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Lecture – 01 Properties, Modelling Approaches, Process Modelling and Optimization

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Hello everybody. Now I will start this module 1 of Finite Element modeling of welding processes. We can start the module 1, the content of the module 1 is that first is introduction to welding processes and it have been the different components. Introduction; first we will try to introduce basically the associated with the welding processes different welding processes and may be materials and the different. Properties of the which may be required for for the development of the numerical model.

So, that we will try to discuss and make us in the classification; that means, what we can classify the fusion welding processes, then what are the different fusion welding processes, how the brazing and soldering are different from the welding processes apart from that solid state welding processes we will discuss and then advanced welding processes.

The advanced welding processes also we will try to discuss and then finally, wire additive manufacturing processes. So, basically in this module we will try to look into the basics of the different welding processes and of course, we analyse the welding processes in the prospective of the physics behind this welding process or physical mechanisms we will try to understand associated with welding processes. But it is not intended to look into the complete description the welding process the advantage this not like that.

We will try to understand the welding processes the in the light of the physical mechanism involved in a particular welding process. Such that it will be easier for us if we understand this six physical mechanism then we will be able to develop some kind of the model. So, using the tool finite element method. So, that is a objective of this module 1.

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Introduction - Materials processing technologies

Materials processing - manufacture of raw-materials into finished goods

Industrial processes - various mechanical or chemical procedures, and produce large quantities or batches.

Raw materials - either extracted from minerals or produced from basic chemicals or natural substances.

Additional processes - smelting and alloying are used to produce the metal that is to be fabricated into parts that are eventually assembled into a product

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Now, start with a very basic things that material processing technologies. So in general we can say that this material processing technology the what a we can generate the raw materials first. And from the raw materials basically the engineer will try to produce from the raw materials to the some finished good or some product which we can directly use this product we can use, but there is a several steps involved to conversation from the raw materials to the final product.

So, then that is associated with the different kind of the manufacturing processes for it may be involved some casting, machining, welding, joining, heat treatment, so many processes may be involved in between. So, that is in general we can say that it is a material processing technologies. Now in [vocalized-noise] industrial processes means; its the industrial scaling of all this manufacturing processes, but they aims to produce in the larger amount larger

scale; that means, it is associated with the various chemical mechanical processes and, but try to produce as a large quantity in a batch production.

So, that is why that follow the industrial processes. Of course, industrial processes definitely if it is also involved included some all of the manufacturing processes. Then raw materials is basically we understand the raw materials is normally produced either extracted from the minerals or it can be produced from the basic chemicals or natural substances.

So, there are several procedure to extract from the ore to a getting the raw materials and that raw materials after that we process it that is following through series of the manufacturing processes and then it reach to the final product. But apart from these things all these series of the manufacturing processes we discuss the several manufacturing processes involved in this conversation from raw material to the finished product.

It is also associated some additional processes. For example, smelting and alloying, but sometimes it is necessary to characterise or to get some specific properties of this particular material or metals the alloying of the metals is also required and sometimes we made we can produce a composite materials also for that purpose to achieve some specific properties which may be required for a particular application

But sometimes we what we do? Alloying are used to produce the metal that to be fabricated in two parts were finally, has to be assemble and then it after assemble we can get the particular product so; that means, it means that some alloying of the metals is also possible such that it can achieve on a particular properties ah when [vocalized-noise] and which is may be aim to a particular application. So, this is the overall we can say that there are several material processing technologies are also involved.

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Now, before understanding the processes any manufacturing process we should know that this what are the common materials and alloy system is normally used from that prospective here I am presenting some common alloy, engineering alloy and most of the cases there is a huge application of all these particular alloy or metals.

So, in that case its comes first that ferrous metals it say simply iron as a main main constitute that is that we say it is a ferrous metals. After that nonferrous metals also there other than iron as a main constitute. There are several nonferrous metals ah we can see that alloy aluminium alloy, nickel, titanium alloy, all are nonferrous metals and there are having the different different applications.

So, we use all these particular metals and alloys and simply we are dealing in the manufacturing industry also, most of the cases we dealing with these things this particular metals and alloy. But this is not enough may be other kind of metals and alloy may are also used in these things, but I am try to get some overall view on this what kind of metals normally used in the manufacturing industry.

So, steel can huge application of the steels components are also there in the manufacturing industry and normally the steel we can define carbon is having less than 2 percent then we can categorise this steel and carbon having more than 2 percent we say it is a simply a cast iron. Both are having their use in industry. Then copper alloy; copper alloy is the there are so many application of the copper alloy, but which is comes into in your mind that pure copper is electrical industry mostly use the copper and copper alloy.

Then aluminium alloy mostly used in the automotive industry main application, but definitely is having some other applications also. But mostly we use in this automotive frame or automotive applications. The nickel based alloy is outstanding strength and concentrate is the main properties of nickel based alloy, but there are huge application [vocalized-noise] nickel based alloy in several applications we see.

Similarly titanium alloy also. Titanium alloy is having very good ah strength to a ratio and of course it is normally designed the high temperature engineering materials we considered in that way and there is a huge application of titanium alloy one of is that even aerospace industry as well as the medical industry we can use the titanium alloy.

Apart from that that is super alloy also super alloy having the specific property then high strength keep resistance oxidation properties we will look into that what are the different properties normally used to ah evaluate the materials before use of this particular material for a particular application.

