**Thermo-Mechanical and Thermo-Chemical Processes**
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**Lecture-20**
**Constitutive Analysis: Case Study**

Hello friends we are continuing with our discussion on constitutive analysis. Today I am going to take one case study here. So, we have already discussed how to develop constitutive equation and what are the different constitutive equations for different material processes. This case study is basically our own work and one particular thing we were trying to highlight that is what is I am going to present here.

So, this work is on actually on zirconium niobium alloys. These are some structural material for nuclear plants so the zirconium niobium tubes are there in the nuclear power plants where the fuel bundles are kept. So, of course if you want to know you can look at it on the internet there is lot of literature available on zirconium niobium alloys. So, the processing of these alloys is one of the main issue we were trying to understand.

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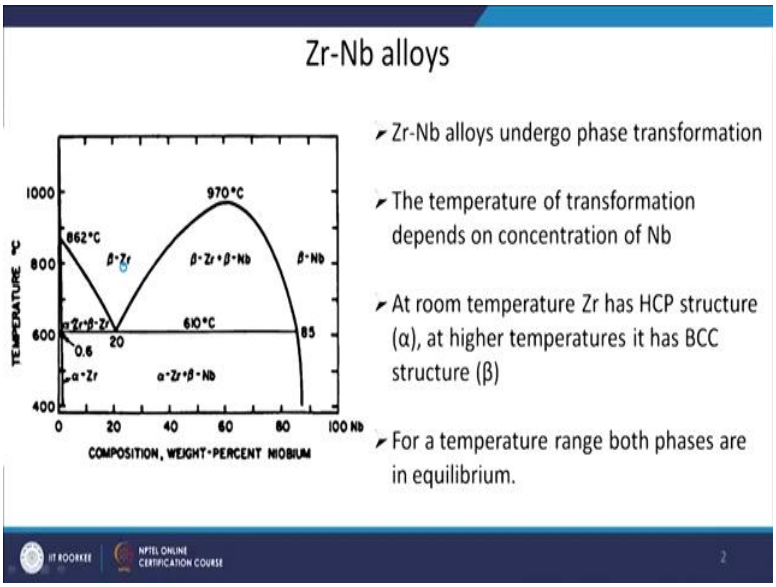


And there is one phase diagram is shown here for zirconium niobium alloys. Of course, niobium is increasing in wt. % in this direction and on the y-axis, you have temperature and of course it has two different phases. The α-phase which is stable below 600°C that has HCP structure that means hexagonal closed pack structure and the β-zirconium which is stable at higher temperatures it has body cantered cubic, BCC structure.

So, there is a of course a phase transition and the two phases will be in equilibrium in the temperature range and of course this temperature will change as a function of percentage of niobium. So, the idea is that you have two phases in equilibrium in this particular temperature range from 600°C to somewhere between 800°C. Usually the alloys which we studied was zirconium 2.5 niobium or zirconium 1 niobium.

So, you can understand the complete transformation to β-phase will happen somewhere around 850°C. So, we studied the whole transformation range here for deformation behaviour and what we saw in the literature is that people are developing constitutive equations without taking into account different phases present at different temperature. So, for example I can do deformation at different temperatures here all these what I am pointing are may be let us say temperatures (refer to above figure).

And the constitutive equation will be developed for all the temperatures together without taking into account the different crystal structure present at different temperatures and that we feel is going to put lot of error in the calculation because different phases behave in a different fashion. Their dislocation glide phenomena of course slip system will change, diffusional values will change depending upon the phase with the crystal structure which is there.

So, we proposed that we should develop constitutive equation based on the phases present. So, we should develop one constitutive equation for β-phase for example, one constitutive equation for α+β phase i.e. two-phase region and one constitutive equation for α-phase. So, independent phases and incidentally the most of the processing which takes place for these particular alloys is in the two-phase region. So, this region is important for processing.

