Mathematical Modeling of Manufacturing Processes

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Lecture - 03
Physics Based Modeling Approach at Different Scale – Continuum to Nano

So, in the first module, now we have the overall different types of the manufacturing process we have already discussed, their properties, what type of properties, all we have discussed. Now, we try to look into that the next component of this module is the physics based modelling approach at the different scale. Here, I will try to explain the different approaches and more focused on the physics based approaches.

And the construction of a particular model, what are the different components we need to understand before developing of a mathematical model.

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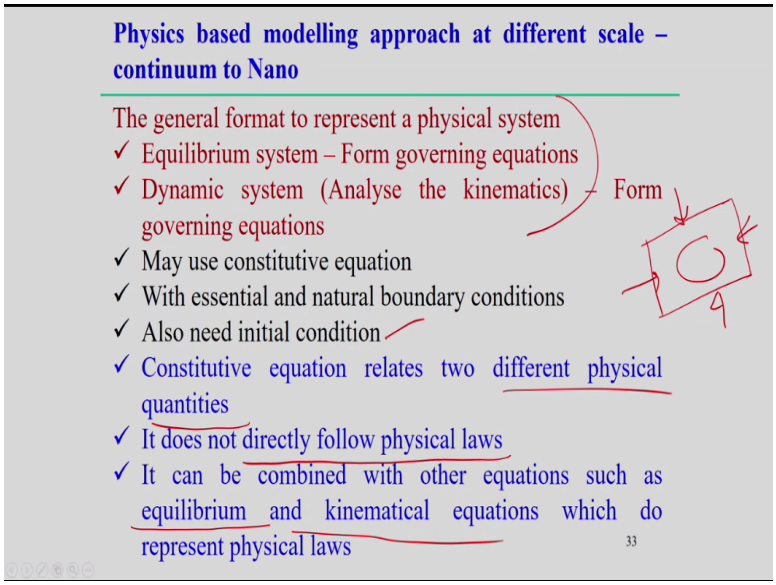

So, to start with that we can look into that what are the approaches, normally if we try to make some physics based modelling approach and of course this general purpose to develop a physical system but first thing is that what the physical system represents, we represent a domain, we first fix a domain of the analysis.

So, this is the solution domain and we try to look into once we fix the domain within this domain, what are the physical phenomena is happening with this domain and what we can represent all the physical phenomena within this domain and of course what we represent in

the mathematical sense. So, normally the representation or general format to the represent particular physical system, the first is the, the one way is the equilibrium system.

The system is in equilibrium conditions, we normally assume that equilibrium condition and once is the equilibrium conditions then we try to look into the what are the governing equations normally acting on this particular process. So, for example if it is a static system and we can say in the most of the cases we assume the heat conduction equation is prevail. So, 3-dimensional heat conduction equation is the standard equation.

And that we assume it is an under equilibrium condition, this equation is satisfied and once we know the heat conduction equation with this domain, we just solve this governing equation and we can get the solution in the form of the temperature. Of course, rather the heat conduction equation I can say that better to represent in terms of the energy equation. So, from the energy equation, we can solve the temperature distribution for example.

That if you look into the momentum equation that is valid within this solution domain and from the momentum equation if we solve in case of fluid flow analysis, we can get the velocity field as the output within this domain. Of course, this is the one system or the system maybe dynamic system also and of course this dynamic system must analyze what are the kinematical behaviour also within this dynamic system.

And this dynamic system can be represented in terms of governing equations, so once we represents a particular system in terms of the governing equations, then we try to find out the solution of this equation. So, once we get the solution of the equation, we can get the distribution of this variable. So, this governing equation can be solved numerically, can be solved analytically.

But when there is no solution of the analytical solution because of the complexity of the following we can go for the numerical solution and of course once we look into this form of the governing equation either equilibrium system or dynamic system to represent in the form of the governing equation, then to represent certain phenomena or we using this governing equation in some part there may be the possibility of using the constitutive equation or constitutive relation.

But of course along with the natural and boundary condition that is also part of the system because the governing equation is valid within this but boundary interaction is also important to specify and that boundary interaction, spatial boundary interaction may be possible but the boundary interaction in the form of a, as a function of the time that is also possible but that normally we do in case of transient problem, we need the time dependent boundary condition that can be represent in terms of the initial condition or other kind of boundary condition.

But if it is a, we assume is a steady state situation that means all equation is happening within the system under steady state condition, that means is independent of the time, then spatial boundary condition must be defined to get the solution of a particular system of the equation. Now, I am talking about this thing apart from this equilibrium system and dynamic system representation, there is a role of some constitutive equation also.

Then, constitutive equation actually relates two different physical quantities between two constitutes, what this physical quantity relates, for example constitutive relationship between stress and strain. What I can relate between the stress and strain? In that way, we can form the constitutive relation this two physical quantities. So, they are called it does not directly, not necessary always try to follow the physical.

Or rather it can be combined with other equations such as this constitutive equation can be used in combining with other equations. For example, the equilibrium equation or kinematical equation which do represent the physical laws. Actually, by representing the equilibrium equation on kinematical equation that actually represent the physical law but constitutive equation may not follow the physical law.

But what way we can form the constitutive equation? We can get some example to form the constitutive equation.

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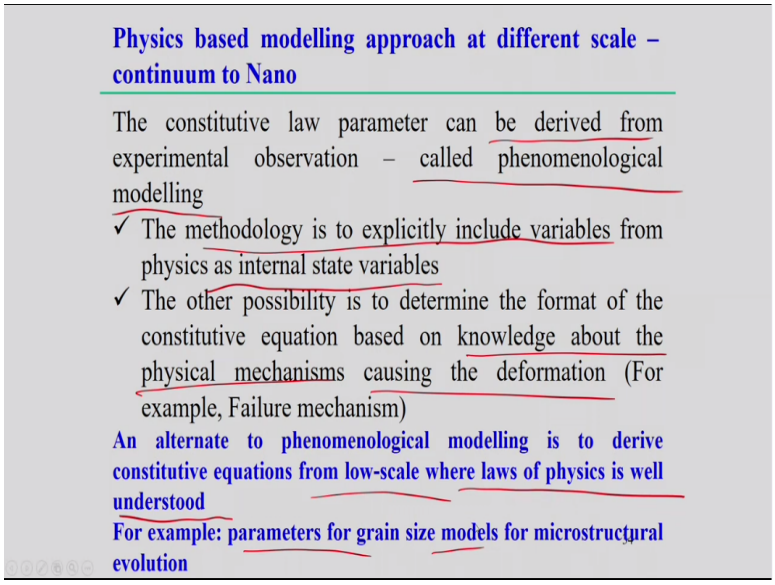

So, the constitutive law parameter in this equation can be derived from the experimental observation that constitutive law with the help of the experimental observation we can relate between these two physical quantities to make some constitutive relation and that is often called the phenomenological modelling approach.