Now corrosion resistance, fatigue resistance all combination of all of these kind of properties is having a combination of good properties that is normally design the super alloy system. The super alloy system can be nickel based super alloy base metal is nickel and other alloying elements are there. So, that it is possible to achieve particular properties in a particular application.

Similarly iron based cobalt based super alloy also possible are have been developed. But main application we can find in our mind that super alloy can be used jet in engine rocket and nuclear applications or huge applications. So, that is why there is a so many engineering materials are available and but they are having the different applications and the for the particular purpose or different purposes.

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Now, these are the just overall view of the different kind of metals we normally use. Now if you look into that properties of this now once we use particular material then we should have some knowledge about the properties of this particular material and what are the different properties normally when evaluate to analysis for a particular manufacturing process that is

also necessary because to adopt a particular manufacturing processes we need to know the particular specific properties of a particular material.

Now what are the physical properties? We can see that I have listed few of them the different kind of the properties; one is the thermal conductivity is the simply property of a material to conduct the heat flow, that is the one property. Thermal conductivity it is very important property and because, this important property characterise different weld behaviour in specific to welding properties.

So, they definitely thermal conductivity of a particular material is very significant very important parameter. For example, high thermal conductivity material copper, aluminium, silver, gold, these are the mainly the high thermal conductivity material other way low conductivity material having the thermal low thermal conductance; that is polymer, alumina, they are having the low thermal conduction.

So, I want to mention here that material having the high thermal conductivity and material having the low thermal conductivity. So, in these two cases the application of the welding technology can be different since their properties are completely different. So, it is necessary to analyse to have some knowledge about the different kind of the properties normal common properties of the particular material. Then thermal expansion is the another kind of properties because it actually decide there is a mismatch plastic deformation may happen after welding process.

So, in that case it is also necessary to understand what is thermal expansion or that related property coefficient thermal expansion is necessary to explain the different kind of the thermal strain or residual stress strain associated with a welding process better to explain all these phenomena. Now thermal expansion we say change in volume with response to the change in temperature associated with the [vocalized-noise] change temperature and this change may happen in a very localized area.

It creates the thermal strain in solid definitely there is a change with the application of the temperature or presence of the temperature gradient then definitely it clears some kind of the thermal strain in a solid.

Now degree of expansion per unit change in temperature is simply defined the materials properties these properties we normally measure that is the coefficients of thermal expansion that we measure, but even the coefficients of thermal expansion can also vary with respect to temperature; that means, the different temperature, the coefficients of thermal expansion may also differs.

So, should have some knowledge about the coefficient of thermal expansion value in this perspective.

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Now, if we look in to the mechanical properties of a particular material that we define this different material properties or we can evaluate with this different material properties. One is the strain; the change in dimension per unit original dimension. So, with the application of the mechanical load or with the application of the thermal load in a structure; what is a change in dimension per unit with respect to the original dimension that indicates the strain.

Similarly stress can be defined applied force per unit area and stress can be mode normal stress as well as the shear stress. So, normal stress can be defined in such a way that application the load is applied which is perpendicular to the surface of a particular material. In that cases the stress is defined as a normal stress.

And shear stress means, applied load is parallel to the surface of this particular material. So, in that case this is also define the stress load divided by area, but in this case the area can be defined that load and area are parallel with respect to each other. So, this way we can differentiate what is normal stress and what is shear stress value.

So, that knowledge is required may be to understand the different modelling approaches ah then elasticity can be defined the we know the elasticity means if we apply the load particular component and after removal of the load it will come back to the initial position.

So, that property is call mainly defined as a elasticity, but why elasticity is important? Because elasticity can be defined such that it helps to define what is the yield stress; that means, if you cross that value over that value then material deforms there is a permanent deformations we can observe in a particular components.

So, that is why property of the elasticity is defined in that way. Then plasticity simply we understand the if there is a permanent difference with the application and then plastic deformation will happen in the structure if it cross the elastic limit, then only plastic deformation we can observed. Then toughness is the property of the material to resist fracture due to the high impact that property is associated with the if there is a impact load is there then how much energy is observed before fracture that is the measure of the toughness.

So, that toughness properties is is also necessary to define in a particular metal to understand that how metal behaves with the application of the dynamic load or may be impact load. Then resilience is the what is the amount of the energy when deformed elastically and release upon the unloading. So, when elastically deform the material then when you release the load then it will release the some amount of the energy.

So, that energy is the measure of the resilience, but of course, the deformation should not cross the elastic limit it should be below the elastics limit; that means, resilience is associated with the amount of the energy elastically not with the plastically.

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Similarly, another important parameter is the creep properties. So, creep properties is another important parameters when the material is [vocalized-noise] having some application and the high temperature application. So, at high temperature at the same time it is associated some amount of the constant load, then creep properties is important. What we can define?

The material is subjected to a constant load stress at elevated temperature for a long period of time; that means, it creates some slow and permanent deformation in the structure. So, that indicates the creep properties.

So, creep properties is properties at elevated temperature subjected to constant load normally in that way we can define the creep properties. Now tensile specimen elongate continuously until rapture occurs even the application of the stress below the yield point. So, it is like that only ah suppose one sample is in the room temperature and then you apply there is a application of the load. So, metal will deform plastically once it cross the elastic limit.

But creep is different because creep even it is not reaching the yield point then then permanent deformation may happens in this structure and this is the, but this creep property so we define what that means this permanent deformation at constant load is there below the even it is below the yield point that may happen at the high elevated temperature.