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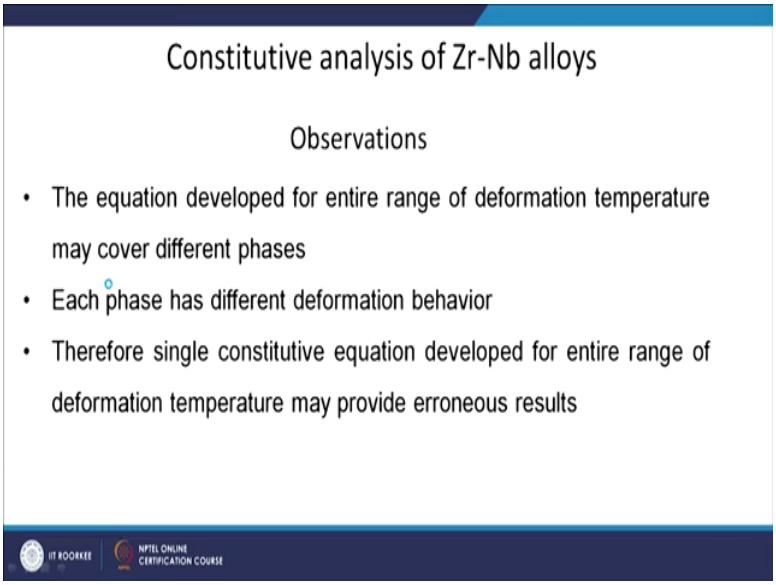


So, observations which we found out from the literature that the equation developed were for entire range of deformation temperature as I told you which covers different phases. Of course each phase has different deformation behaviour, therefore a single constitutive equation developed for entire range of deformation temperature may provide erroneous result. So, when we develop this constitute equation and then we will use it for some modelling.

The modelling will not be able to give you accurate output that is what we felt. So, what we provided as solution that constitutive equation should be developed in as a function of phase that means different phase region should have different constitutive equation. Now, how to know that whether what we are doing is correct or not and that we try to validate it using some FEM simulation, the constitutive equation developed for different phases.

And basically, prediction of ram force for hot extrusion was used as a process to simulate these constitutive equations were used there and we try to simulate and try to compare the result with actual data. So, that is how we were trying to validate whether what we are doing is correct or not.

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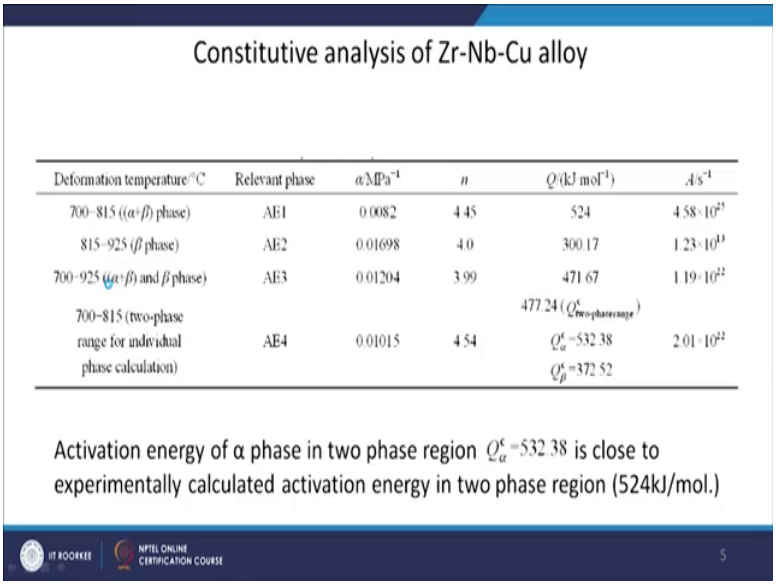


So, for example first work which we did was on zirconium niobium copper alloy, 0.5% copper is there zirconium 2.5 niobium and these are called ZNC alloys also. These are all published literature. And the deformation temperature which we did for different phases, so, α+β was between 700°C to 815°C, β-phase from 815°C to 925°C. So, this is the one two phase region (α+β) for one constitutive equation. So, you can see (refer to above figure) all the parameters are there which we have already discussed when we were discussing how to develop constitutive equations.

