Smart Structures

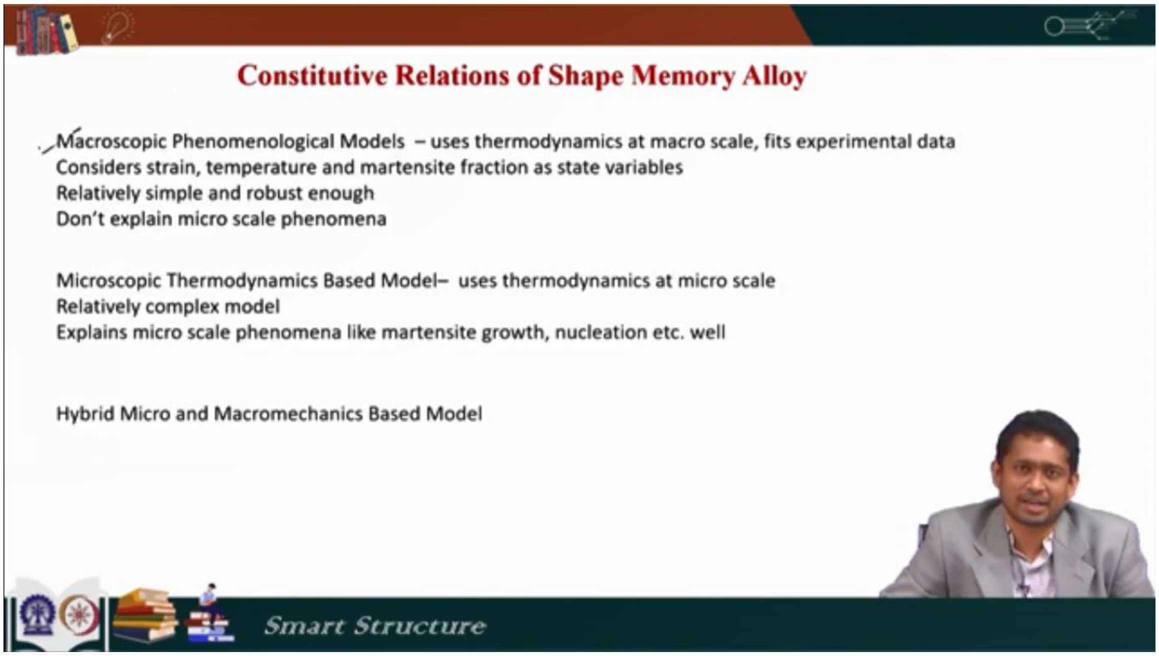
Professor Mohammed Rabius Sunny
Department of Aerospace Engineering
Indian Institute of Technology, Kharagpur
Week - 09
Lecture No - 45

Constitutive Relations of Shape Memory Alloys

Welcome to the 9th week. In this week we will talk about Constitutive Relations of Shape Memory Alloys. When we talked about the constitutive relations of piezoelectric materials, we saw that there are various approaches. So, today before starting with the constitutive modeling, we will see some of the approaches that have been used so far by various researchers for constitutive modeling of shape memory alloys. Here are some of the approaches. First one is macroscopic phenomenological model.

These models as the name suggests they are macroscopic and they used thermodynamics at the macro scale. And the thermodynamics gives the structure of the constitutive relation and then by using experiments we find out the actual coefficients. And in these models generally the state variables are strain, martensite fraction and temperature and these models are relatively simple. So, they can be easily applied to engineering problems and they are robust enough they capture good amount of physics.

(Refer slide time: 2:19)



Constitutive Relations of Shape Memory Alloy

Macroscopic Phenomenological Models – uses thermodynamics at macro scale, fits experimental data
Considers strain, temperature and martensite fraction as state variables
Relatively simple and robust enough
Don't explain micro scale phenomena

Microscopic Thermodynamics Based Model– uses thermodynamics at micro scale
Relatively complex model
Explains micro scale phenomena like martensite growth, nucleation etc. well