So, that is why it is a normal temperature, the room temperature creep properties may not significant, but metal is having application at the high temperature then creep properties is important or creep properties significant. So, in that case we can analyse the creep properties. For example, gas turbine, power plant, high temperature pressure vessel when you apply we choose particular material in this particular application then definitely it is important to know what is the creep properties of this particular material.

Similarly fatigue also other properties when metals is subjected to some kind of the cyclic loading conditions in that cases the failure may happen even it is the yield point of a particular material. Why it is like that? Because yield point we normally measure as a simple tensile testing machine. So, simple uniaxial tensile testing machine we measure the yield point for a particular material.

Now once wants the load condition because in tensile testing machine there is a we put the continuous load and the rate may be very slow so; that means, almost study state it reaching. So, in that condition we measure the yield stress. Now when the load condition changes them it is not necessary the metal will behaves same as what we got in the simple tensile testing normally done at room temperature value.

So, that is why fatigue also we can define this one [vocalized-noise] property is a kind of properties when there is a application of the cyclic load in a on this material. So, it may fail below the yield point stress. So, basically in that cases the endurance limit we normally evaluate in a during a cyclic loading of a structure. Also the hardness properties also define the resistance to the scratching or resistance to the wire based on that we can measure the hardness of a particular material.

So, all this mechanical properties is also important and sometimes it is necessary to define hardly beforehand if you try to develop particular model. So, this values of all these material properties may be important and sometimes all this kind of mechanical or other physical properties as a function of temperature is also required when you try to develop the model of the welding process. So, that is why we discuss all this different kind of the properties of the materials.

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Property evaluation Physical properties: Standard experimental methodologies **Microstructural measurement:** Average grain size and distribution - line intercept method Residual stress - X-ray diffraction (XRD) method, Neutron diffraction Chemical composition of a metallic sample - Energy Dispersive X-Ray Analysis (EDX) Various phases in component - XRD method

And of course, discussion is mainly focused on the; I just forgot to mention that it is focused only on the metallic materials. So, we will not focus on the what is happening all these modelling approaches is particular to the polymeric or plastic material. Now, what way we can evaluate all these?

So, we now we understand the there are several properties are there which is associated with the material and it can be thermal properties, it can be mechanical properties and may be other properties, but what we can evaluate this properties how we can measure all these properties.

For example, physical properties; there are standard experimental methodologies are there and that we can get any reference we will get what are the different and standard methodologies to measure the different physical properties. So, that is not in the scope of analysis for this in in this process in this module.

Now we can look into the microstructural measurement can be done that in this sense the average grain size and distribution we can use the line intercept method can be used to understand the average grain size and distribution.

Apart from that residual stress we normally use the XRD method, X-ray diffraction method commonly neutron diffraction method can also be used or other mechanical methods can also be used to measure the residual stress also. Then chemical composition of the metallic material normally use the energy EDX analysis and even various phases in a particular component some XRD method can also be used.

So, here apart from that other physical properties; for example, universal testing machine what we can measure the hardness properties this is while said and while understood [vocalized-noise] available. Apart from that we can there are several other methodologies what we can about the different we can characterise the microstructure get their phases in a particular component or samples which is process by following some kind of the manufacturing process and here it is a specific to the welding process.

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Other properties also in associated with the modelling approaches for example, latent heat of material. So, it is associated with the phase change from liquid phase to solid phase or vice versa. So, from solid phase to liquid phase or latent heat of solidification, both are important that can also be measured.

Then apart from that thermal diffusivity is a one significant parameter which is open used in the heat transfer analysis. Then viscosity if you want to look into that the fluid flow analysis then viscosity property is necessary. Then electrical conductivity and resistivity. In this case this electrical conductivity or resistivities may be useful when you try to look into the modelling approach in case of the resistance of resistance spot welding processes, there it will be this property is useful there.

And the whatever we can generate the heat that we can relay just looking into the electrical resistivity property. Similarly, magnetic properties is may be significant if you try to analyse the induction welding process. So, all these properties having may be this specific properties is may be significant associated with particular welding process.

Apart from that in machining welding and casting in general we can say that thermal properties of the work is important parameter is very important in machining, welding and casting. If you look into the case casting and the welding process the there is a material flow is there and solidification is also there. So, once the material flow is there basically have some idea about the what are the fluid properties is associated in the flow of the material associated with the casting and the welding processes.

Apart from that semiconductor manufacturing there it is also necessary the electrical properties of the silicon is important parameter, they are the electrical properties is important in this particular manufacturing processes. Apart from this for example, mass diffusion coefficient. This particular property is important in case of the surface hardening or when you try to analyse the diffusion welding process; we have some idea what is the mass diffusion coefficient associated with this welding processes.

So, we can see that when you try to analyse the different welding processes and then it always associated some kind of the physical properties of these things and that physical properties in some point of time is possible to measure using some standard methodology or standard experimental techniques are there and by following that things we can measure the physical properties of this particular welding process or other kind of the manufacturing processes.

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Now, once you understand the different properties all these things which property is important at what type of the welding processes or what kind of the analysis. Now it is also important to understand that what are the different physics based modelling approach. Because here the core structure we say finite welding modelling of the welding processes, but to understand the welding processes, when you try to develop the finite element welding processes we need to understand what are the physical mechanism or physics in a welding process is involved.

So, to understand that now we will try to discuss the different perspective in the since what are the different physics based modelling approaches normally we follow and overall in this modelling approaches, that will helps to understand to get overall view of the different

modelling approaches or definitely physics based modelling approaches and then will be easy to apply in kind of in specific with the welding processes.

