Thermo-Mechanical and Thermo-Chemical Processes
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Lecture-19
Constitutive Based Model: Physical Based Model

Hello friends, we were discussing constitutive analysis. So, continuing with that we have already discussed the phenomenological model and in that we have discussed creep as well as high strain rate deformation. So, Johnson Cook model in that and then we were we have discussed for hot working, Arrhenius type of sine hyperbolic relationship between stress and strain rate. So, these are couple of models which comes under phenomenological model used extensively, though they have empirical nature.

But it is easy to kind of fit all the parameters and get some constitutive equation which can be used easily in any modelling work or to predict stress at any other temperature and strain rate. So, we will now discuss this physical based model. Again, I am not discussing again, you can see, if you go to any review paper, there are tens of models, but I am just giving you a flavour of what type of modelling is done when you are basing it on the physical phenomena.

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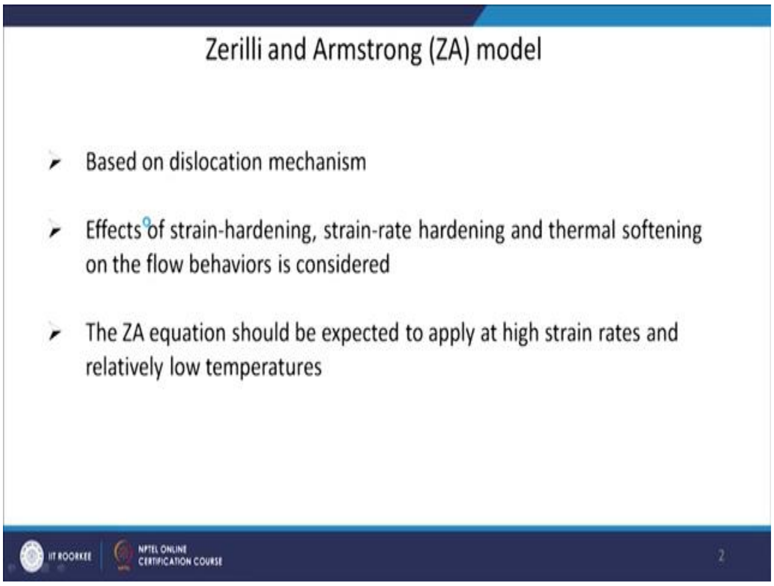

Zerilli and Armstrong (ZA) model

- Based on dislocation mechanism
- Effects of strain-hardening, strain-rate hardening and thermal softening on the flow behaviors is considered
- The ZA equation should be expected to apply at high strain rates and relatively low temperatures

So, in this first is this ZA model, Zerilli Armstrong model and this model is based on dislocation mechanism that how dislocation multiplication is taking place or dislocation recovery is taking place and so on. So, as you can see that now we are directly relating our constitutive equation with the actual deformation mechanism, which we were not doing earlier. So, this is based on dislocation mechanism, effect of strain hardening, strain rate hardening and softening on the flow behaviour is considered.

So, from physical basis, they have included all these three parameters. This particular model you can consider it for any high strain rate and relatively low temperature kind of condition. You can apply this particular model to develop constitutive equation.

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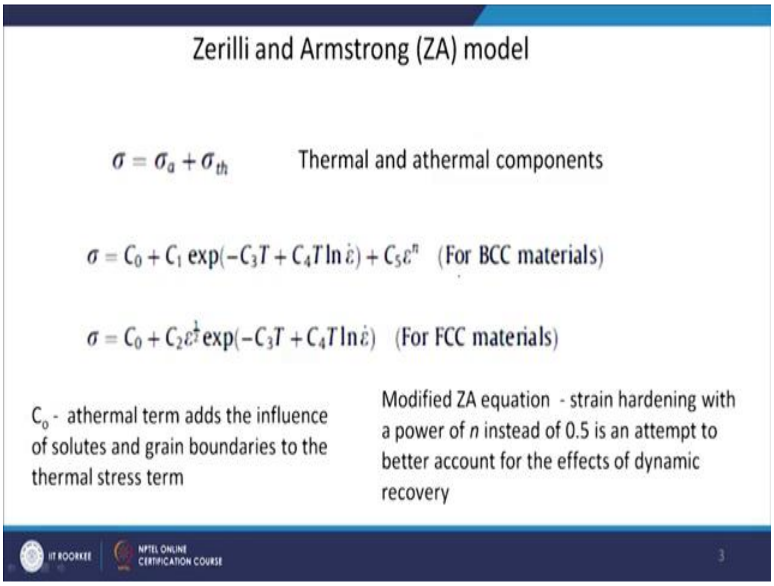