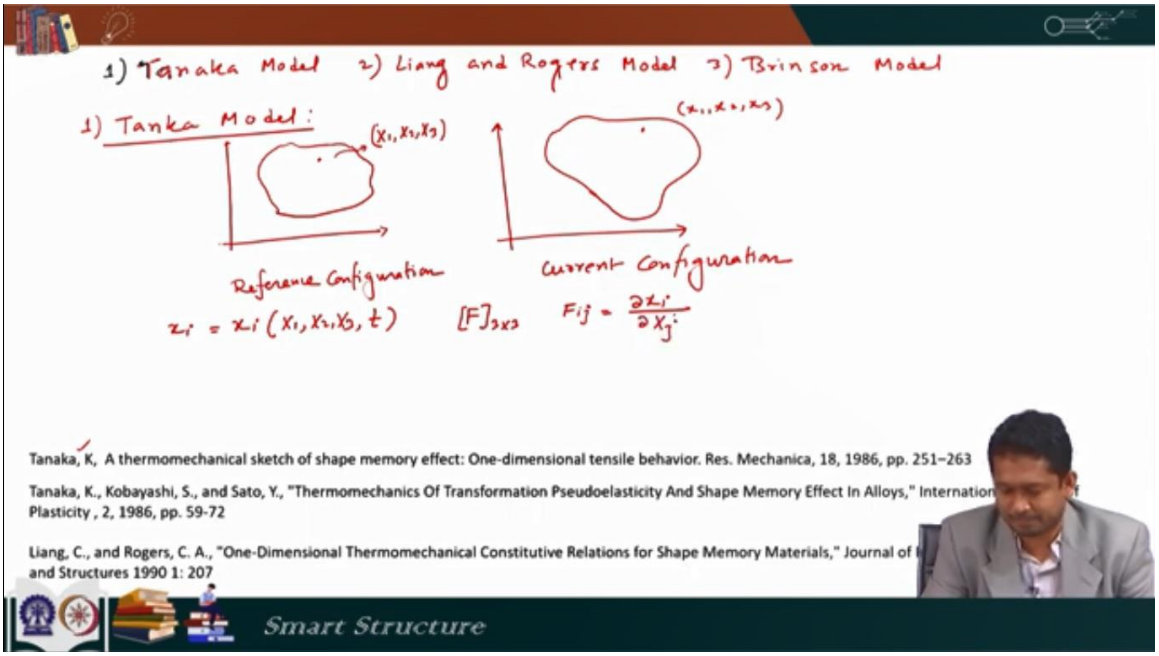
Hybrid Micro and Macromechanics Based Model

However, they do not capture the micro scale phenomena. So, to capture the micro scale phenomena there are microscopic approaches where thermodynamic laws are applied at the micro scale. Now, in those models there are more complexities. So, they are not good for large scale applications, but for micro scale phenomena like martensite growth, nucleation etcetera they capture very well and they are successfully applied for those kind of problems. And there is problem there are other models which are kind of hybridization between these two approaches.

So, in this course we will talk about the microscopic models. Now, we have seen that a shape memory alloy shows both one way and two-way memory, but in this model we generally take care of only the one-way memory one-way shape memory effect. And these models we will restrict our self to one dimensional models because shape memory alloys are mostly used in wire forms. So, one dimensional models would suffice for those applications. So, we will talk about three models which are macroscopic phenomenological models.

One is Tanaka model, Tanaka model then there is Liang and Rogers model and the third one is Brinson model. So, let us start with the first one that is the Tanaka model. Now, Tanaka model is described with sufficient details in this paper by Tanaka, the thermo mechanical sketch of shape memory effect one dimensional tensile behavior. And also the other paper by Tanaka and his co-authors thermomechanics of transformation pseudo elasticity and shape memory effect in alloys shows good details of this model. And apart from that this paper by Liang and Rogers also talks about the Tanaka model with sufficient details.

(Refer slide time: 7:13)



1) Tanaka Model 2) Liang and Rogers Model 3) Brinson Model

1) Tanka Model:

$x_i = x_i(X_1, X_2, X_3, t)$ $[F]_{3\times3}$ $F_{ij} = \frac{\partial x_i}{\partial X_j}$

Tanaka, K, A thermomechanical sketch of shape memory effect: One-dimensional tensile behavior. Res. Mechanica, 18, 1986, pp. 251–263

Tanaka, K., Kobayashi, S., and Sato, Y., "Thermomechanics Of Transformation Pseudoelasticity And Shape Memory Effect In Alloys," Internation
Plasticity , 2, 1986, pp. 59-72