So, one set of these parameter were developed for two phase region α + β. Another set of these parameter were developed for single β-phase field and one was developed for the entire temperature range. And the third calculation which we did also wanted to know when you are in two phase region that which phase is dominating the deformation behaviour. Whether α phase is the one which is deciding how the flow stresses will be there or what will be the response of the material. So, the two-phase region also we try to divide into two phases that how independent phases will behave and the activation energy for independent phases were calculated. The idea which we used here I will just tell you in the next slide maybe.

So, what we found out is that activation energy of α phase in two phase region is this, the calculated activation energy from the data of α phase in the two phase region (refer to above figure). I will tell you how we did that. So, this was coming around 500 kJ/mole so Qαc is for calculated, if it is experimental we did not put any suffix here and the experimented calculated activation energy in the two-phase region was 524 kJ/mole.

So, you can see these two values are very close to each other that means that the activation energy of deformation of α phase is very close to the activation energy for the deformation of which we found experimentally in two-phase region. That means the α phase is the dominant phase in the two-phase region, that is the one which decides that how the deformation is going to take place.

So, one very important outcome of this work was this that we were able to identify the phase which is dominating the deformation process in the two-phase region.

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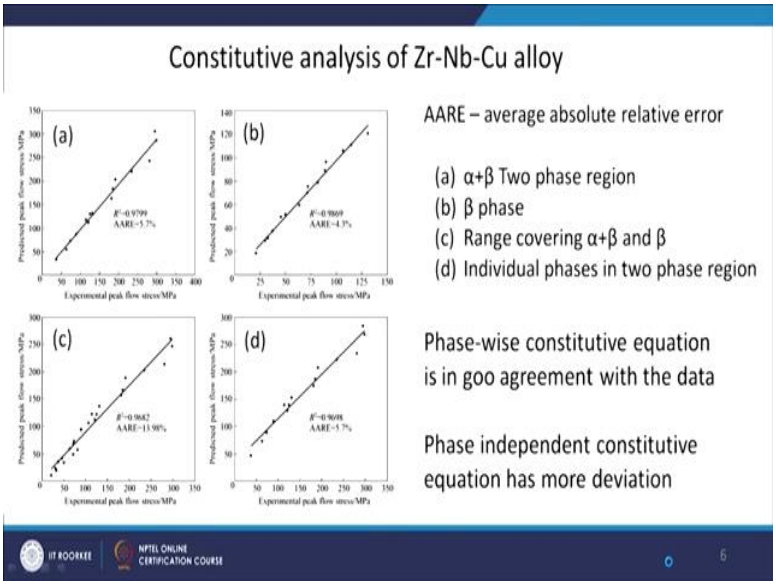


So basically, I was trying to tell you that how we found out this data for the two-phase region. I am just dividing different temperature regions so this is my temperature scale (refer to above figure) and flow stress data is here temperature is increasing here and flow stress data is like this and this is where you have α phase, this is where you α + β and this is where I have β phase.

So, suppose flow stress is decreasing as a function of temperature, but slope may be different in different region. So, let us say you have something like this (refer to above figure) and so what we were trying to do is we extrapolated the flow stress of A which we were calculating in lower temperature range into the two phase region and to do that we used a simple logarithmic dependence of stress on the temperature which you can easily get that how the flow stress is dependent on temperature.

And there is a logarithmic dependence so that is extrapolated for let say of A into the two-phase region. Similarly, for β phase the flow stress was extrapolated in the lower temperature range.

So, what we did for α, we did for the higher temperature range and for β lower temperature range. So, we could go into the two-phase region and then we calculated the values of all these parameters through this data.

And to know that whether this data is correct or not we also found out using a rule of mixture kind of idea that what will be the flow stress if I combine the flow stress of α with the β whether I am able to get the flow stress of the actual experimental results and which we found out is coming very close to the actual flow stress results that means I could extrapolate it. And if I combine both I am able to get what we are getting through experimental data, the flow stress in the two-phase region. So, that is how we calculated the activation energy for α and β and we could show that the α phase is the dominant phase.