Zerilli and Armstrong (ZA) model

$\sigma = \sigma_a + \sigma_{th}$ Thermal and athermal components

$\sigma = C_0 + C_1 \exp(-C_3 T + C_4 T \ln \dot{\varepsilon}) + C_5 \varepsilon^n$ (For BCC materials)

$\sigma = C_0 + C_2 \varepsilon^{\frac{1}{2}} \exp(-C_3 T + C_4 T \ln \dot{\varepsilon})$ (For FCC materials)

C_0 - athermal term adds the influence of solutes and grain boundaries to the thermal stress term

Modified ZA equation - strain hardening with a power of *n* instead of 0.5 is an attempt to better account for the effects of dynamic recovery

Now, what it actually does is, the stress is calculated by considering two contribution to the stress. So, one contribution is a thermal contribution and another contribution is athermal contribution which does not depend on the temperature. So, by doing these two or combining these two different effects of stress, you are trying to find out the flow stress of the material.

Of course, then you have to develop these particular models and equations (refer to above figure). So, you can see that these two equations are shown here, one for BCC material, another one for FCC material and as we promised in the first lecture of constitutive equation that you will have more constants when you are dealing with physical models. So, you can see here there are the numbers of constants have increased.

So, you have from C_0 to C_5 which earlier we had only 2-3 and on top of that, you have these exponents also. Similarly, for FCC material you have C_0, C_2, C_3, C_4, and so on. So, basically again you can see that it is bringing down the effect of strain hardening with a strain hardening exponent here also, the effect of strain rate and effect of temperature.

And that is how they are able to predict that what will be the flow stress for a BCC material. Similarly, they have proposed another equation for FCC materials where there is a slight change in the way they have introduced the strain component in exponent, instead of exponent n now it has a exponent of half that is 0.5 and it is already multiplied in the exponential term earlier it was as a separate term (refer to above figure).

Now, it is a single term here with the temperature and a strain rate. So, these are the two equations developed for two different set of materials. So, C_0 is basically the athermal term which aids the influence of solute and grain boundary to the thermal stressed term. So, this is our athermal component which we were trying to see in the first equation. So, you have athermal and thermal component.

Now of course, as for any other model equation people have modified this Zerilli Armstrong model also. So, what these modified ZA equations usually are trying to do is actually with the strain hardening exponent. If you see in the FCC material, they have kept it as a constant 0.5. So, strain hardening exponent they are changing with some variable n that means, it can have different values instead of only a constant value 0.5 which is proposed by this ZA model.

So, this is to take into account in a better way the dynamic recovery which is taking place during the deformation process. So, the other model is that which consider dynamic recovery and so, it is concentrated more on the recovery part.

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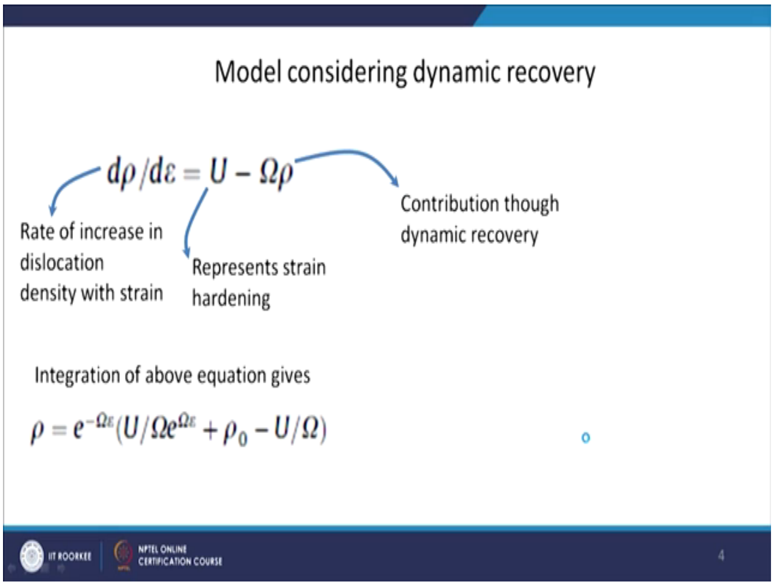