So, phenomenological modelling approach means we normally observe through the experiments what the phenomenological things happening during this process and there from this through large number of experiments normally we try to relate between the two physical quantity and that is normally call the constitutive relation between this but this constitutive relation can be linked with a physical law.

But physical law is normally represented in a dynamic or equilibrium system, so that under the equilibrium system we can link with the constitutive relation and we can further solve the different kind of the problem. So, therefore constitutive law parameter can be derived from the experimental observation and it is called phenomenological modelling but the methodology is to explicitly include the variables from the physics as the internal state variable.

For example, when we try to explain that phenomenological modelling say recrystallization modelling for example, recrystallization modelling and which is associated to metal deformation process. So, when we deform a particular component in material deformation process and in metal forming processes that we represent the deformation process as a function of strain rate or as a function of strain and or as a function of temperature.

Now, all these 3 are variables here. Now, the internal state variable can be represented in this process represent that recrystallization mechanism that internal variable can be the dislocation density. Now, during the deformation process, how dislocation density evolves that can be linked with the parameters in terms of the strain, in terms of the strain rate or as a function of temperature but the internal variable in this case is the dislocation density.

Now, we try to look into that this based on this dislocation density considering as an internal variable during the recrystallization process and we can predict what is the average recrystallized grain size after the deformation process once finished or at a particular state what are the amount of the stress generate during through the recrystallization process. So, this way, we can develop one particular model.

But when a phenomenological model, we try to represent all these things, say in terms of some internal variable, internal state variable which are to represent. Of course, the state variable can be included in the recrystallization model as a grain size also, average grain size can be a state variable as well. So, therefore other possibility to determine the format of a constitution based on the knowledge about the physical mechanism and causing the deformation.

If you identify that what are the physical mechanisms responsible for the deformation process and that physical mechanism can be represented in terms some other parameter, in the form of one parameter and that parameter can be included in this for the development of the constitutive model. So, therefore an alternate to the phenomenological modelling is to derive the constitutive equation from the low scale.

Of course, in the phenomenological modelling, we try to derive some physical mechanism is responsible here that can be look in that can be derived from the very low scale or the low scale physics is basically we can rely on the low scale physics because the low scale laws or the laws of the physics is well understood at very low scale. So, we can take the information from the low scale and then we develop the, we can decide the constitutive equation by the information from the low scale mechanism.

For example, parameters for the grain size methods, so therefore parameters for the grain size methods, we look into the microstructural evolution and we can evaluate what are the parameters and that actually responsible to predict the grain size, that is the one example just by looking to decide the parameters at the low scale.

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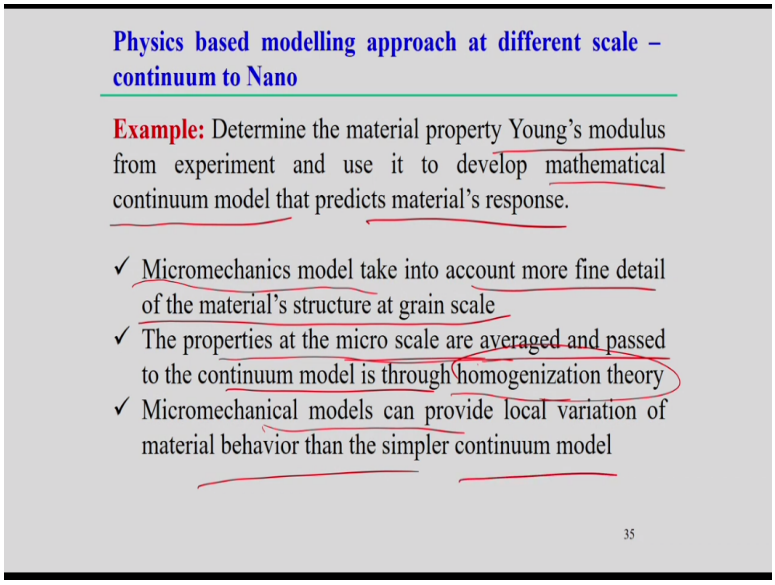

Now, we can give another example, for example determine the material properties Young's modulus, we know the Young's modulus we can easily measure in a particular material through experiments just by looking into the universal tensile testing machine for a particular material and therefore that value Young's modulus can be used some mathematical model in the continuum model, trying to develop the stress analysis for elastic stress for a particular material.

Then, when we try to look into the elastic stress analysis, in that case there is requirement of the Young's modulus for this particular material. So, therefore using this value that from the experimental measurement and give the input property to the model and then model can predict the output in terms of the material response. So, of course Young's modulus once we measure that from the universal tensile testing machine for a tensile specimen.

That information is actually usable at the continuum scale that means we cannot use this information probably in the lower scale prediction. So, then in that cases we need to look for example we cannot use Young's modulus for a bulk of material what we extract from the universal tensile testing machine. It is not possible to use when we try to predict the single crystal structure what is the Young's modulus.

So, that in that cases we need to refine the experimental procedure to get to find out the Young's modulus and for this particular cases and there is another difficulty also because when you try to look into the lower scale, for example in the single crystal structure, the atomic arrangement may be different in the different direction, so therefore that E value can be different direction.

So, in that cases if you look into to conduct experiment of the different direction, so then we can get the elastic behaviour that means different values of the E at the different direction but when you do at the macroscale experiment to find out the tensile specimen the Young's modulus with tensile specimen, we apply one single direction and in that direction, there is the value of the Young's modulus.

