacement is the fine displacement in atomistic scale but in continuum scale the continuum displacement probably it is not very find coarse, so in this case we can consider atoms as not the main elements but atoms can be considered as the subset in the continuum scale. Particle velocity in atomistic scale includes the high frequency vibration but continuum scale only low frequency vibration relevant. Particle forces probably in atomistic scale represented by the atomic forces point wise an atomic forces but point wise it is discrete, but in continuum scale the particle forces can be represented in terms of the continuum forces but that is the distributed.

So there is a huge difference to represent of the difference property at the different scales therefore it is necessary to develop the filter algorithm in the handshake region is essential and also the energy conserving formulas so energy conserving formulas at the handshake

regions for both molecular dynamics and finite element methods when you try to link between these two scales.

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Now the two scales of analysis continuum atomistic scale of course difficult but since atomistic contain information that continuum does not provide or only indirectly I think in terms of temperature, so atomistic region that is the one point and therefore averaging stress displacement and the statistical mechanics, once real dynamical trajectory is know then we can using the filter we can get the useful information, but still boundary effect is very critical through link in between two scales.

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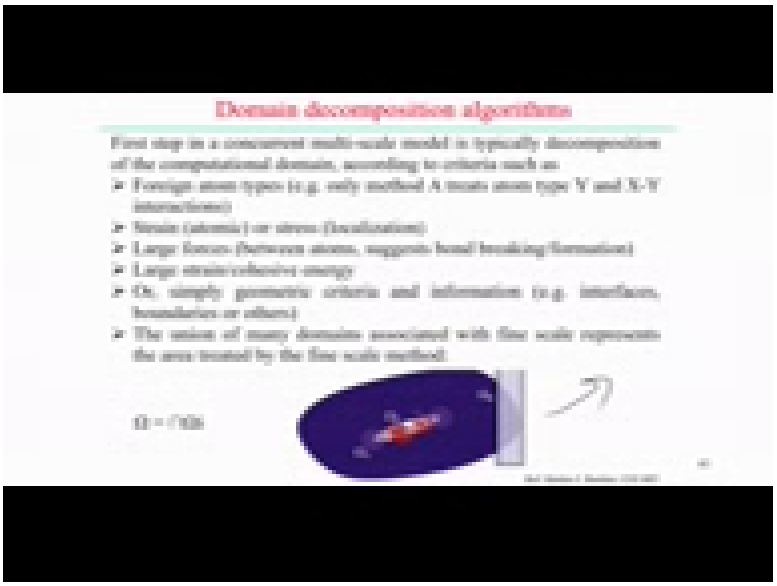

Domain decomposition is one of the probably algorithm in multi-scale approach is the domain decomposition algorithm, so it says as simply as that the first step of the concurrent multi-scale model is typically decomposition of the computational domain according to the several criteria we can follow, so how we can decompose the different domains, so there are several criteria, first criteria is the for a atoms types, probably the only method (())(86:04) atom type y and xy interaction. Second is the atomic strain or the stress localization based on the we can divide the different domain large forces between the atoms suggests bond breaking or formation, bond formation so that can be based on that criteria, we can divide the different domain large strain or (())(86:29) energy based on that or simply geometric criteria or an information that means interfaces, boundaries or others.

That criteria that is impossible to decompose the different domains so finally the union of the many domains associated with the fine scale particles represents the area treated by the fine scale methods. If we look into that figure that different zone of interest, having the different uhh different following the different criteria so it is possible to discretize the domain of small small domains and that actually union of the whole domain, and accordingly we can analyze, we can predict the behavior or individual uhh for individual domain probably we can use the different theory in that scale level and finally we can link it. So this is the one way, simple way that the domain decomposition algorithm.