Model considering dynamic recovery

$$d\rho/d\varepsilon = U - \Omega\rho$$

Rate of increase in dislocation density with strain

Represents strain hardening

Contribution though dynamic recovery

Integration of above equation gives

$$\rho = e^{-\Omega\varepsilon}(U/\Omega e^{\Omega\varepsilon} + \rho_0 - U/\Omega)$$

So, basically what we are trying to do here is that the change in the dislocation density as a function of a strain is related with two terms here U-Ωρ (refer to above figure), U represent the strain hardening part and ρ is the contribution through dynamic recovery. So, that is why it has a negative term as recovery will takes place, the dislocation density will decrease. The rate of dislocation density increases a function of strain this should have a negative influence on that.

Now, if you integrate above equation you get the ρ term in this form (refer to above figure) that how the ρ will change as a function of strain.

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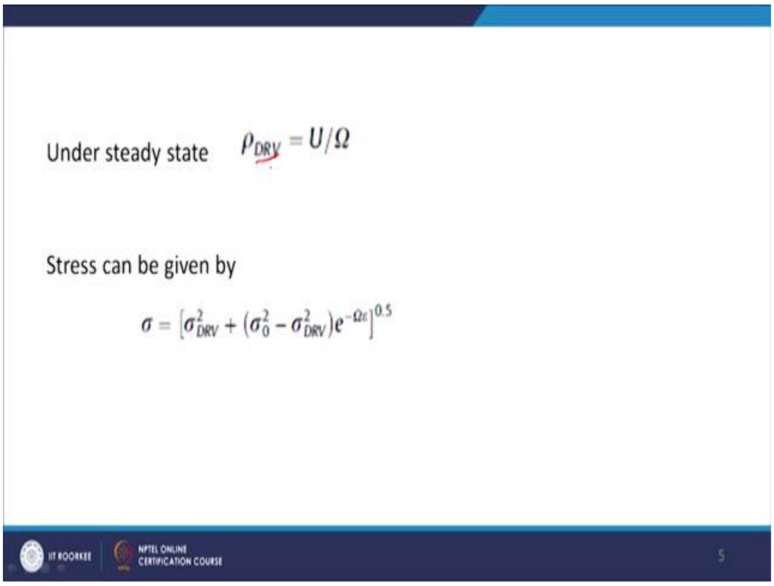

Under steady state $\rho_{DRV} = U/\Omega$

Stress can be given by

$$\sigma = \left[\sigma_{DRV}^2 + (\sigma_0^2 - \sigma_{DRV}^2)e^{-\Omega\varepsilon}\right]^{0.5}$$

So, under a steady state the ρ i.e. dynamic recovery, what will be the dislocation density is dependent on the on these two term U and Ω and stress can be given by an equation like this (refer to above figure).

I will tell you all this that what do we mean by σ_{DRV} and so on and it is an exponent of 0.5 and that is a strain term in the exponential. So, from physical based model you can predict now that what will be the flow stress of the material if you know σ_{DRV} and so on. So, this is the model based on dynamic recovery.

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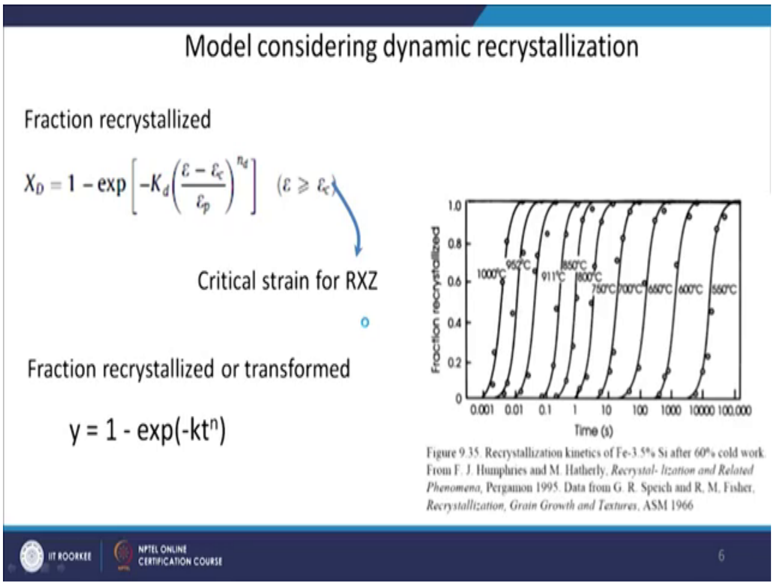