So, now we developed the constitutive equations and then we were trying to compare the experimental flow stresses which are shown with these data points (refer to above figure) with the predicted flow stress. So, constitutive equation can give you an equation which you can use to plot a line here for example, so these are predicted peak flow stress. This particular line is from the constitutive equation. So, this is a standard exercise people do after developing constitutive equation that whether using that constitutive equation I am able to predict the flow stress or not and when I am predicting it whether these values are coming very close to the actual flow stress or not.

So, these were compared. So, the $R^2$ value is 0.97 in the first cases where you we have taken α + β two-phase region, 0.98 when we did for only the β-phase and .96 when we use the whole range of the entire temperature range without looking at the flow stress data. And 0.96 when individual phases in two phase region were used to find out the flow stress. Their average absolute relative error is also calculated 5.7%, 4.3%, 13.98% and 5.7% respectively. So, you can see that the error in the predicted and the experimental value is very high when we considered the whole temperature range.

Whereas when we developed the constitutive equation for individual phase region, our errors were very small. Similarly, when we did with the data of extrapolated values and we then combine them together to get the flow stress of or the activation energy of the two phase region, again the values were very small or the error was small. So, this kind of result told us that phase wise constitution is in good agreement with the data.

Whereas phase independent constitutive equation has more deviation from the actual values, so when we are developing this constitutive equation we should take care of this phase information also.

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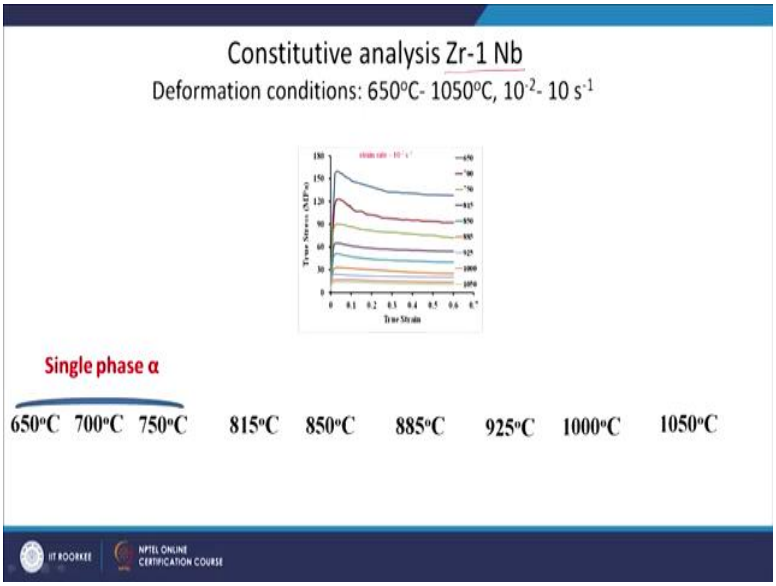


Now, this is another work which we did in zirconium 1 niobium alloys. So, earlier work was on zirconium 2.5 niobium 0.5% carbon. In this case also we did as previously, so you have from 650°C to 750°C single phase α, two phase region from 815°C to 885°C and single phase β from 925°C to 1050°C and one constitutive equation was developed for all the phases considered together.

So, you actually for each strain rate we deformed the material at different temperatures and these (refer to above figure) are the flow stress curves for the deformation process. Of course, you can see at lower temperature the deformation behaviour is different than the deformation behaviour at high temperature, it looks like as a single peak and then the steady-state condition is being reached. So, it is like a discontinuous dynamic recrystallization.

And as you go toward higher temperature the deformation behaviour is changing to kind of dynamic recovery where you do not get a peak in the stress. But there is a steady-state behaviour which is typical of dynamic recovery. So, you can also see that the deformation behaviour is also so it can be understood that as a function of temperature the deformation behaviour is changing.

You can also argue that the deformation behaviour is changing as the phase transfer or the phase present at particular temperature is shifting from one type of phase to another type of phase. So, you can see as you are going toward β phase or maybe in the β phase, the dynamic recovery is the dominant deformation mechanism and in the α phase the dynamic recrystallization is the dominant deformation mechanism.

So, it can be argued that as a function of phase also this kind of change is taking place. Now one thing I told you at that time but did not brought out and that was about the adiabatic temperature rise.