And we assume that most of cases say homogenous structure at the microscopic point of view. So, therefore if we change the scale, we need to refine the experiment to get the information. So, therefore when we look into the continuum model, some information from the micromechanics models can be incorporated account and more detail from the material structure at the grain scale.

At the grain scale what are the material structure? We can look into the micromechanics available at a grain scale and that information can be used, can be supplied to the model for the development of the continuum scale or the microscale. So, therefore properties are the microscale but properties we can get, just I have given example if we measure the Young's modulus in a 110 direction for a single crystal structure and 111 direction and maybe other direction and 110 direction.

Then, in that case is will get huge variation of the Young's modulus is possible because crystal structures are different. So, therefore what this variability, normally we can do the averaging out and we can give the average Young's modulus to the next scale to find out the, to develop a particular model. So, that means, that is called the lower scale are averaged and passed the value to the continuum model.

And that is normally done through the homogenization theory, so I am not going into that what theory can be, details about this theory. So, therefore micromechanics model or

micromechanical model can provide some local variation and that of the behaviour and then we can pass the local variation in the average form to the continuum model for development of the next scale model in the larger scale model.

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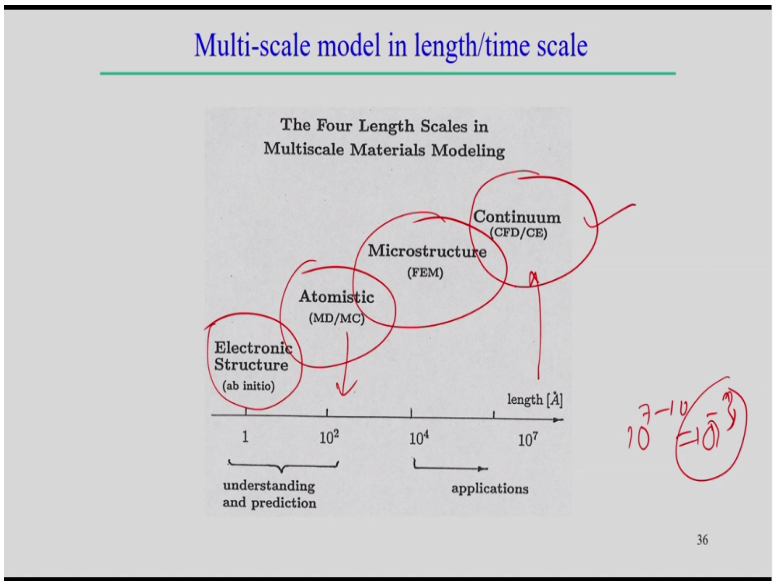

So, now we can look into when we try to link the one scale to other scale and then people have developed that multi-scale modelling in the length and time scale also, both multi-scale modelling is possible. So, now people are working in this different scale modelling approaches. So, normally 4 length scale in multi-scale materials modelling normally happens; one is the electronic structure we can look in the very lower scale, understanding and prediction.

Then atomistic scale, then we look into the microstructure, finite element method can be used. At atomistic scale, we can use some molecular dynamics or some statistical physics also we can use to make the model at this scale and finally we normally use for example we say we are using the governing heat conduction equation and we are solving, that is actually we are doing in case of that scale, continuum scale.

So, there are 4 hierarchy level of the modelling, different scale modelling approach. So, length scale we can see the length scale is 10 to the power 7 that means 10 to the power 7-10=10 to the power -3 in that scale so that means millimeter scale we can get the continuum's model and of course this continuum model we can use the CFD method, computational fluid dynamics.

Even we can use finite element method also, this numerical techniques we can use to develop model at the continuum scale.

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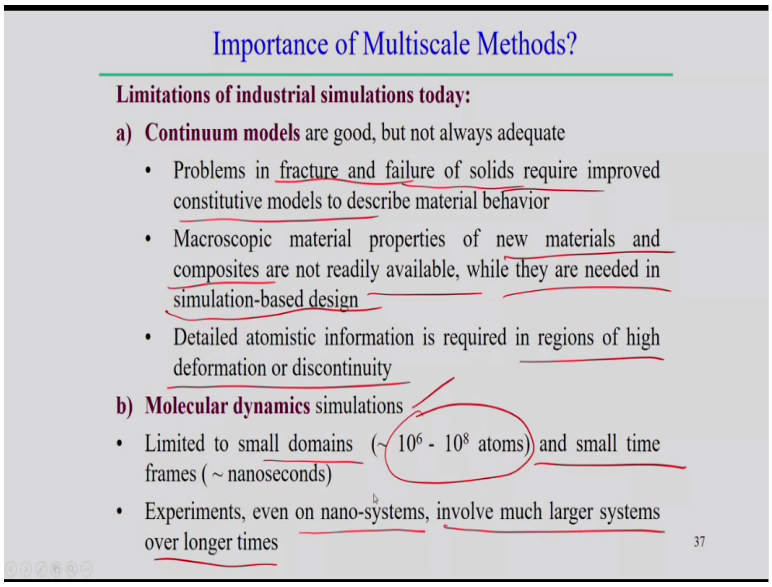

Now, importance of the multi-scale methods; now limitation of the industrial simulation today is the continuum models are good but not always adequate because for example problems in the fracture and failure of the solids require the improved constitutive models because when you try to predict the fracture and failure it is very difficult to represent this thing using some kind of governing equation there.

Rather it depends more on the some constitutive equation but it is a best if we analyze the fracture and failure mode from the continuum scale or micro scale approach then it is very difficult to predict this behaviour. So, therefore in this case, there is a requirement to look back to the lower scale model to predict the fracture behaviour of a particular material.

And so therefore macroscopic material properties of the new materials this is another composites which are not readily available while they are not needed in the simulation when we try to look into the simulation based designs. So, composite material is varied in that cases probably we can get the material properties by analyzing at the lower scale. Therefore, detailed atomistic information is required in regions of the high deformation of the discontinuity.