Model considering dynamic recrystallization

Fraction recrystallized

$$X_D = 1 - \exp\left[-K_d\left(\frac{\varepsilon - \varepsilon_c}{\varepsilon_p}\right)^{n_d}\right] \quad (\varepsilon \geqslant \varepsilon_c)$$

Critical strain for RXZ

Fraction recrystallized or transformed

$$y = 1 - \exp(-kt^n)$$

Figure 9.35. Recrystallization kinetics of Fe-3.5% Si after 60% cold work. From F. J. Humphries and M. Hatherly, *Recrystal- lization and Related Phenomena*, Pergamon 1995. Data from G. R. Speich and R. M. Fisher, *Recrystallization, Grain Growth and Textures*, ASM 1966

Now, there are model which is also consider dynamic recrystallization. In this what they are trying to do is they are trying to find out the fraction recrystallized. So, to find out the fraction recrystallized they have some parameters here. So, the equation is like this

X_p = 1-exp[-K_d($\frac{\varepsilon-\varepsilon_c}{\varepsilon_p}$)] and ε is more than ε_c.

So, what is ε_c it is a critical strain for recrystallization, which we have already seen earlier.

If you remember that when we were discussing the dynamic recrystallization, we discussed about this particular term. So, you this is your peak stress σ_p. So, obviously, the strain corresponding to that will be ε_p and the recrystallization will start at some point here and this we call as ε_c the critical strain to initiate recrystallization and obviously, the stress associated with that is σ_c.

And so, basically idea is that the strain should be more than the critical strain and then only the recrystallization will happen and then only you will be able to calculate the fraction recrystallized. So, some parameters are there K_d and n_d here, which depends on the deformation condition. So, if you see actually the recrystallization process that how this equation has come. This equation has come from this kind of the Avrami equation, where it has a typical a shape of curve.

And this type of curve you will see in large number of processes not only metallurgical processes for example, growth in bacteria's, if you have you are doing some culture of bacteria. So, there will be some incubation time, then the bacterial growth will increase suddenly and it will increase exponentially and as the volume of whatever system you have the ingredients are getting exhausted then the population will again become saturated and it will start decreasing and become saturated.

This kind of curve you will also see in the phase transformation that for a phase there is a incubation time before the new phase, by the time which the nucleation takes place then there is a sudden increase in the nucleation as well as growth. So, fraction of phase transformation increases and then as the amount of volume becoming smaller and smaller of the parent phase, so again the kinetics decrease.

So, you have a very typical this S shape curve like this, initially increasing exponentially and then decreasing and this kind of behaviour can be nicely shown with an equation like this

$$1-\exp(-Kt^n)$$

This bring out both these behaviours very nicely and it gives you the fraction either recrystallized or fraction transformed if you are doing a phase transformation. So, you can see that it has very nice similarity with this (refer to above equation) the equation is shown in the very similar way only the parameters which are used in exponential has to be different depending upon what is your process you want to know.

So, as you can see here fraction recrystallization shown on y-axis, x-axis has time. So, as you increase the temperature recrystallization kinetics is increasing, it is starting at lower time and finishing also at lower time and all the curves they have this kind of S shaped curve. So, they have found out the fraction recrystallized from the idea of this Avrami type of equation.

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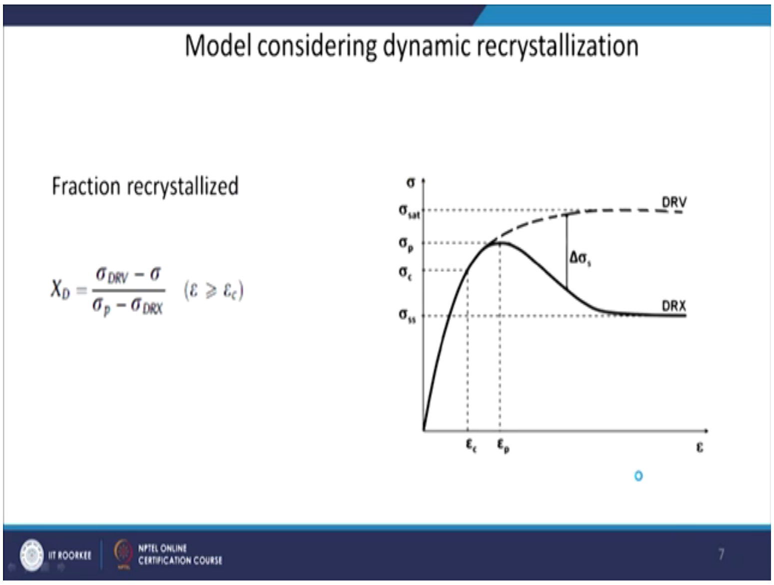