Now what are we represents the general format to represent the physical system. The we normally represent the physical system assuming there some equilibrium system exist. When we assuming the equilibrium system, then from there it is associated with some kind of the governing equations along with the boundary conditions are also there.

Now even it is not equilibrium system if it is dynamic system also then also it is possible to represent the dynamic system in the form of a governing equation of course, in this cases the we analyse the kinematics for this particular process and it also form the governing equations.

Now once we represent the system assuming it is a either in the form of equilibrium system or either in the form of a dynamic systems all we try to represents the in the form of a governing equations. Now finite element is the tool once we represent the governing equation. So, tool will help to solve this particular governing equation by using the specific boundary conditions and that boundary conditions may different from the different processes.

For example, the heat transfer analysis may be associated both in welding processes and heat transfer analysis may associated with the machining process or casting processes. So, all these processes we will be solving the same heat conduction equation, but since process are different their boundary condition can be different and finally, we will be getting the temperature distribution.

So, that is way we can develop in particular system, then we define the governing equations, then we try to find out the what way we can solve this [vocalised-noise] governing equation such that we will be able to solution of this equation in the form of a some intended variable. So, in case of heat transfer analysis we will be getting the temperature distribution is in case of fluid flow analysis we will be getting the velocity distribution in case of stress analysis or thermomechanical model we will be able to get the temperature as well as the displacement field both will be getting from a couple thermomechanical analysis.

So, but all these cases we have to develop either in the form of a governing equation and some cases it is also necessary to develop some kind of the constitutive relation we will coming that point also.

So, some system we represents the in the form a constitutive equation along with the some cases we need it in a we try to represents there is the there are some variables may be they relate following some constitutive relations apart from that definitely we already mentioned that some essential or natural boundary condition has to be depend associated with the particular process.

And also need the initial condition means; if we are solving some transient problem then some initial condition has to be defined. Now what we can look into the constitutive relation between the different two physical quantities and actually the constitutive equation when it relates between the two physical quantities.

For example, stress and strain relation we relate between stress and strain that different from assume the constitutive relation, but it may not follow some directly follow the physical laws.

Apart from that it can be combined with the other equations such as equilibrium and kinematical equations. So, that constitutive equation can be combined with the equilibrium and kinematical equations will show that what we can formulate the stress analysis model in the associated with the welding process.

And there we will able to explain that how the constitutive equation are basically linked with the equilibrium and kinematical equations to solve some kind of the to represents the physical laws associated with the particular process.

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Physics based modelling approach

The constitutive law parameter can be derived from experimental observation - called phenomenological modelling

- \checkmark The methodology is to explicitly include variables from physics as internal state variables
- \checkmark The other possibility is to determine the format of the constitutive equation based on knowledge about the physical mechanisms causing the deformation (For example, Failure mechanism)

An alternate to phenomenological modelling is to derive constitutive equations from low-scale where laws of physics is well understood

For example: parameters for grain size models for microstructural evolution

Now, constitutive law parameters it can be derived from the experimental observation; that is possible to do and this normally call the phenomenological modelling. So, experimental observation what we can do these things, the methodology is to explicitly include the variables from the physics as the internal state variables. For example, suppose we want to discuss the recrystallization model, recrystallization phenomena we want to explain that happens in the particular grain scale or meso scale modelling approach.

So, in this case that we can take the what are the dislocation density walls this particular as a function of temperature extended or only the deformation only the strength. So, this here we can incorporate the grain size evolving with respect to the in the recrystalization mechanism as a internal state variables or this density can be represent as a dislocation density can be represent as a state of internal that is called the internal state variables.

And how it evolves? We can track on these things and this internally depends on the phenomenological behaviour normally happening in to the recrystallization process. So, it means that phenomenological modelling can be done and we can look into the constitutive laws which can be represents as a function of some internal state variables and certain parameters we can measured experimentally, that is also possible and ah by doing some experiments.

We can give this way or this is a one way other way possibility of the format of the constitutive equation. For example, we assume some particular in material science, in particular process we uses the Arrhenius type of equation that link the stress, strain, [vocalized-noise] temperature and particular may be some internal state variables we try to evaluate these things. But in this case when you represents particular process using this equations Arrhenius type of equation but it is associated to with some amount of constant term.

So, to evaluate this constant term it is necessary to do some kind of the experimental and that particular scale may be grain scale we need to do some kind of the experiment. So, that we can define this parameters. So, this is a another approach and here with giving some example also constitutive equation based on the knowledge about the physical mechanism. For example, causing the deformation in case of fracture failure mechanism.

How the material fails and it is the particular ah with the application of the mechanical load that in this cases if we look into the physical mechanism and we can look back some constitute relation the material behaviour we can represent or some internal state variable. So, can we can predict the failure mechanism using some kind these kind of modelling approaches phenomenological modelling approaches.

Now apart from this and alternate to phenomenological modelling is to derive the constitutive equations we can derive the constitutive equation, but which information from the low scale. We can get the information from the low scale or we are analysing the what is happening at the low scale lower scale taking the information from that then we can develop some kind of the constitute model that is the another route also.

At, but at the low scale they are following some kind of the physics particular, but therefore, some physical law it is following in that particular and then that physical law has to be understand bit carefully if we want to develop some kind of the lower scale model and the taking the information from the low scale to develop some constitutive model in the next scale that upper scale model. Here you we can give some example parameters for the grain scale models can be used for the micro structural evolution.