Liang, C., and Rogers, C. A., "One-Dimensional Thermomechanical Constitutive Relations for Shape Memory Materials," Journal of
and Structures 1990 1: 207

$$x_i = x_i(X_1, X_2, X_3, t)$$

$$[F]_{3\times3}F_{ij} = \frac{\partial x_i}{\partial x_j}$$

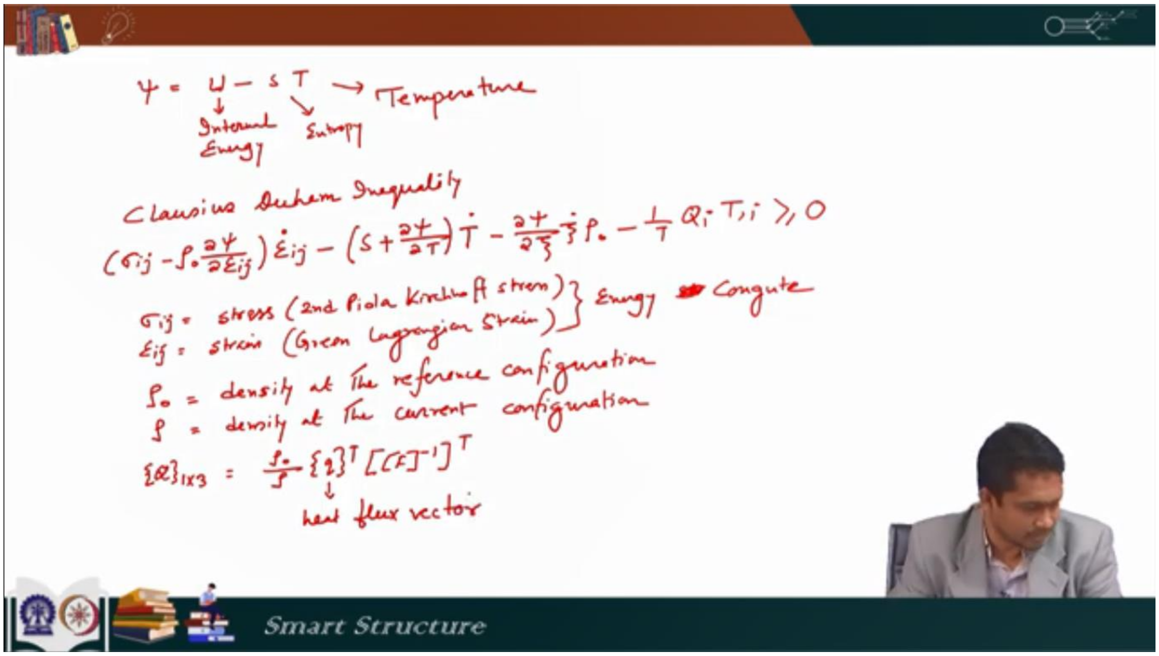
Now, when we talked about the constitutive relations in piezoelectric materials we restricted ourselves to small strain problems. So, we made the assumption of small deformation and accordingly we could simplify few things. However, in shape memory alloy most of the applications involved large strain because we have seen that a material like nitinol can expand up to 8 percent and it can easily recover that. So, at those at that range of strain the problems are non-linear. However, a full treatment of non-linearity is not in the scope of this course generally a course like continuum mechanics treats those things in full details.

Here we look into those a non-linear effect very briefly so that we can explain the models. So, when we deal with large deformation problems we talk about two configurations a configuration which is before the deformation and a configuration which is after the deformation. So, this we can call is this is generally called a reference configuration and this is generally called a current configuration. Now, if we have a point here in the reference configuration and if this point has a coordinate capital X 1 capital X 2 capital X 3 in 3D. Now please understand although for simplicity it is drawn in a 2D plane, but these bodies are 3D in general and then let us imagine that after deformation the same point has a new coordinate that is small x 1 small x 2 small x 3.

In that way each and every point has a corresponding unique point in the current configuration. So, each configuration the reference configuration has a unique point in the current configuration. So, we can say that x i is equal to I mean x i is a function of the coordinate in the reference configuration and as well as t because with time the deformed shape changes. So, with time small x 1 small x 2 small x 3 changes. Now with this we can define the matrix F and that is a 3 by 3 matrix where F i j is equal to partial of small x i by partial of capital X j and this is called deformation gradient.