Model considering dynamic recrystallization

Fraction recrystallized

$$X_D = \frac{\sigma_{DRV} - \sigma}{\sigma_p - \sigma_{DRX}} \quad (\varepsilon \geqslant \varepsilon_c)$$

Then they also find out the same that how the fraction recrystallized can be can be derived or can be calculated from the flow stress curve. So, here we will see how it is done by flow stress curve and here also you will be able to see that what we were discussing in physical based model that what do we mean by σ_{DRV}. So, there are two curves shown here (refer to above figure), one is with a broad peak, which you see for the dynamic recrystallization. So, stress increases then you get a hump and then you have this dynamic recrystallization, if dynamic recrystallization is not taking place, only dynamic recovery is taking place the curve will go something like this. And the difference between the two is given by some $\Delta\sigma$ the initiation of recrystallization is happening at ε_c and corresponding stress is σ_c, peak stress is at ε_p and σ_p and this σ_{DRV} is you can say saturation stress.

And what you are getting after dynamics recrystallization, you can say it has a steady state. So, from this also you can calculate the fraction recrystallized which is shown here (refer to above figure). So, what they are saying is that whatever is stress,

$$\frac{\sigma_{DRV}-\sigma}{\sigma_p-\sigma_{DRX}}$$

So, this is actually the total drop in the stress because of the recrystallization.

So σ_p - σ_{DRX} is the drop because of the complete recrystallization in the material once it is recrystallized it drops to that from σ_p. So, that is you can say is the total recrystallization σ_{DRV} – σ whatever sigma you are at it to find out the fraction recrystallized that $\Delta\sigma$ is the amount of recrystallization which has happened that is why the stress has come down from this σ_{DRV} level to $\Delta\sigma$ level. And at this point the recrystallization will be complete.

So, this ratio of $\frac{\sigma_{DRV}-\sigma}{\sigma_p-\sigma_{DRX}}$ should give me the that how much is the fraction recrystallized because by that amount the stress will come down again we are talking about strain more than ε_c. So, now you have fraction recrystallized from two different ideas one from the stress strain curve one from the Avrami type of kinetics.

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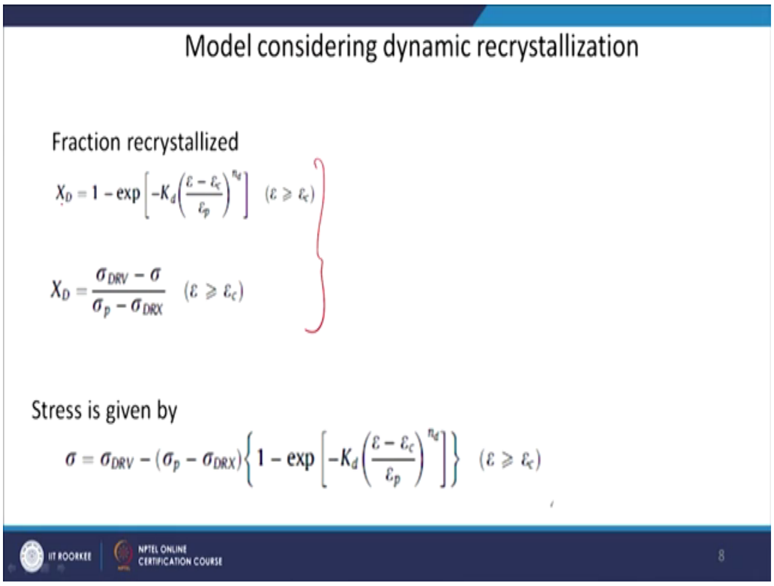

Model considering dynamic recrystallization

Fraction recrystallized

$$X_D = 1 - \exp\left[-K_d\left(\frac{\varepsilon - \varepsilon_c}{\varepsilon_p}\right)^{n_d}\right] \quad (\varepsilon \geqslant \varepsilon_c)$$

$$X_D = \frac{\sigma_{DRV} - \sigma}{\sigma_p - \sigma_{DRX}} \quad (\varepsilon \geqslant \varepsilon_c)$$