So, this can be one example of the that using the lower scale information to develop or to derive some kind of the constitutive models by understanding the physical mechanism involve is a particular low scale approach.

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Now, we can give one example also; for example, determine the material property Young's modulus, we know that Young's modulus we can from the experiment we can easily determine the Young's modulus simply we can do that simple tensile testing for a particular sample. And that parameter or that value Young's modulus is may be significant to develop some kind of the mathematical model and that mathematical model is basically represents the material response.

So, to do that we have some knowledge, with some data associated with the Young's module for this particular. It means that some particular parameters is some particular properties has to fed to the model, such that it will be able to predict the similar kind of the behaviour. So, that means; we cannot exclude the experimental procedure completely once it when we try to develop some kind of the mathematical model. We need some information from the experimental analysis as well.

Specifically from the experimental analysis which what kind of material properties we measure that can be input to the numerical model. Now, micromechanics model take into account more detail about the material structure at the grain scale. Definitely what we can measure the macro scale universal tensile testing we can define different parameters, but that may not be able to explain what is happening at the ah micro scale.

So, therefore, if we able to track for the micromechanical behavior at the micro scale the behavior of the grain they are interacting, how they are growing is there any nucleation or all this phenomena grain scale structure if we analyze all these phenomena and then making the average properties all these things that is the representation of the material response at the next scale may be in the continuum scale.

So, therefore, the properties at the micro scale is basically averaged and passed to the continuum model is through homogenization theory segments micro scale model we analyze all these things then information passed in the average properties values is passed to the next scale modelling approach.

So, in that way there is a development of the different multi-scale model is there and it means that it is necessary to analyze what is happening each and every scale will try to look how there is a development of the micro scale and the what are the different approaches also try to look into that.

Now micromechanical model can also provide some vary local variation particular which may not be able to capture this variation in the local variation or of the properties at the next scale may be continuum scale to look into this variation.

So, therefore, is a simpler continuum model is also possible to develop simply by taking its a what is the information happening in the micro scale and we simply averaging this phenomena at the micro scale and all properties values and this gives the input to the continuum model to develop the or to get the output from this particular model.

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That is why multi-scale model at the different length and time scale can be divide in broadly in this four categories the four length scale in the multiscale materials modelling. Here you can see that starting from the electronic structure. Electronic structure basically exists in this thing at the very lower scale in the may be nanometer or less than nanometer scale.

There look into the electronic structure of particular material then we will predict something by looking into the electronic structure, but we cannot directly predict the link between the continuum model from the electronic structure. Now if we analyze the scale. What is happening in the next scale?

Then atomistic scale scale may be it is on the range of 10 nanometer in that scale, that is molecular dynamic simulation. If you do the molecular dynamic simulation we take the information from the electronic structure then we will predict some behavior, but that prediction of the behavior is basically valid at this particular scale in the molecular dynamic scale in that nanometer scale basically. Now, if you understand the microstructure model if you using some for example, finite element method.

We can take the input from the molecular dynamics taking at the input for the microstructure model then it is possible to predict more precisely the microstructure in a for a particular material. And then if you see the microstructure analysis or this model can be develop the higher scale, maybe we can say the in the range of the micrometer scale.

Then continuum scale; that you can use the safety method also or may be finite element method can also be use the continuum scale can be applied, but is a analysis properties is basically the resolution of the properties in the continuum scale means is the millimeters scale may be millimeter scale we are doing all these analysis. That means, the resolution of this modelling approach at the continuum scale able to predict what is happening at the millimeter scale.

But if you analyze the continuum scale of you look develops some model in the continuum scale it will not be able to predict what is happening in the electronic structure; that means, with the atomistic scale that is not possible to predict what is happening at the lower scale.

Now, this multiscale modeling approach is possible to develop, but our model most of the cases we normally we analyze our focus is not the this is the lower scale model, but our focus is what is happening in the continuum scale model using the finite element method; that means, what is happening at the millimeter scale, all these things.

Because most of the material properties we normally measure at the millimeter scale for example, in Young's modulus what is the yield point this is nothing to do with the at the this is not able to predict the properties this is not associated with the microstructure may be micrometer scale, but this properties is very much associated with the millimeter scale.

So, that is why that properties we measure it this is useful for the development of the model in the continuum scale or may be in the millimeter scale model.

So, multiscale modelling is the there are several approaches are also there, but I am presenting here in such way that we get some idea that over all idea; what are the different modelling approaches may be you can follow to understand the processes and what particular processes, what is the necessary, what is the limitation of a particular process in the modelling approach and what is a resolution of this particular model or at the what scale we can analyze all these phenomena.

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Now, what is the importance of the multiscale methods? Multiscale method is simply what we can link at the different scale; that is the multiscale method. But there is a limitation of industrial simulations today; first is the continuum models are good, but not always adequate because problems in the fracture. Basically by continuum scale we will not be able to understand what is the mechanism of the fracture or failure for at particular material of solids.

And in this cases most of the cases we can use some kind of the constitutive relation models to describe the material behaviour.

Then we will be able to explain these thing in the continuum scale, but when you analyze the material behaviour the constitutive model should describe the material behaviour then we have to going back to the next scale level modelling approach. For example, to understand the what is happening in the microstructural level then we will be able to predict the fracture and failure mechanism using the analysis only on the continuum scale.