Now this quantity will be useful when we go to the constitutive relation its derivation. Now the basic principle behind deriving the constitutive relation is same while dealing with piezoelectric materials we saw that we write the Clausius Duhem inequality and in that inequality we use a suitable thermodynamic potential and we apply all the conservation laws and then using that inequality we get a certain form of the equation and that equation form gives us the constitutive relation same thing we do here. So, in Tanaka's model the thermodynamic potential that is used is Helmerth potential which is written as psi is equal to U minus s T where U is the internal energy, s as we defined before entropy, T is temperature. Now if we write Clausius Duhem inequality for this case it looks like this we have sigma i j minus rho 0 multiplied by del psi by del epsilon i j multiplied by E i j dot minus S plus del psi by del T multiplied by T dot minus del psi by del xi multiplied by xi dot rho 0 minus 1 by T Q i T comma i which is greater than equal to 0. Now here we have some few newer terms first of all sigma i j sigma i j is stress and epsilon i j is strain.

(Refer slide time: 12:33)



$\psi = U - S\,T$ → Temperature

U ↓ Internal Energy

S ↘ Entropy

Clausius Duhem Inequality

$$\left(\sigma_{ij} - \rho_0 \frac{\partial \psi}{\partial \varepsilon_{ij}}\right)\dot{\varepsilon}_{ij} - \left(S + \frac{\partial \psi}{\partial T}\right)\dot{T} - \frac{\partial \psi}{\partial \zeta}\dot{\zeta}\rho_0 - \frac{1}{T} Q_i T_{,i} \geq 0$$

σ_{ij} = stress (2nd Piola Kirchhoff stress) } Energy Congute

ε_{ij} = strain (Green Lagrangian Strain) }

ρ_0 = density at the reference configuration

ρ = density at the current configuration

$\{Q\}_{1\times3} = \frac{\rho_0}{\rho}\{q\}^T[[F]^{-1}]^T$

q ↓ heat flux vector

$$\psi = U - ST$$

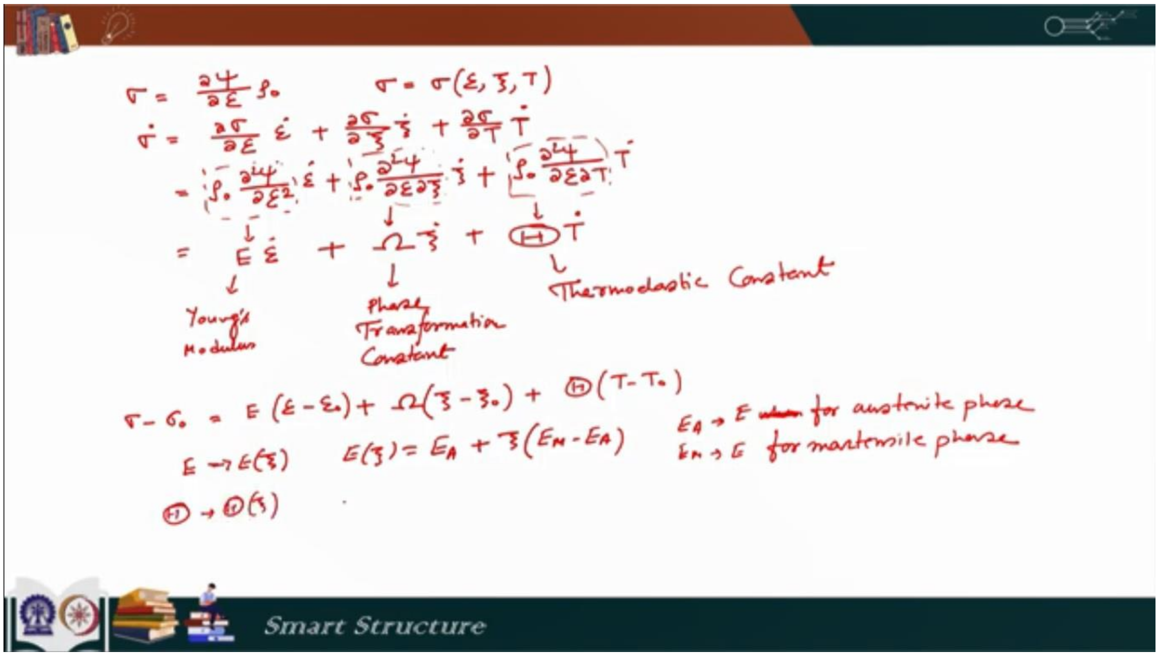
$$(\sigma_{ij} - \rho_0 \frac{\partial \psi}{\partial \varepsilon_{ij}})\dot{\varepsilon}_{ij} - \left(S + \frac{\partial \psi}{\partial T}\right)\dot{T} - \frac{\partial \psi}{\partial \zeta}\dot{\zeta}\rho_0 - \frac{1}{T} Q_i T_i \geq 0$$