So, when try to predict the discontinuity, deformation behaviour. So, in that cases, it is better go for, we can predict the material behaviour just looking, look back to the lower scale

approach. Similarly, molecular dynamics simulation also done, nowadays the scale is limited to the small dimension that means 10 to the power 6 to 10 to the power 8 atoms. So, you know that the size of radius of the atom is less than nanometer.

Therefore, in that scale the domain is very small and that is time frame, of course the time scale also when we try to molecular dynamics simulation, the time scale also lower scale, times scale is in the nanosecond level. So, that nanosecond level time scale and the domain is in the 10 to the power 6 to 10 to the power 8 atoms the smaller domain. So, in that domain if we do the simulation process, so that simulation result directly cannot use to the continuum model.

So, therefore that information may be necessary to develop model in the next scale, say maybe in the meso scale model the information or atomistic scale model we can get, we can give this input and we can develop the model and of course experiments, even the analysis molecular dynamics exist in the very small time scale in the nanosecond level but when you try to do the actual experiment of the nano system is not exactly much longer time is required actually to conduct the experiment.

That means nanosecond phenomena not necessary, the nanosecond phenomena, the experiments can be conducted within the time frame. So, time frame can be much more. So, these are the typical issues associated with the different type of the multi-scale methods but most important of the multi-scale method is that how to link one scale to another scale.

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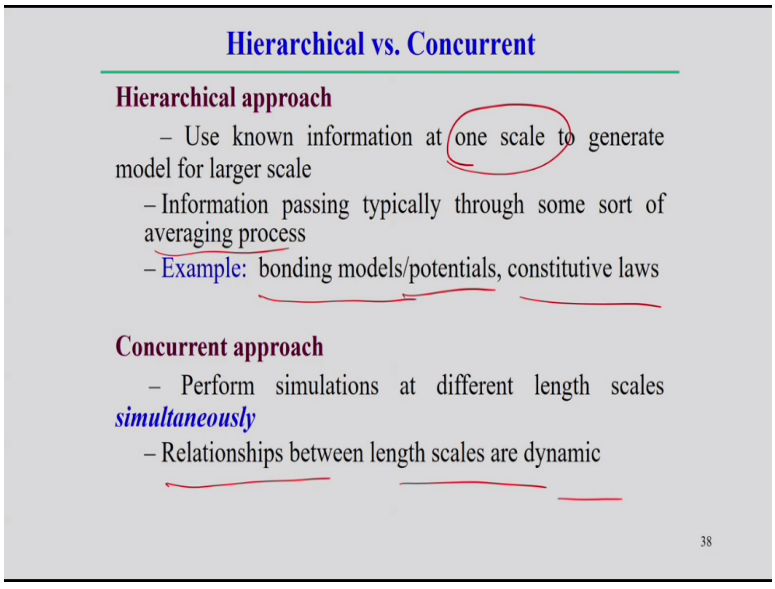

So, therefore two approaches we follow in multi-scale modelling approach. One is the hierarchical approach, so hierarchical approach means known information at one scale and to generate the model for the larger scale. Therefore, information passing typically through some sort of averaging process. Therefore, at the lower scale, we make the properties; we make the information, get the information at lower scale output from the model.

And then we averaging out the properties and then it passes to the next scale, so that is the typical approach in hierarchical approach. For example, in that case is bonding models, potential and constitutive laws can be developed just by looking into the model into the lower scale. Concurrent approach performs simulations at different length scale simultaneously.

So, therefore at a time at the different length scale if we perform the simulation but difficulty is the how to link, how to get the performance of one scale, information from one scale to another scale. So, therefore relationship between the length scale in this case is mostly are dynamic in nature, so they pass the information in this one scale to another scale is the major issue in case of the concurrent approach.

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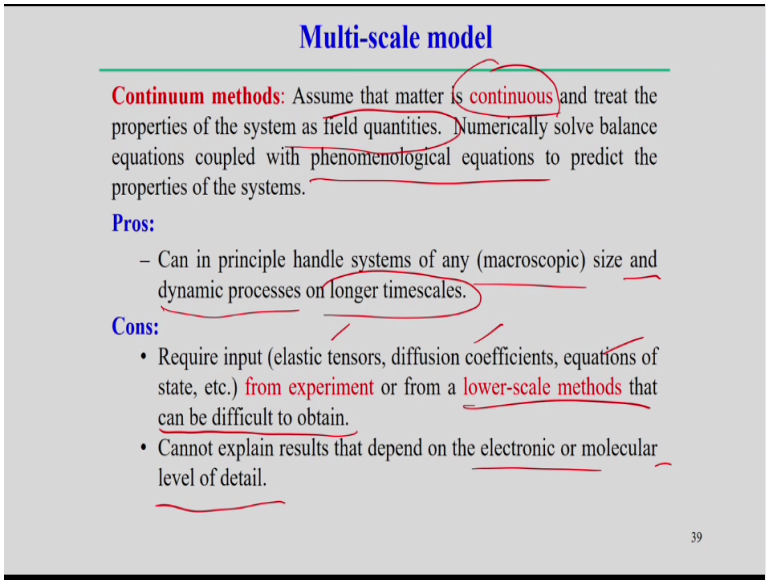

Now, multi-scale model, if we look into the continuum methods because most of the cases we use this continuum methods and of course the method of modeling of manufacturing process is mostly based on this continuum methods that means just finding out the equilibrium equation and try to solve the equilibrium equation to get the output variable. So, therefore continuum methods we try to look into and assume the continuous media basically and treat the properties of the system at the field quantities.

Say properties of the system at the field quantities and therefore numerically solve the balance equation or coupled equation we can solve. For example, thermomechanical, thermal and mechanical analysis, even coupled it and then we can solve this, we can get the output variable and of course couple with some phenomenological equation can also be used here and of course along with the governing equation some constitutive relation can also be used.

For example, thermomechanical analysis, thermal analysis can be based on the governing equation but when you look into the mechanical analysis it is mostly develop based on the constitutive relation. So, therefore and if we incorporate some lower scale, the prediction of the certain variable.