Similarly, macroscopic material properties of the new materials and the composites are not readily available. We have we necessary for a particular new materials going to analyze going to develop the model then we should know what are the material properties of this particular metal at this particular scale also and then it is possible to develop some kind of the simulation.

And next detail atomistic trans information is required in regions of the high deformation or discontinuity. So, therefore, if you want to predict using the continuum models high particular zone on the deformation zone or discontinuity or deformation happens, why localized deformation anything we want to predict all these things; it is always we have to link with the previous scale modelling approaches. It may be atomistic scale, it may be microstructural scale all these information is may be required.

So, that we can develop the continuum models in the more precisely. So, that information is required. But question is that, what we can interface the one scale to another scale model. Because time scale all these thing are different and the analysis are different the analysis physical law, physical behaviour are different at the at two different scale.

So, the main challenge is the linking of the different scale to develop a multiscale model. Another example we can take the molecular dynamic simulation. For example, that is the one continuum scale this is the higher scale may be in millimeter scale and the one is a molecular dynamic simulation in the nanometer scale.

In this case what we do? Limited to very small domains it has to be covered we normally consider only 10 to the power 6 to 10 to the power 8 atoms and small time frames only the nanosecond level that kind of analysis can be done in the molecular dynamic simulations.

But at the same time if you want to do even molecular dynamic simulation and it is also required some kind of the experimental data to do the simulation and, but all this experiment has to be done in the nano scale also, because we are analyzing we are developing this model at the nano scale level.

So, therefore, properties would be depend at the nano scale. So, definitely; obviously, the main difficulty is the all to at the develop or to do some kind of the experiments are the nano scale is the very much expensive. So, that is why in that sense it takes much larger time, long time, costly experimental setups are required to get all these properties in the molecular dynamic simulation. So, that is why these are the different challenges normally we face in case of the at the lower scale modelling approach.

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Now, it just definition which on the hierarchical approach and concurrent approaches. So, hierarchical approach use the known information at one scale and to generate the model for the larger scale. Basically we get the information in the lower scale and the supply this information to the larger scale to develop that model.

Information passing through the some sort of averaging process already explained when you try to link one to different scale the one is the lower scale which simply making the properties in the average and then we feed to the properties to the next scale to get the good simulation for these things. Example bonding models, potential, some kind of the constitutive models it is a microstructure constitutive models we develop and that model we fed to the continuum scale we use this thing.

So, that in the continuum scale we will be able to get good very good model development. Similarly concurrent approach means in this cases perform simulation and different lengths scale simultaneously, but in this cases the relationship between these two scales are dynamic, mostly two different length scale are very much in dynamic in nature. So, basically in that sense it clear some kind of the difficulty because it is a relationship completely dynamic in that approaches.

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Continuum methods therefore, this method is assume that the matter is continuous and this treat the properties of the system as a field quantities. Numerically solve the balance equations coupled with the phenomenological equations to predict the properties of a particular system.

So, when you try to get the properties then we have to follow some kind of the phenomenological equations and that equation from that equation we evaluate the properties and we can fed to the continuum models and this is the already discussed this is the milli scale model. Now advantage disadvantage is that for example, in principle handle the system of the macroscopic size.

So, everything is defined in the macroscopic scale and of course, dynamic processes can be solved using this or continuum methods, but it takes relatively longer time. So, dynamic problems can also be solved in this case.

But difficulties is that; require input for example, elastic tensors different coefficients, diffusion coefficients, equations of the state all these kind can be the input to this distance and most of the cases with the coefficients value elastic components may be this most of the properties can be evaluated experimentally that data is required.

Either experimentally or some polynomial time it may be required to the data from the lower scale method; that means, macroscopic scale method we can follow in that micro scale model from there some data is required for these things we sometimes is very difficult and it may be required extensive experiments or simulations is also required. So, that is the main difficulties in this continuum methods.

Apart from that it cannot explain the results that depend on the electronic or molecular level of the details. So, certain structure all these thing that depend on the molecular or electronic level then that particular that it is the continuum methods cannot explain that kind of in detail or material viewer of this particular material which depends on the entirely depends on the or dependent on the lower scale detail.

Multi-scale model

Connection between the scales: Upscaling

Using results from a lower-scale calculation to obtain parameters for a higher-scale method. This is relatively easy to do; deductive approach. Examples:

• Calculation of phenomenological coefficients (e.g. elastic tensors, viscosities, diffusivities) from atomistic simulations for later use in a continuum model.

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Connections between the scales it can be that upscaling and downscaling with two different scale, there are two approach in the connecting to difference scale; one is the using the results from the lower scale. Calculation to obtain the parameters for the higher scale model method and this is called the upscaling these things. And this is relatively easy to do and it is also called the deductive approach.

For example, calculations of the phenomenological coefficients for example, elastic viscosities, diffusivities and from atomistic simulation for the later use in the continuum model. For example, this is the deductive approach for; that means, it the simply where evaluate the properties from the lower scale simulation atomistic simulation and then that data we are feeding to the upscaling; that means, higher scaling at the continuum scaling method or continuum scaling model.

So, this is called the upscaling. So, simply that upscaling means using the data taking the data from lower scaling to develop the model in the upper scale.

Similarly, downscaling using the higher scale information to build the parameters for the lower scale method and of course, this is more difficult due to the non uniqueness of the problem and we can give some example also, but it is a few cases; that means, for example, results from the mesoscale simulation definitely mesoscale simulation or grain scale simulation do not having the atomistic details. Therefore, it would be desirable to be able to use such results to return the atomistic simulation in some information in some point of view.