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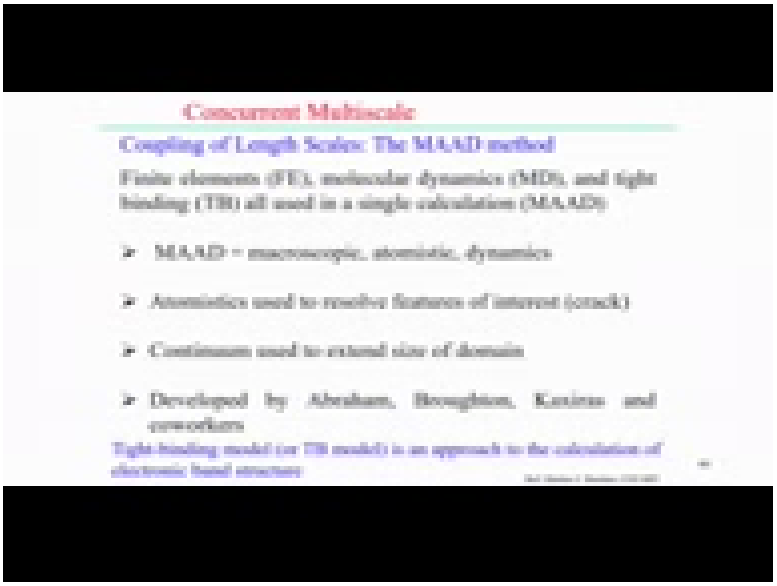

Another is the concurrent multi-scale method, the coupling of the length scale, so that is typically called the MAAD method, so it is the typical links between the finite elements

molecular dynamic and the type binding all used in the single calculation. So that MAAD methods actually is called microscopic atomistic behavior and the dynamic behavior is captures in a single calculation. So type bonding means here type bonding model generally is an approach to the calculation of the electronics band structure that is uses. So in MAAD model or maybe MAAD method probably we can use all these three different scale information, microscopic atomistic and dynamics.

Atomistic used to resolve features of the interest for example crack and the continuum used to extend the size of the domain, so taking the advantage of this continuum and atomistic and individual area of interest, merging in these thing that is the MAAD algorithm or MAAD method has been developed.

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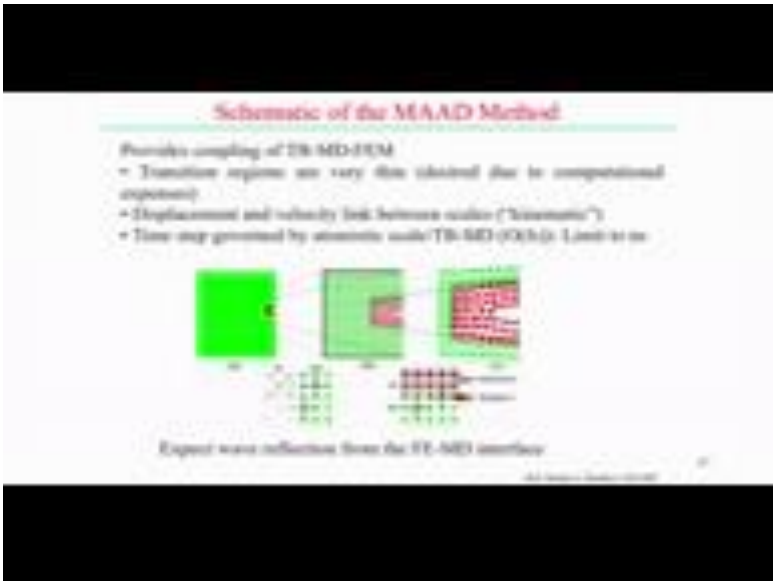

So this is the schematic diagram for the MAAD method if you see the simply coupling, how it is coupling the tight binding molecular dynamics and the finite element method. If you see that thing the transition regions are very think desired of course due to the computational expenses. So displacement and velocity link uhh between the scales based on the kinematic and the time steps governed by the atomistic scale or tight binding or molecular dynamics and time scale generally follow in the order of femtoseconds, but it is limited to up to nanoseconds. Except wave reflection from the finite element and molecular dynamics interface probably this method (())(89:52).

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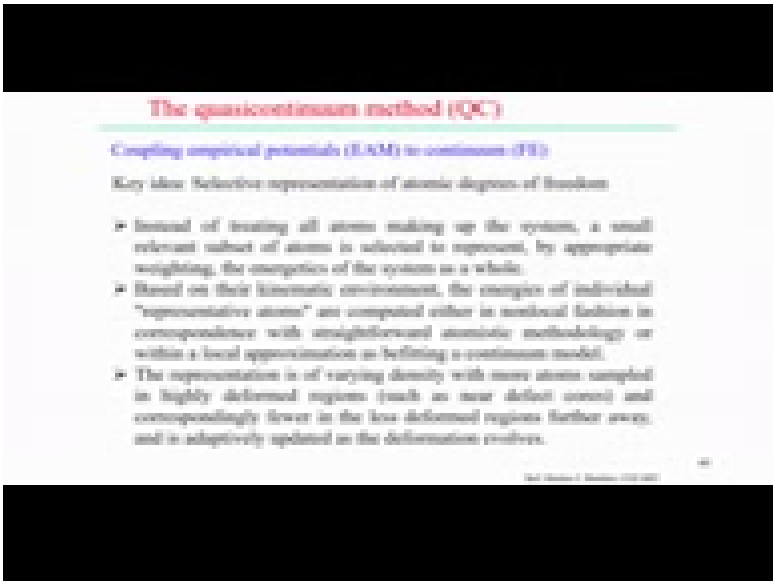