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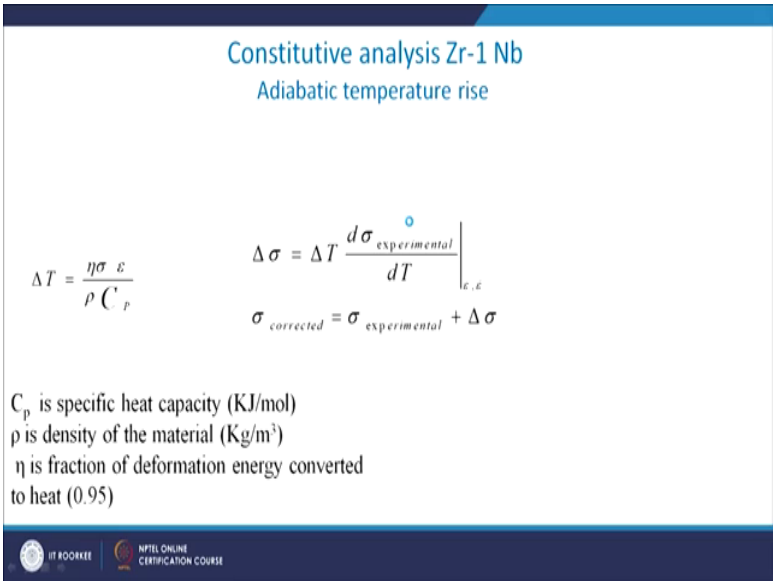


So, basically adiabatic temperature rise $\Delta T$ can be given by an expression like this (refer to above figure) so η is your friction of deformation energy converted to heat, σ is of course flow stress, ε the strain, ρ is density of the material and $C_P$ is the specific heat capacity. So, the $\Delta\sigma$ can be calculated from the slope of variation of stress as a function of temperatures so $\frac{d\sigma}{dT}$ and multiplied by $\Delta T$.

So, you can do a correction to the flow stress. So, this is my experimental flow stress and this is the change in the flow stress because of the rise in the temperature during the deformation process (refer to above figure). So, you have to do a correction for that so the flow stresses must have come down if there is any adiabatic heating because the temperature must be more. So, you have to do a correction for the temperature rise, that means the flow stress what you have measured is actually lower.

But the actual flow stress should have been higher for that temperature which you have considered and you can see that is what is done here.

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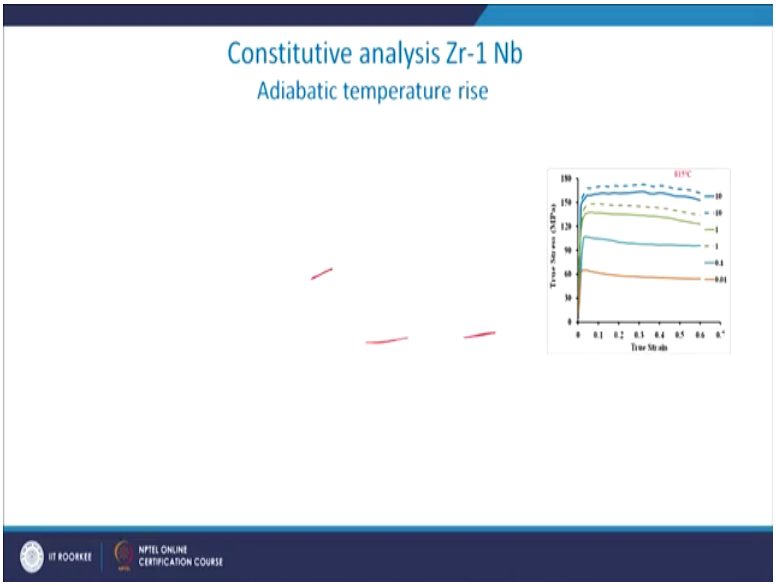


And especially as I told you that at higher strain rates, only this particular problem will occur because strain rate is very high and you are not giving enough time to for heat to dissipate. So, you can see that this (refer to above figure) is my flow stress which is measured experimentally but as we are expecting that temperature rise must have taken place the flow stress for that temperature should be this one.