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It is possible to get the what is the information in this mesoscale simulation. Some parameter is sometimes useful to develop the model or information from this mesoscale passed to the atomistic scale. And then that atomistic scale method can be useful, but it is not a very precision or good approach to follow all these things and this is also called the inductive approach.

We can give an example also. For example, stress strain curve for randomly oriented polycrystal we can know that is stress strain curve for an randomly oriented polycrystal is easily to define if we define this oriented polycrystals, but this information stress strain curve can be used to predict the shear stress and shear strain curve for a single crystal structure.

It is basically higher scale to the information persists from the higher scale to lower scale approach; that means, it is a one example of the downscaling approach or we can say the [vocalized-noise] ah inductive approach. Here if see that x there they are having some relation between these two shear stress and shear strain in the term of the Taylor factor and here the normal stress and the shear stress can be used using the Taylor factor.

So; that means, the using this higher scale; that means, data at the higher scale is the stress strain curve randomly oriented polycrystal this is probably is possible to fetch to the lower scale. So, that we will be able to predict the single crystal, because experiment for the single crystal structure and evaluate evolution of this stress strain diagram of single crystal structure is more difficult.

Rather I say that polycrystalline material the evolution of the stress strain diagram is little bit easier. So, the in that sense this is one of the example for the inductive approaches.

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Now, what is the challenges in the multiscale modelling? In general we can say the large number of degrees of freedom at the atomic scale. So, it is more computational time is involved, more computer basically is involved in this case. Then interfaces; what we get represents the interface? That is also another challenging task. So, there may be possible return mismatch of the dynamic properties and other issues because of the improper defining of the interfaces.

And of course, some it is very difficult to averaging in sometimes because there are multiple time scales are involved in this multiscale modelling approaches. Interdisciplinary nature of the multiscale method. For example, continuum mechanics is involved at the same time classical particle dynamics lattice mechanisms may also involve quantum mechanics mechanisms and quantum chemistry also involved thermodynamics strategical physics.

So, linking all these one scale to another scale is basically difficult at the same time the handling of all these kind of the different scale as a single platform is very difficult to handle basically. For example, atomistic, scale plasticity, lattice dislocations may be different mechanism physical law as follow as compared to the, but we know the continuums plasticity bond mesoscale yield criteria and then plasticity model in the continuum scale can be different or should be different from the atomic scale plasticity.

Then what we can link all these things? That is the one of the main question mark I can say associated with the linking of this different scales.

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Now, some little bit on this statistical because we have discussed the different physical based modelling approaches and this physics may be involved at the different scales also and what we can link all these scales that is the physics based modelling approaches that was. Now

what is the statistical and data driven modelling approach? This is different aspect to make you understand that how the different modelling approach which is different from the any kind of the physics based modelling approach.

So, statistical and data driven modelling approaches may be the most important first is the what we can call it the data from the sensor. May be from the through experiments we can collect the data and then we analyze the data, such that we can link the input data to the output data, but it may not follow any kind of the physical law involved. It is simply that what we this is a handling of all the several data by means of some kind of the statistical relationships between the input and output. That is the overview of the statistical and data driven modelling approach.

Now, sensor to provide the data any kind of sensor can be used through the data acquisition system. Then, in the it can be in the form of the current voltage or directly temperature may be I have talking about the in prospective of the welding process. So, sensor data can be used for online monitoring as well also, but it may be collected the data and then for online monitoring it is passes through the robotic system. So, that we can monitor the system on the online monitoring system.

So, that way we can use or other way we can offline we can analyze all these sensor data, but there is a necessary to collect the data through the data acquisition system and then storing of this data. One example of the sensor acquisition data is that for example, measuring of the temperature. Now we can use the thermocouple or non contact mode for example, thermal vision camera or may be infrared camera method both are can be used to collect the data, but infrared camera uneven surface thermal emission becomes an issue.

So, that is the one difficulty of infrared thermometer, but however, we can use the data infrared thermometers is more reliable as compared to the thermocouple, because infrared the thermometers having the faster response as compared to the thermocouples. So, once we try do decides the online monitoring of the systems then its better to acquire the data from the infrared camera as compared to the thermocoupled data. So, that is the difference of the collecting the data and what kind of the sensor we can use for a particular process.

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Now, once data acquisition. So, sensor data is collected some sample rate basically data and we can store in the buffer or temporary memory and it depends on the what way we can sample rate and transfer of the data is controlled by the CPU or the microprocessor; that means, rate per unit time how many data's can be collected that is decided by the CPU or microprocessor it depends on that.

But, my point is that its a one important parameter to consider for a particular when you try to use some kind of the sensor to collect the data.

Now, once the discrete data points has been collected evaluated through the different property evaluation techniques, that now the next step is the what we can evaluate all these data; that means, what we can analyze the data to develop some kind of the mathematical model that does not deal with the some kind of the physical laws in this process.

For example, the strength properties of the weld joint or hardness and the surface roughness of a machined surface can be linked input parameter because, where in stress strain what is the weld joint properties.

So, we can conduct the experiments at the several input process parameters several experiments and we can experimental level at what are the joint properties. Now, we have this data. Now we just correlate between what is the input and what is the joint properties like that. Same thing may happens also measuring process also surface hardness and surface roughness with measuring surface with respect to this the input parameter. But how to link between the input and output parameter? There are several techniques; we can look into that one example that is called the process modelling and optimization.