Now if we look into another basic method that is Quasi continuum method. That is also coupling the empirical potential to the continuum models, so key idea is the selective representation of atomic degrees of freedom, not necessary to consider all degrees of freedom in the atomic scale probably if we more selective we can that selective scale probably representative on that molecular dynamic scale. Therefore instead of treating all atoms making up the system is small cross subset of the atoms which is selected to represent by appropriate waiting the energy of the system as a whole. So only system of the atoms represents the energy of the whole system. In this case if it is needed we can use the appropriate waiting of all the atoms.

Based on the kinematic environment the energy of the individual representative atoms are computed either in non local fashion in the corresponds to the state for atomistic methodology or within the local approximation as befitting in out continuum model. So assuming the local approximation of the befitting of the continuum model since few atoms represents the whole system. The representation is of varying density of more atoms in highly deform regions such as near defect. It says strategically if high deform or high deformation gradient to which that point probably we can increase representative atoms more to capture the phenomena more precisely and corresponding the pure or less deform regions further is adaptively updated to the deformation evolves in that way probably we can conduct this experiment.

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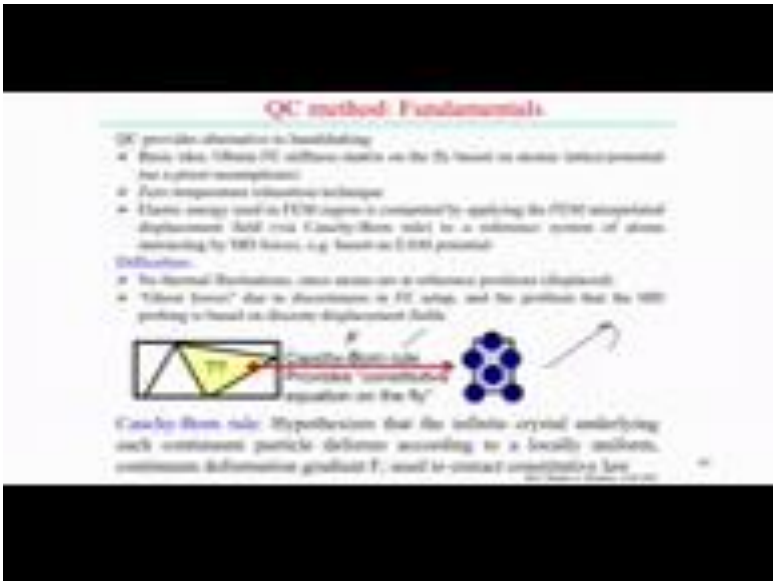

We can conduct probably that is the basic philosophy of this method. Now quasi continuum method actually provides the alternative to the hand shaking, you see the basic idea was like that obtain the finite element stiffness matrix on the (())(92:03) based on the atomic lattice or potential not required any uhh prior assumptions. Zero temperature relaxation technique this is elastic energy used in finite element region is computed by applying the finite element methods interpolated displacement field using the Cauchy Born for example to a reference system of atoms interacting by the molecular dynamics forces based on the finite EEAM potential.

But difficulty is that no thermal fluctuations since atoms are at reference position therefore sometimes go forces due to the discreteness of in FE system and the problem that the molecular dynamics is based on the discrete displacement field, so if we look into that one continuum model, we link the MD model probably based on the discrete displacement field and that using following the Cauchy Born rule and provide the constitute equation the fly. So Cauchy Born rule states that the infinite crystal under lying each continuum particle deforms according to a local uniform continuum deformation gradient m that is used to extract that constitute law.