Similarly this is the flow stress at strain rate of 10 we have measured and this is what we have done the compensation for the temperature rise. So, now flow stress is more for that particular temperature. So, this kind of correction for temperature rise we should do for deformation where we are doing deformation at higher strain rates. At lower strain rate as you can see, we are not doing any correction. So, usually at greater than one we start putting the correction.

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Constitutive analysis Zr-1 Nb

Material constants and activation energy of different modes using peak flow stress

| Parameters | Mode-1 | Mode-2 | | |
|---|---|---|---|---|
| | Full temperature range | α Phase | (α+β) Two Phase | β Phase |
| α | 0.01575 | 0.00534 | 0.01340 | 0.03150 |
| n | 4.52 | 6.20 | 5.17 | 4.89 |
| s | 13.07 | 6.45 | 17.42 | 7.22 |
| Q | 490.67 | 332.58 | 748.99 | 293.31 |
| Ln A | 53.07 | 38.83 | 77.96 | 25.86 |

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Now these are the material constants which we have measured. So, you can see that we have all these α, n and Q and all these parameters were measured for full temperature range here. So, this is my activation energy. In this case (refer to above figure) this is for only the α phase and this is the activation energy, for two phase region α + β this is the activation energy and the β phase for which the activation energy is this one.

So, independent constitutive equations are developed for different phases and now how to know that whether what we have developed is accurate.

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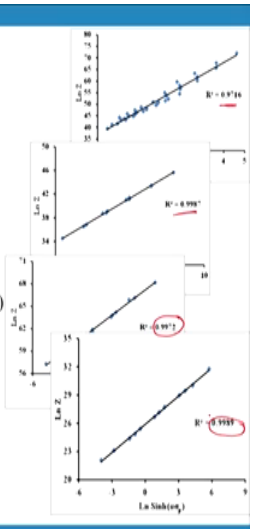
Different constitutive equations – phase wise

$$\dot{\varepsilon} = 1.12\times10^{21}[\sinh(0.01575\times\sigma_p)^{4.52}]\exp\left(-\frac{490670}{RT}\right) \quad (\textit{for All Temperature Range})$$

$$\dot{\varepsilon} = 7.32\times10^{16}[\sinh(0.00534\times\sigma_p)^{6.20}]\exp\left(-\frac{332580}{RT}\right) \quad (\textit{for Alpha Phase})$$

$$\dot{\varepsilon} = 7.19\times10^{33}[\sinh(0.01340\times\sigma_p)^{5.17}]\exp\left(-\frac{748990}{RT}\right) \quad (\textit{for Two Phase})$$

$$\dot{\varepsilon} = 1.700\times10^{11}[\sinh(0.03150\times\sigma_p)^{4.89}]\exp\left(-\frac{293310}{RT}\right) \quad (\textit{for Beta Phase})$$



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So, actually these are the different constitutive equations (refer to above figure). So, you have for only the for all temperature range $R^2$ value is around 0.97 for α phase, the $R^2$ value is 0.99 for two-phase region, and for β phase again the $R^2$ value is 0.99. So, you can see that when we

are developing the constitutive equation for independent phases or phase region the $R^2$ value is quite high, very close to 1 whereas when we are developing for the entire temperature range the $R^2$ value is coming low. Now how low is very low and how high is very high. we cannot some time tell from these values directly. A better approach as I told you is to validate this constitutive equation with the maybe actual experiments.