For example, predict the failure behaviour then in that case is if you want to predict the failure behaviour from the thermomechanical analysis then we need to incorporate some kind of the phenomenological modelling approach there by introducing some sort of state variable there. Now, the advantage and disadvantage of these things and of course continuum model can in principle it can handle the system of any even for macroscopic scale also.

Size can also be handled by using this continuum model and of course it is in the continuum model can also handle the dynamic processes also and the dynamic processes may exist over a time scale. For example, in atomistic model or in that molecular dynamics model in that case is the time scale is very lower, very low so that relation statistical valid over a very small time scale but this continuum's model is another sense.

It can be valid for longer time scales that is the main advantage of continuum models and but require input, for example diffusion coefficients, some elastic properties of a material and particular equation of state from experiment that is the input to the model. So, therefore when you define some material properties that material properties normally evaluate from the experiments and we give the inputs to the experiments, we give the input to the model that is one approach.

Or these properties can be evaluated just by looking back to the lower scale methods. So, from the lower scale methods we can predict the properties and that can be given to this

material but lower scale that can be difficult to obtain because in that case is we need the develop the model at the lower scale to predict the properties of the particular material.

And of course this continuum based method cannot explain the electronic and the molecular level in detail so this getting no information and nothing prediction, what is happening at the molecular structure detail of a particular material. So that information we cannot get from the continuum methods.

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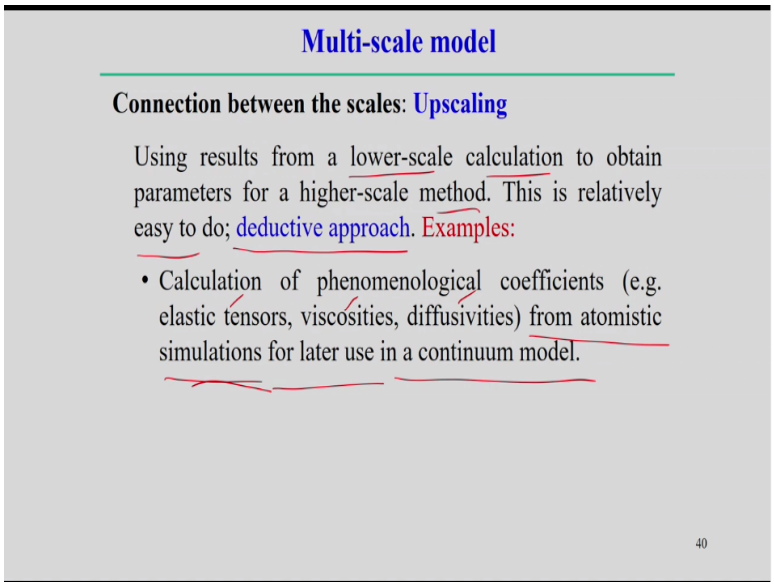

Now, connection how we can connect the different scale that is one is the upscaling method, for example upscaling means that using results from a lower scale calculation. So, we can use the results from the lower scale calculations to obtain the parameters for a higher scale method. So, therefore first use the lower scale calculation and we get the parameters and we use this for the higher scale method.

This is relatively easy to do and of course this is called the detective approach and in this upscaling method relatively easier because we get the information in details in the lower scale and that predict the properties, we average out the properties and that properties can give to the next scale, so from lower scale to the higher scale it is easy to move from this upscaling method, for example calculation of the phenomenological coefficients.

For example, the elastic tensor, viscosities, diffusivities, all these coefficients are for this particular properties. Then, that can be done from the atomistic simulation, from the atomistic simulation it can be done for later use in a continuum model. So, that we can give the

upscaling one, example of the upscaling is the phenomenological coefficients, may be when you try to predict the elastic tensor which may be associated some kind of the coefficient viscosities, the properties or diffusivities properties.

And diffusivity sometimes represent in terms of the some coefficients also introduce, so that values are values of all these parameters that can be evaluated from the atomistic model, atomistic simulation model and that model can be stored and that data can be used for the continuum. This is the one approach or this is the one advantage of the upscaling during the multi-scale modelling approach.

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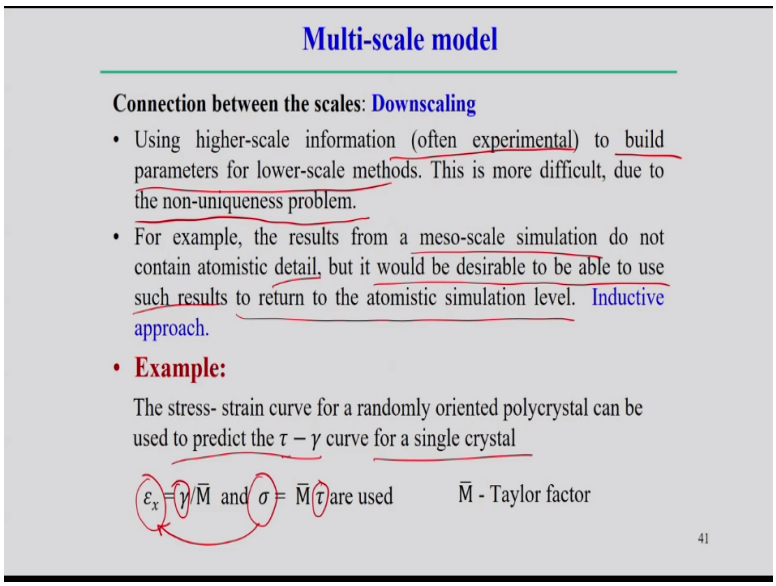

Now, it can be downscaling approach can also be possible in the multi-scale model. So, then in this case is higher scale information, so in this case is higher scale information passed to the lower scale information. So, that is higher scale information normally we can observe from the experiment, often experimental. So, that means it is easy to obtain, to conduct the experiment at the higher scale.

For example, if we look into the macroscopic scale, in the macroscopic scale we can obtain the experimental results and that information can be passed to build or develop the lower scale, so here the only advantage is the doing the because we have the scope to easily do the experiments and that information can pass from the higher scale to develop the model at the lower scale, to build the parameters for the lower scale.