Stress is given by

$$\sigma = \sigma_{DRV} - (\sigma_p - \sigma_{DRX})\left\{1 - \exp\left[-K_d\left(\frac{\varepsilon - \varepsilon_c}{\varepsilon_p}\right)^{n_d}\right]\right\} \quad (\varepsilon \geqslant \varepsilon_c)$$

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And if you combine this together, you will get an equation like this

$$\sigma = \sigma_{DRV} - (\sigma_p - \sigma_{DRX})\{1\text{-}\exp[\text{-}K_d(\frac{\varepsilon-\varepsilon_c}{\varepsilon_p})^{nd}]\}$$

So, they found out the fraction recrystallized from two different ideas and then they equated it and from there they found out the what will be the stress of the system at a particular point.

So, this is a model physical based model which is considering dynamic recrystallization. Now, there are some time a as I told you artificial neural network based models also.

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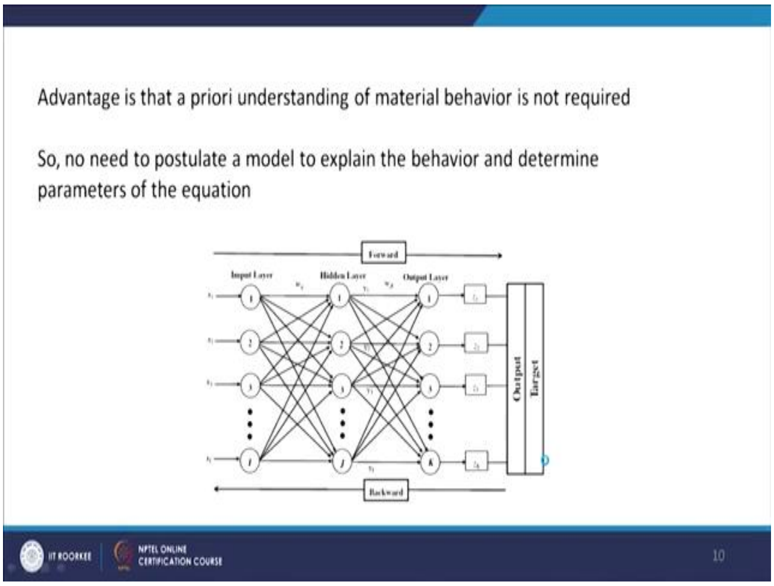

Advantage is that a priori understanding of material behavior is not required

So, no need to postulate a model to explain the behavior and determine parameters of the equation

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So, ANN based model, the advantage is that you do not have to know the material behaviour or actual deformation mechanism, you do not need that. Also, I do not need to know that which model I should be using for this particular material. So, I do not have to postulate a model. I do not have to determine the parameters of the equation because we are not talking about any equation here, what we are doing is we are inputting.

For example, in our case I am putting input of if it is a steady state condition my strain will not come in picture. So, I am inputting the stress at different strain rate and temperature. So, strain rate and temperature are your input and the output is your flow stress. So, basically your ANN model will be trained with the data which you have initially inputted and what actually ANN does in between it fits lot of polynomial equation to your data.

And from there it is it try to minimise the error. So that it gets it gets a curve which can be used to predict the flow stress for any other condition. So, strain rate and temperature will be used to get the flow of stress and you can use ANN model for doing that. Right now because ANN model is something in which there is no physics involved we cannot discuss that in greater detail.

But if you are familiar with ANN model and all these ideas of machine learning and so on, you should be able to collect lot of data maybe from literature if you do not want to do experiments yourself, collect lot of data from the published literature, use that to train the model and then try to predict the flow stress for some other condition which you have not used to make the model.

Then you will be able to say with confidence your model is working. So, with this we have kind of completed the constitutive models, based on phenomenological model, physical based model and ANN model. We have used on a few models to bring out the flavour of each of these categories and also, we have tried to understand that why we want to develop constitutive equation, the idea is to know the material behaviour. So that you can also design material accordingly and to use this for doing any FEM based modelling or so, for your actual industrial process. So, once you know all the constitutive equation parameter, you will be able to do that. So thank you for your attention.

Key words- Constitutive equation, Zerilli Armstrong model, Avrami equation.