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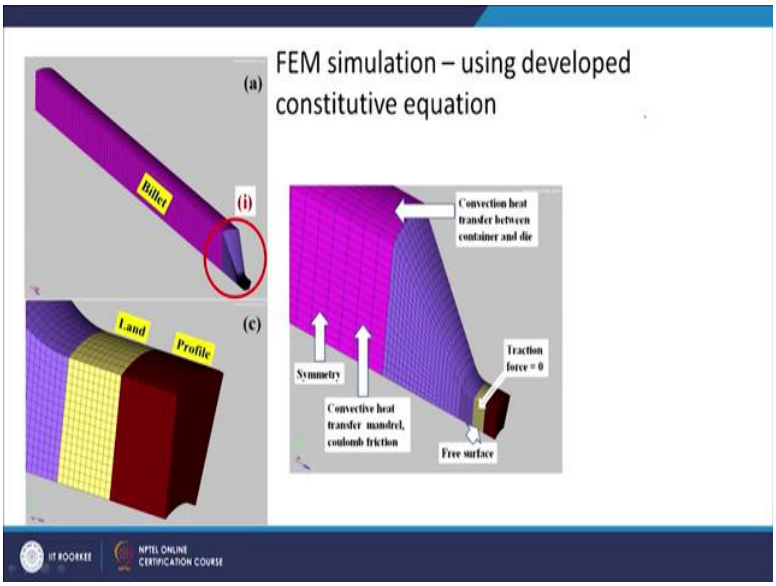


And to do that we have done the FEM simulation of a hot extrusion process. So, as you may be knowing if I look at the hot extrusion process, basically the billet will be put here and it will be deformed, the cross-sectional area will reduce (refer to above figure). So, this is my output which I am going to get and this is my input and of course there will be a ram here to push through that and the material will come out.

And there will be deformation, the cross-sectional area is reducing and so on. So, what will be the ram force will be required for deformation of these, this data was acquired from actual shop floor where a big billet is extruded at a higher temperature and you are deforming it, so how much how much ram force is required to do the deformation that already is measured in the actual shop floor.

So, this process was simulated using finite element analysis and these are the grid which you put on the on the billet for measurement of the stresses and strain during the deformation process. And we have used the constitutive equation developed by us to do this simulation.

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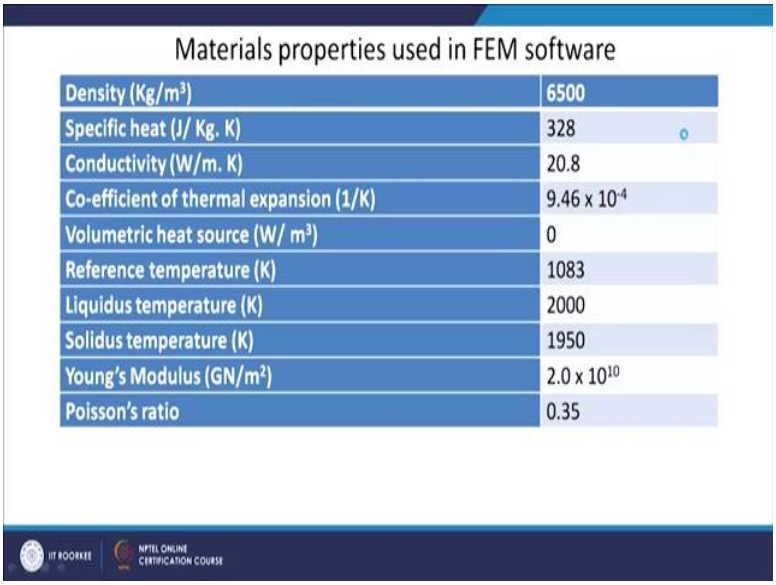


These (refer to above figure) are the properties used in FEM software that what material property you are giving to FEM software and of course we are also using the constitutive equation that how the material behaves during the deformation process. So, the main input to the FEM simulation was what we call as lookup table. So, lookup table means if we give the input as only the stress as a function of strain, strain rate and temperature.

So, one way to do is that you make a table, so your stress will come here (refer to above figure) and all other parameter will come here and you are giving these for different strain rates and temperature, what is the values of stress. So, that is kind of a table and the software has some artificial neural network-based model within the software itself. And the software which we used is called hyper extrude, it is a commercial software.

So, the software also has some ANN model built in as we have already discussed during constitutive equation that this is another approach to develop but in that case, you do not know and you do not understand the material behaviour it does within inside. So, either you can give lookup table like this that you have measured the flow stress at different strain, strain rate, temperature and that data you give to the software and it develops ANN model and that the software uses for FEM simulation.