But this is more difficult as compared to the upscaling due to the non-uniqueness of the problem. So, non-uniqueness of the problem because if there is a uniqueness in the sense that if you want to develop the fracture model and by looking into the information from the higher scale data basically that if we correlate the fracture model in the responsible parameter for the fracture of a particular material.

So, then that correlation can done with the continuum scale or the macroscale modelling approach but this information cannot be used to develop the model for the lower scale because the fracture normally happens; sometimes it is kind of catastrophic failure may happen during the application of the fatigue loading in a material deformation process. So, therefore for example the results from the meso-scale simulation do not contain the atomistic detail.

Definitely meso-scale model do not contain the atomistic detail but it would be desirable to be able to use such result to return the atomistic simulation level. So, inductive approach that means you can compare the results by some assumptions and this inductive approach may not be very convincing to develop the downscaling modelling approach. For example, we can give an example also, the stress-strain curve for a randomly oriented polycrystal.

So, we can easily predict the randomly oriented polycrystal can be used to predict the shear stress, shear strain curve for a single crystal. So, we can use this relation, for example the strain and this stress, the stress and strain for the polycrystalline material we can easily find out this stress versus strain graph for polycrystalline material.

But this polycrystalline information from the stress-strain diagram polycrystalline material that information can be used to predict the lower scale, that means for lower scale in the sense that for single crystal structure. Single crystal structure, the variable is the shear stress and shear strain is more important in the single crystal structure because normally slip happens due to the application of the shear stress there and critical shear stress may be responsible there.

So, therefore shear stress and shear strain diagram is more important in case of the single crystal structure to predict the failure behaviour of the single crystal structure or yielding behaviour of a single crystal structure. Now, here this conversion is possible by using some

Taylor factor but this Taylor factor, it is the average value of the Taylor factor, so basically the local behaviour by passing the information from higher scale to the lower scale.

Basically, we are suppressing the behaviour at the lower scale rather we can passing only the averaging value from higher scale to the lower scale and this to some extent can be represented by this, this is suppose stress strain something like that and if you have a single crystal structure, it is a strain and it is a shear strain, it can be something like that just to maintain the average value of the Taylor factor and average value of the Taylor factor actually comes from the types of the grain distribution basically in a polycrystalline material.

So, this Taylor factor can be estimated for a randomly oriented polycrystalline. So, here the downscaling of the modelling approach is little bit is not very much convincing for downscaling approach as compared to the upscaling approach. So, normally in the simulation process mostly we follow in the upscaling approach in case of multi-scale model.

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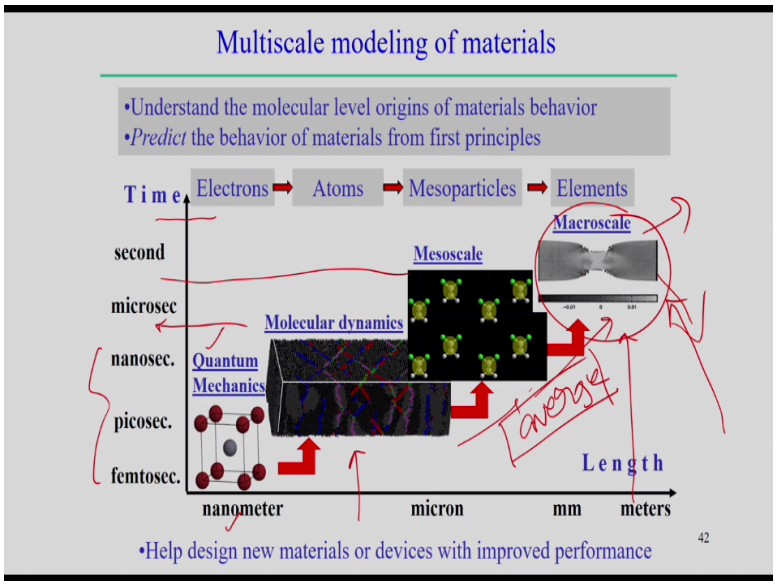

Here, we can see that multi-scale modelling of the materials, they understand the molecular level of the origin in the materials behaviour, we can see that also and predict the behaviour of the materials from the first principle. So, we can use the basic law and we can link from the one scale to another scale. Here, we can see the quantum mechanics is responsible in the nanometer scale.

And of course within the femtosecond, picosecond and nanosecond, with that time scale this model is valid. When we go for molecular dynamics, scale goes little bit the nanometer and

micrometer range and then scale is little bit, time scale is little bit increasing here, then once from molecular dynamics too it can reached link with the meso-scale, model development.

So, model development or we can say the grain scale model development and then the time scale also increasing here and finally from meso-scale to we can reach the macroscale model. So, this macroscale model we can see is the little bit higher time scale and length scale also in terms of the meter within the millimeter to meter in that range.

So, therefore with this level of linking, in the multi-scale modelling approach is the main the different process methodology has been developed that how we can get the information from the lower scale, pass the information from the lower scale to higher scale but when you pass the information from lower scale to higher scale mostly in the averaging by averaging the properties.

So, then the average value we can pass from the meso-scale to microscale and based on that different level of the scale has been developed and we can analyze the different scale of the models and of course we can link the different scale of the models to finally predict this think so but how it is significant because when we try to develop some kind of the new material, so understanding of the different scale multi-scale modelling is to predict that expected behaviour of particular material.

So, then based on the multi-scale modelling approach is the most suitable modelling approach to predict the behaviour of a new material when you try to develop on particular material and therefore try to analyze their performance. So, therefore we need to understand the link and the understanding the mechanical properties or other kind of properties at the different scale but most of the cases we normally focus on this macroscale modelling approach.

And we can do all the tensile testing, universal tensile testing or hardness measurement, all kind of information normally we can do for the development of the macroscopic limit and here we supply in microscale only product, here we supply all the material properties but that material properties normally evaluated in case of at the macroscale.