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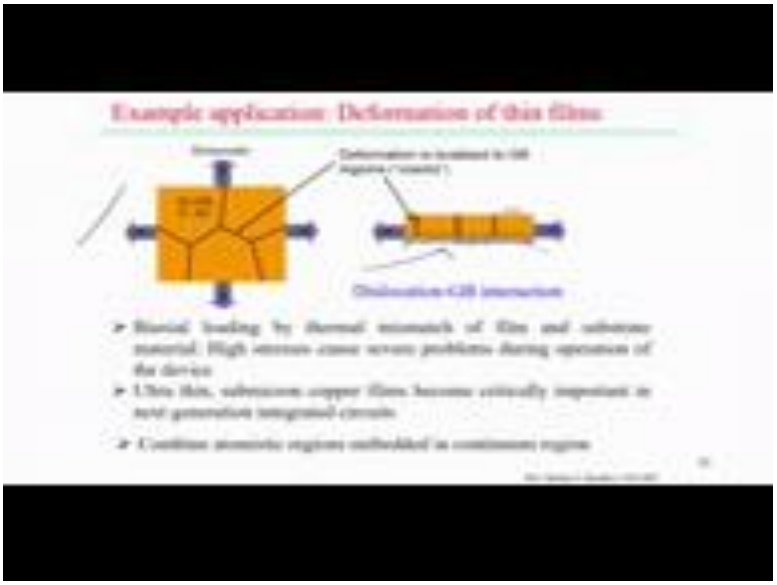

So another example application that is deformation of the thin films probably if you see that the biaxial loading by thermal mismatch of field and subsequent metal, so actually high stress cause the severe problem during the operation of the device. So schematically if you the see the biaxial stress subjected to a polycrystal structure, now deformation is localized actually the deformation is localized at the grain boundary and so in this case the dislocation and the grain boundary interaction is important to know and if you see that idealize system in the polycrystal form probably you can represent this thing, stress and if you see that near about the grain boundary there is a plaster of the dislocation and there is a probably there is a deformation is localized near about the grain boundary region.

So it is important practically because sub-micron copper film because critically important in the next generation integrated circuit. So in this case probably the combine atomistic regions embedded in the continuum region and by following the multi-scale modeling approach we can adjust this kind of problem.

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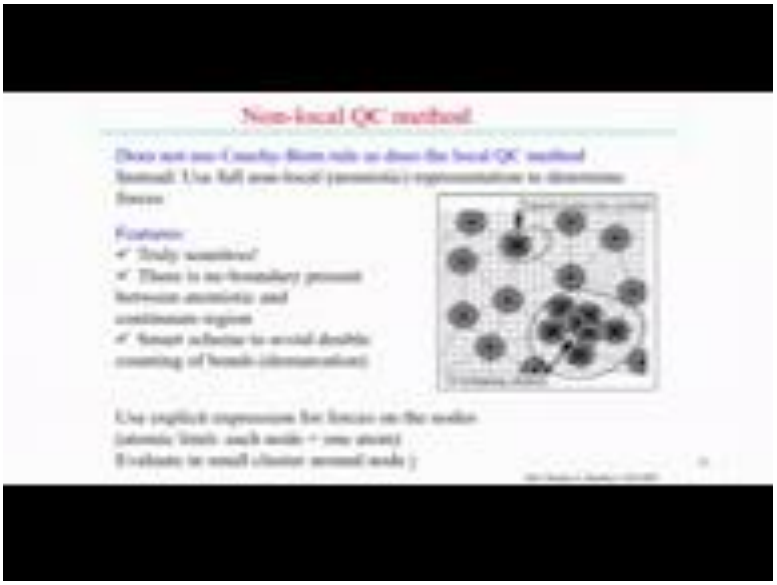

But non local qc method in this case if you see it does not use the Cauchy Born rule as thus the local qc method, but instead use full non local representation to determine the forces. So what are the features of this non local qc method, here if you see that it is truly seamless that there is no boundary present between the atomistic and the continuum region but it is a very smart thing to avoid double counting of the bonds. Use the explicit expression of the forces on the nodes atomic limit each node and one atom evaluate the small cluster around the node j. Here if you see that typical cluster there is no overlap, and it is a overlapping cluster so this is basically one kind nonlocal qc method and most important features is that no boundary present between the atomistic and continuum (())(95:54) so this approach can be used to solve the multi-scale modeling problem.