Another approach is to develop the constitutive equation and then you feed that constitutive equation. So, you are not giving data but you are giving the material constants and then from constitutive equation the software will be able to calculate the stress at different strain, strain rate and temperature.

So now the output of the FEM simulation will depend heavily on the accuracy of the constitutive equations. So, that gives us confidence in that whether what we are developing or what we are doing or what we are proposing is good enough or not.

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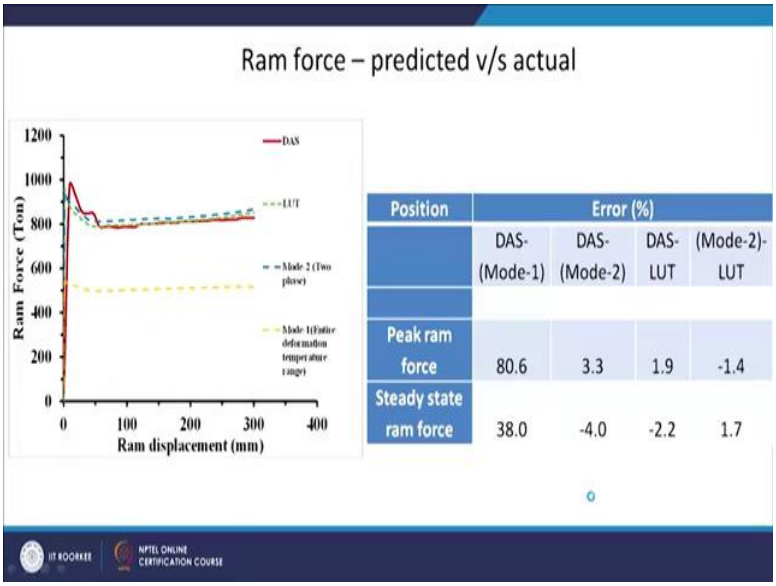


| Position | Error (%) | | | |
|---|---|---|---|---|
| | DAS-(Mode-1) | DAS-(Mode-2) | DAS-LUT | (Mode-2)-LUT |
| Peak ram force | 80.6 | 3.3 | 1.9 | -1.4 |
| Steady state ram force | 38.0 | -4.0 | -2.2 | 1.7 |

So, to do that we have done the simulation, so as you can see this red one which is showing (refer to above figure), this is the shop floor data or shop floor measurement of ram force as a function of ram displacement. So, this is the actual measurement of course they must have some load cell or some transducers to measure the force. This green one LUT as I told you through lookup table, so the software uses some ANN model here and predicts the equation and using that one it tries to predict that what will be the ram force.

So, as you can see it is also very closely following the actual shop flow data, the peak ram force and the steady state ram force are very close to the actual data. This (refer to above figure) is the equation because this particular deformation takes place in the in the two-phase region, the temperature is corresponding to two phase region, so we gave the constitutive equation which we have developed for two phase region.

And this blue one also you can see very closely following the shop floor data as well as what you get from the ANN model and this yellow one here this is for the entire deformation temperature range, the peak ram force and the steady state ram force are much lower than the actual values or the predicted values through the constitutive equation of two-phase region and the lookup table.

So you can understand that what constitutive equation we were trying to develop. It is able to predict a very close value to the actual shop floor data as well as what we have got from the ANN model so that gave give us the confidence that the idea which we are proposing it is able to predict the actual or the constitutive equation which we are developing is more accurate than if we consider the whole temperature range where different phases will dominating at different temperatures, that is not a not a right way to develop the constitutive equations.

So, this is one of the case studies using constitutive analysis which we have done in our work and this is actually one of the PhD theses work and the project was sponsored by BRNS. And the PhD thesis was from Kuldeep Saxena. He did all this work. I should have mentioned the papers and all that here.

I could not do that but anyway you can go to the reference can be given in the next lectures that which papers we are using for presenting this particular lecture. So, with that I think the constitutive equation and development and analysis is complete. And now we will go to the next module which is on processing maps so that we will try to understand. Thank you.

**Key words**- Constitutive equation, Zirconium niobium alloys, ANN model