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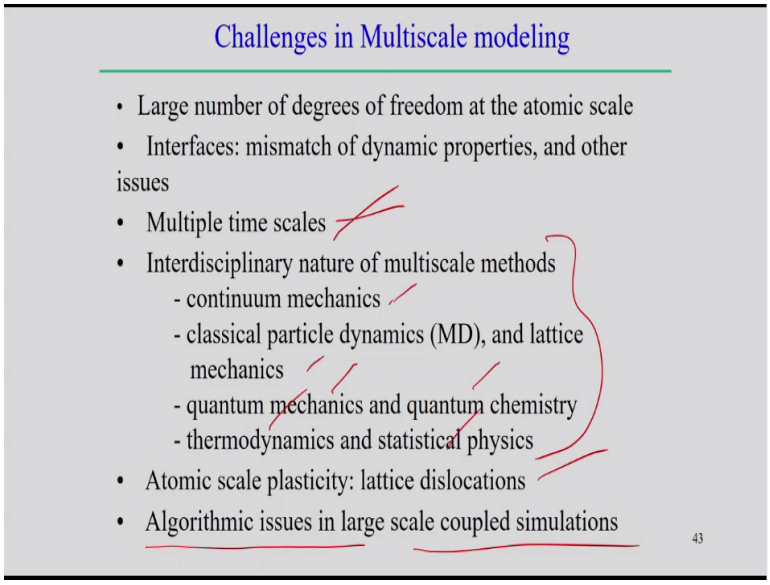

But in general what are the challenges in multi-scale modelling, we can point wise we can say that of course if we lower down the scale then for large number of degrees of freedom large number of variables actually involved at the atomic scale; however, if we go to the higher scale the degrees of freedom gradually decreases. Other difficulties in multi-scale modelling is the interfaces, basically how to represent the interfaces and mismatch of the dynamic properties.

Because interfaces actually act through dynamic behaviour, so therefore it is often quite possible to mismatch of the dynamic properties at the interfaces, that is the one difficulty in multi-scale modelling approach and of course we try to link with the different scale so analysis can be done at the different scale. So, therefore for example if we try to analyze for example laser welding processes and this thing.

So, this laser welding processes, if it is pulse laser welding process, so we can analyze the pulse laser welding process, maybe time period, if it is a pulse, duration maybe or the order of the microsecond, then in the microsecond in that time scale we can analyze this process but for example if we try to analyze the ultrashort pulse laser welding process, then ultrashort pulse the pulse duration maybe in the of the order of femtosecond and picosecond.

So, therefore we need to bring the analysis and reduce the time scale in that second and this analysis so once we change time scale, so analysis procedure can be different. So, therefore for example this ultrashort pulse laser welding process we cannot apply simply the heat

conduction equation, Fourier's law of heat conduction, so we have to analyze in the different scale, so that is why there is a different multiple time scale.

The analysis behaviour will be different and of course the interdisciplinary nature of the multi-scale methods, continuum mechanics, therefore classical particle dynamics and the lattice mechanics these are the all mechanism are different, we need to understand all these mechanisms. So, we have to link these mechanism, the quantum mechanics also, quantum chemistry, thermodynamics and statistical physics.

So, analysis of all these is required to develop a model, to understand this model to develop the interdisciplinary nature of multi-scale model. So, getting knowledge of all these things is sometimes difficult. Then, if you look into the atomic scale plasticity, then we have to look into the lattice dislocation behaviour. So, we have to analyze all these matter different things if there is a scalar difference.

So, analysis, procedure, modelling approach, all are different and finally the algorithm issues in large scale coupled simulation. When you couple one scale to another scale, how to develop the algorithm that is one issue, maybe in the different time scale or at the same time scale or the different analysis behaviour. For example, thermal and mechanical analysis or thermal and fluid analysis.

So, how we can couple this thermal analysis and fluid analysis because some parameters or variable is a common variable between these two analysis procedure. So, therefore developing of the algorithm for the large-scale simulation is another difficulty in case of multi-scale modelling approach.

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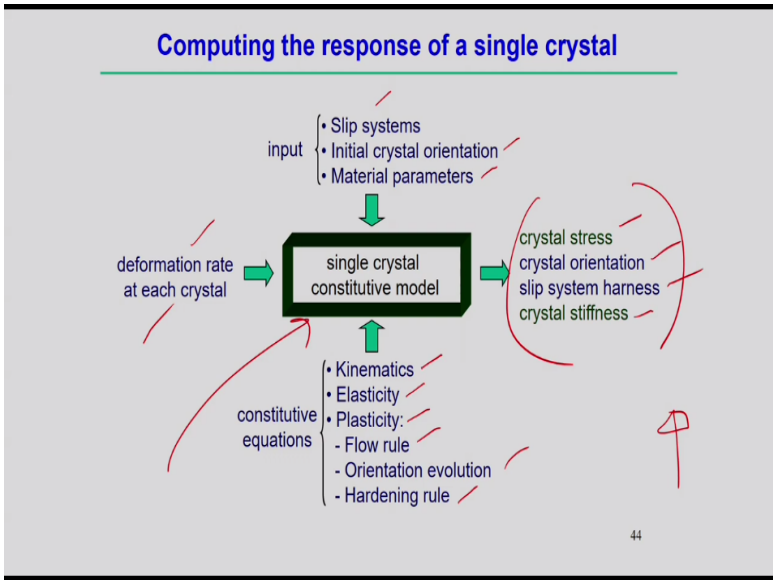

We can give an example also, for example computing the response of a single crystal structure. How we can do this things, what are the input required, if you see the input slip system, we should know for a particular metal what are the slip systems, then what is the initial crystal orientation and what are the material parameters is involved in this things and we should know deformation rate at each crystal what are the deformation rate.

And of course some constitutive equations also is involved get improve, what are the kinetics, following the kinetics. Elasticity; elastic behaviour, how this following. Plasticity behaviour, how we are predicting, representing the plastic behaviour single crystal structure and then even plastic behaviour depends on the flow rule and then orientation evolution of course it depends on hardening rule.

So, all information give to this thing and then it creates the single crystal constitutive model looking into all this type of equation input and these input parameters. Then, develop the single crystal constitutive model then we predict the crystal stress and crystal orientation and then slip system hardness and then finally crystal stiffness. These are the output from all this input, so once taking the input following the different constitutive equation, we can develop the constitutive model single crystal structure.

And we can get the output in the different crystal structure crystal orientation but all these is a particular scale we follow. So, all this phenomena happening at a particular scale, particular time scale.