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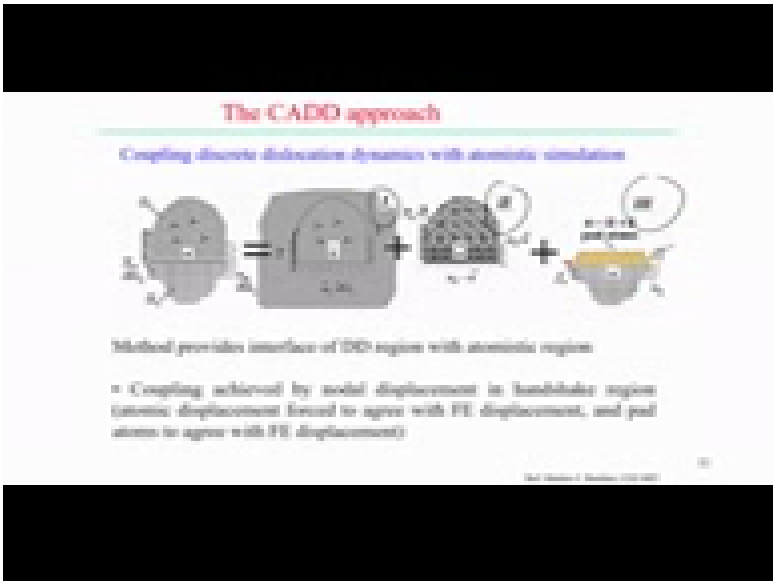

Now another approach is that Cadd approach, the coupling discrete dislocation dynamics with atomistic simulation, here the method provides the interface of the dislocation density agents to the atomistic region. If you see the zone 1, 2 and 3, we can represent the different way that coupling achieved by the nodal displacement in the handshake region, so in terms of the atomic displacement force to agree with the finite element displacement and Cadd atoms to agree with the finite element displacement, so Cadd atoms actually agree to the finite element displacement but coupling happens that in the (())(96:43) region so that the atomic displacement is basically agreed to the finite element displacement. So this is the Cadd approach and we use the coupling discrete dislocation dynamics with the atomistic simulation.

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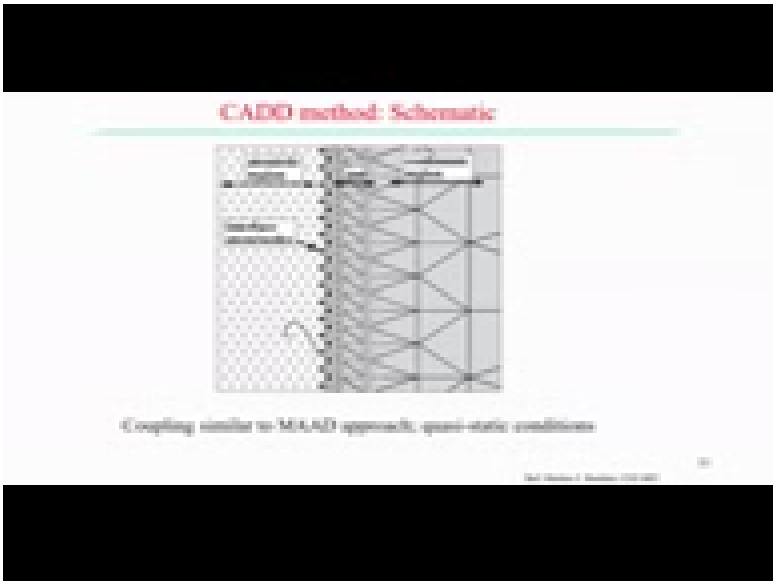

If you see Cadd method schematically that this is the interface atoms and right hand side is the continuum region here and there is a Paad atom, so coupling is similar to Maad approach but it is in the quasi static condition.

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Now another method is that the bridging scale method, we use the multi-scale modeling approach. That actually coupling the atomistic scale to the continuum scale at finite temperature so in this case the finite element representation exist everywhere in the domain even where md is also present, molecular dynamics also present. So use the projector operator to represents the displacement field as orthogonal combinations small scale and the

coarse scale, both we use it but what are the advantage in this reaching scale method, the atomistic at continuum scale do not have to be intricated using the same time step. As we generally is in done in the Maad scheme. But high frequency oscillation naturally disappear when leaving the atomistic core region and where the impedance force. Atomistic region sense finite temperature in the finite element region where the (())(98:24).