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We take one example pertaining to the welding process. The what are the few approaches. So, sensor integration method; that means, it is a collection of the data and analysis of the data method. We can use any artificial intelligent techniques also. We can use several data based techniques; that means, some statistical methods we can use it.

We can use the vision system based method; that means, we can collect the data based on the vision; that means, we can capture the image as a data and then we analyze the data to find the some kind of the correlation.

Now, for example, the modelling of the weld quality using the main spindle motor current signal. So, we can in friction stir welding process we can model the weld quality; that means,

we can evaluate the weld quality, but during the process we collect the data from the motor current signal.

Similarly we can collect the data machine vision based system we can put the camera and from the we can collect the data if there are any defect all these things we can use this data image and we can analyze the image also in the form of a data. And modelling of the weld quality using the sensor integration techniques different sensor data for forces.

For example, we can use the force data also, the force signal in the we collect the data and stored the data and at the same time torque the data from the measurement of the torque in FSW process. So, this is nothing, but the different ways or the putting different sensor. So, we can collect the data.

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And then we can analyze by using the different methods to get the illusion between input and output; that means, few research techniques for example, wavelet packet analysis can be done of all these data collecting data. Hilbert Huang Transformation with the wavelet analysis can be done we can apply the fractal theory also. We can use artificial neural network, we can use support vector machine. So, these are the different techniques we can use to analyze the data to reach some kind of the input and output relationship.

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Now, it will be more easier to understand that what we can do the process modelling and optimization these things ah. We can take an example of the MAG metal active gas welding process and here what we can establish between the input and output relationship. We can simply the regression analysis which is collect the data and as per Taguchi design of the experiment and then we can do the, but regression analysis then we have to look in the ANOVA table also ANOVA method to get all these datas sets statistical data here.

Now, this regression analysis model was basically embedded in the optimization algorithm and then to determine the optimal process parameters.

So, we can link some optimization algorithm also to determine the optimal process parameters in this cases for weld bead geometry specification in this cases suppose we can get the input parameter for MAG lwelding process and we can link the with the what is the weld bead geometry specification. And which geometry to achieve particular geometry what should be the input parameters that can be done using some kind of the optimization algorithm process.

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Now, input parameters can be in a MAG welding process and for example, welding speed, welding voltage, wire feed rate nozzle to plate distance torch angle. This can be done and the output parameters at the different responses for example, a height bead width bead penetration these are the output parameters.

And of course, we can design the experimental also if you follow the full factorial design then huge experimental data if you follow that Taguchi design of experiment then we can define the limited experiments in this case.

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Now, if you use some kind of the combination of optimization technique. For example, genetic algorithm, differential evolution, simulated annealing in this cases we can choose any kind of the method and then set of mathematical equations can be done. For example, linear curvilinear or logarithm equations.

So, we can give the input we do not know which equation is better feed to feed the data then therefore, development of the model relationship between the process variables and the weld geometries can be done in the particular welding process.

Now, optimization algorithm determine the optimal values for the process parameters with respect to any given bead geometry. For any given bead geometry this is the input and using the relationship between input and output some statistical relation then optimization will predict the what is the best input parameters if you want to achieve particular bead geometry. So, that is the purpose of this optimization in this particular process.

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Now, Taguchi DOE is basically adequacies of the models and variance within the confidence less than 95 percent and correlation factor for these models is normally we get the all the data form the ANOVA table. And then choose the superior model among all these parameter all these relationship. For example, we can use the linear curvilinear logarithm and based on that we can choose which relations is better fitting between the input and output data. Therefore, few experiments are used to test the mathematical model to get these things.

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Now, mathematical model provide one to one relationship between the process variables and the weld dimension and it can be used in the two different ways; one is the predicting bead dimension based on the given welding variables. Suppose this is a welding variables, I can give the predict the what is the bead dimension.

In other way also using this relation between the input and output variables if I want to predict that achieve particular bead dimension what should be the input parameters. That information can also we get from this data driven this modelling approach.

So, may be this modelling approach is easy to only analyzing the data all these things, but it does not follow these things. So, therefore, if there is any physical law is involving this local variation of particular govern by process particular there is a change of these things drastic change or the parameters governing the physical law then that kind of phenomena is basically not possible to able to achieve or to capture using this data driven modelling approach.

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Now, in summary for the module 1st lecture of this module 1 we can say that we have discussed the properties of the engineering materials, then we discussed the multiscale modelling approach, the different hierarchical approach may be lower scale to higher scale is the most preferable approach because we use the information lower scale to develop the higher scale model.

It will be easier for these things and of course, multiscale modelling approach each and every scale when you try to look into the particular scale, it is also necessary to do some experimental data is required at this particular scale.

So, that is why it is maybe the challenging into the sense that to link between the two different scales is the most challenging task in case of the multiscale modelling approach apart from this computational time for a particular multiscale model.

Also we have discussed the physics based modelling approaches what are the physics based modelling approaches and definitely we understand that physics based modelling approach we have to understand the what are the physical mechanism involved in this particular process then it will be easier to develop these particular physics based model in pertain to any kind of the manufacturing process.

And finally, we discussed the data driven modelling approach and I hope the difference between the data driven modelling approach and physics based modelling approaches, there is a difference is there and having some limitation of data driven modelling approaches also with respect to the physics based modelling approach.

So, that is why our whole part or analysis of this particular course will be following the physics based modelling approach not the data driven modelling approach.

So, thank you very much for your kind attention.