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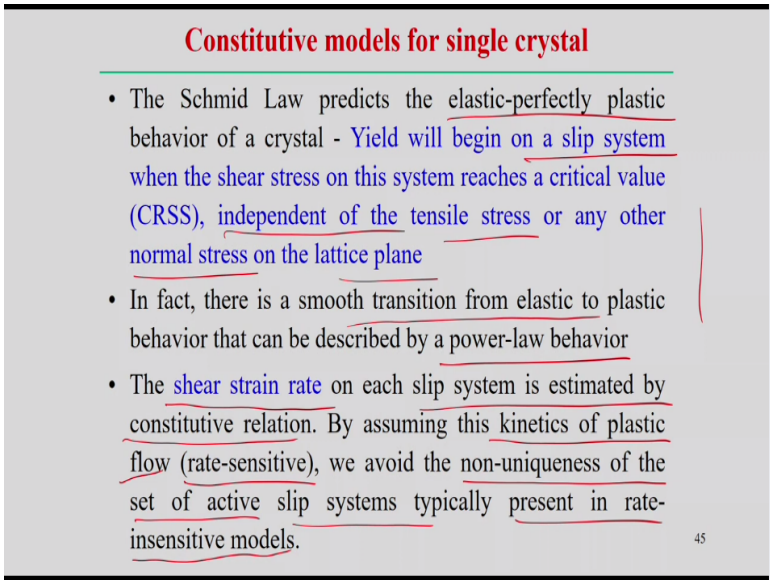

Then, we can give another example, for example if you want to develop the constitutive model for single crystal structure. Then, normally we see what will happen; the Schmid's law predicts the elastic-perfectly plastic. So, the deformation happens during the slip system, slip occurs within the single crystal structure, it is just elastic component and just from elastic to perfectly plastic, this kind of material behaviour normally follow in case of single crystal deformation process.

So, yield will begin on the slip system when you just cross the critical value of the shear stress and that shear stress critical value of the shear stress is independent of the tensile stress or any other normal stress on the lattice plane. If you know this is the yielding behaviour of a particular single crystal structure, then we try to develop the model for the deformation behaviour of the single crystal structure.

So, therefore we see the elastic perfectly plastic behaviour but in that case is the transition from elastic to plastic can be smooth also. So, when you looking into the smooth transition from elastic to plastic behaviour then we can look into the power-law behaviour, we can represent this power-law equation, smooth transition from elastic to plastic. Of course, in these cases, other parameter also can influence that is the shear strain rate. So, rate also in slip system is estimated by the constitutive relation.

That can also be estimated from the constitutive relation but of course kinematics of the plastic flow can be represented by the rate-sensitive or rate insensitive or we can avoid the non-uniqueness of the set of the active slip systems typically present in the rate intensity

model. So, therefore we have to look into the uniqueness of the active slip system because one particular single crystal structure,.

There are so many slip systems and that all the slip systems may or may not active at a time. For example, FCC crystal structure, there are 12 types of the different slip systems may happen. So, therefore 12 slip system may nor active at a particular time. So, therefore we have to look into that how many slip systems, minimum slip systems is required to activate the deformation process.

So, all these matters, when we try to develop the constitutive model for single crystal structure so therefore all this analysis is actually required or information is required.

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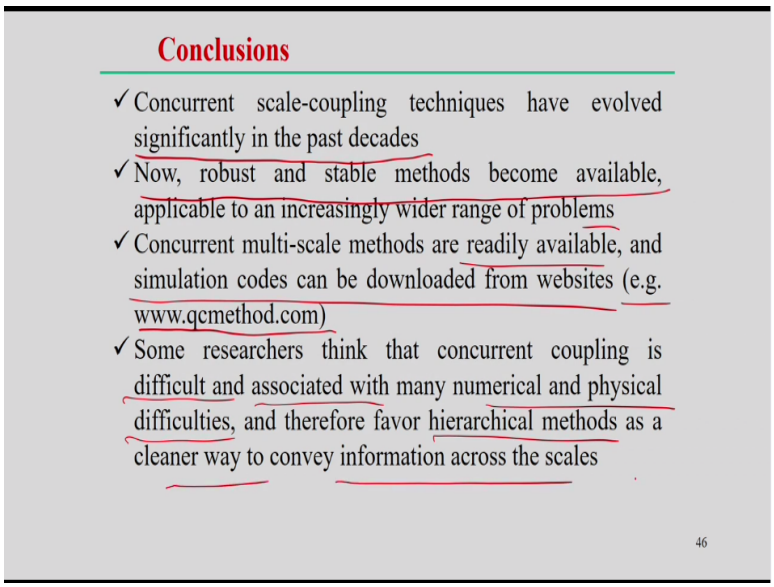

Now, from this modelling approach in different scale, we can make some conclusion also that concurrent scale-coupling, so concurrent scale-coupling techniques have been evolved significantly in the recent decades. So, people have tried to look into that concurrent scale-coupling techniques for the development of the multi-scale model but most robust and the stable methods become available applicable to increasingly wide range of the problem.

So, that I think now it is available the most robust and stable methods becomes available but we need separate study on that to utilize the multi-scale modelling approach. Then, concurrent multi-scale methods are readily available and simulation course can be downloaded from the website also, from this website we can get lots of this thing the concurrent multi-scale approach or model we can get from here also.

And some researchers think that concurrent coupling is difficult and associated with many numerical and physical difficulties to implement all these things. Therefore, they favour the hierarchical methods as a more cleaner way to convey the information across the scale. So, these are the typical I think conclusion for the development of the multi-scale model but of course to understand the multi-scale model, we need to look and understand the physical mechanism behaviour happenings at the different scale this is the first step.

And second step is the how we can link all these scales and of course when we linking all these scales what may be the algorithm we need to follow or any algorithm we need to develop to get prediction of a particular behaviour and of course this multi-scale understanding, all this multi-scale modelling approaches may be more suitable when we try to develop some new materials.

Or may be for particular materials, we try to develop some good, we try to propose certain manufacturing processes, therefore all these approaches required in that cases. So, thank you very much for your kind attention.