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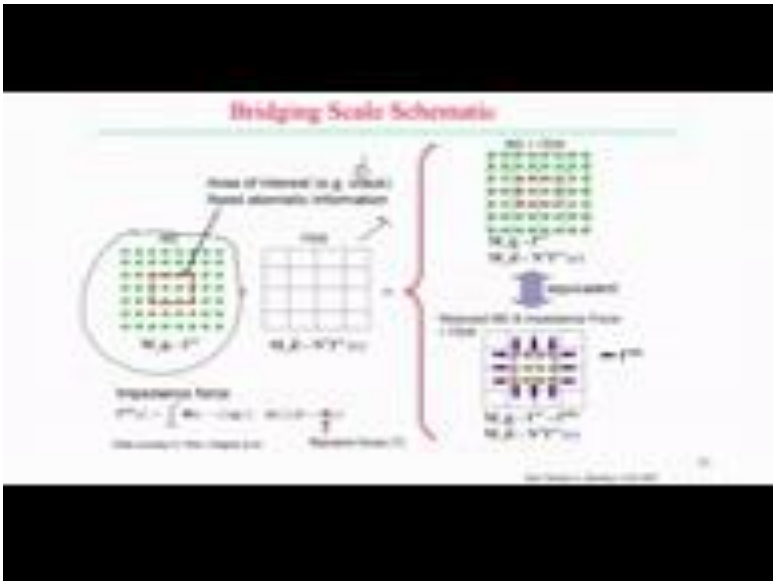

So this is the another typical bridge scale method we generally follow in the polycrystal modeling approach and if we see that area of interest for example if we consider the example of the crack and that molecular dynamics, if we consider the represents of this thing right hand side is the finite element zone in the continuum scale. So if we advertisement this to probably we can represent the md plus fem this zone and that is equivalent form and we represent the correctly that the force actually uhh f, reduce to the md, md and impedance force plus fem is represented correctly. So this is the other way to link bridging the different scale following some specific strategy. So these are the all methods, we try to explain the different methods just to overview on the different methods that actually generally use in the multi-scale modeling approach.

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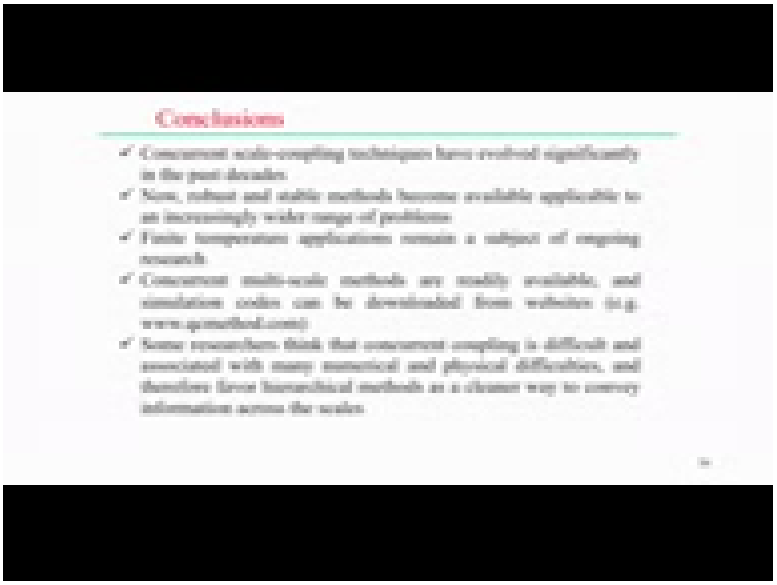

So to do that we can conclude this section like that normally conference scale coupling have evolved significantly in the last (())(99:51) decades and most of the methods developed on the concurrent scaling approach, but now robust and stable method become available applicable to an increasing wide range of the problem, so many (())(100:09) can be done, robust methods also be done. Now-a-days it is available, finite temperature applications of course remain a subject of ongoing research steel and concurrent multi-scale methods of course are readily available and probably simulation course can also been downloaded from the obstacle different methods, if you find interest to do that but some researched still think that concurrent coupling is really difficult and associated with many numerical and physical difficulties so they favor the hierarchical approach method as a cleaner way to convey the information according to the scales.

So thank you very much for your kind attention.