$$\{Q\}_{1\times3} = \frac{\rho_0}{\rho}\{q\}^T[[F]^{-1}]^T$$

Now again when it comes to large deformation problems there are various types of stresses and various types of strain because our initial configuration and different configuration is significantly different. Now in this case this stress is second Piola Kirchhoff stress and this strain is Green Lagrangian strain. Both this stress about this second Piola Kirchhoff stress and Green Lagrangian stress are defined with respect to the undeformed or reference configuration. So, in when you talk about this second Piola Kirchhoff stress the force or area both are taken with respect to the reference configuration and these two stresses are energy conjugates. So, not any stress is energy conjugate of any strain.

So, this stress sigma second Piola Kirchhoff stress is the energy conjugate of Green Lagrangian stress strain. Now we have other quantities like rho 0 rho 0 is density at the reference configuration rho is the density at the current configuration. So, we can see that in this problem we are considering event density to be using two separate variables for the reference and current configuration and then we have a term Q here. So, Q as a vector Q as a 1 by 3 vector can be written as rho 0 divided by rho multiplied by q small q transpose multiplied by deformation gradient f which we defined before its inverse and its transpose where this q is heat flux vector. Now this equation gives us from this equation we can find out the constitutive relation.

(Refer slide time: 18:21)



$$\sigma = \frac{\partial\psi}{\partial\varepsilon}\rho_0 \qquad \sigma = \sigma(\varepsilon,\xi,T)$$

$$\dot\sigma = \frac{\partial\sigma}{\partial\varepsilon}\dot\varepsilon + \frac{\partial\sigma}{\partial\xi}\dot\xi + \frac{\partial\sigma}{\partial T}\dot T$$

$$= \rho_0\frac{\partial^2\psi}{\partial\varepsilon^2}\dot\varepsilon + \rho_0\frac{\partial^2\psi}{\partial\varepsilon\,\partial\xi}\dot\xi + \rho_0\frac{\partial^2\psi}{\partial\varepsilon\,\partial T}\dot T$$

$$= \underbrace{E}_{\text{Young's Modulus}}\dot\varepsilon + \underbrace{\Omega}_{\text{Phase Transformation Constant}}\dot\xi + \underbrace{\Theta}_{\text{Thermoelastic Constant}}\dot T$$

$$\sigma - \sigma_0 = E(\varepsilon-\varepsilon_0) + \Omega(\xi-\xi_0) + \Theta(T-T_0)$$

$E \rightarrow E(\xi)$ $\quad$ $E(\xi) = E_A + \xi(E_M - E_A)$ $\quad$ $E_A \rightarrow E$ ~~when~~ for austenite phase

$E_M \rightarrow E$ for martensite phase

$\Theta \rightarrow \Theta(\xi)$

Smart Structure

$$\sigma = \frac{\partial\psi}{\partial\varepsilon}\rho_0, \sigma = \sigma(\varepsilon,\xi,T)$$

$$\dot\sigma = \frac{\partial\sigma}{\partial\varepsilon}\dot\varepsilon + \frac{\partial\sigma}{\partial\xi}\dot\xi + \frac{\partial\sigma}{\partial T}\dot T = \rho_0\frac{\partial^2\psi}{\partial\varepsilon^2} + \rho_0\frac{\partial^2\psi}{\partial\varepsilon\,\partial\xi} + \rho_0\frac{\partial^2\psi}{\partial\varepsilon\,\partial T}\dot T$$

$$= E\dot\varepsilon + \Omega\dot\xi + \Theta\dot T$$

$$\sigma - \sigma_0 = E(\varepsilon - \varepsilon_0) + \Omega(\xi - \xi_0) + \Theta(T - T_0)$$

$$E(\xi) = E_A + \xi(E_M - E_A)$$

$$\Theta(\xi) = \Theta_A + \xi(\Theta_M - \Theta_A)$$

If we look at this quantity that tells us how the stress is related to the potential and the strain. So, we can write sigma is equal to del psi by del epsilon with rho 0 multiplied. Now here we intentionally dropped out those suffix as those subscripts i j to keep it simple and anyway finally, we will use it for one dimensional cases. So, that is fine. Now rho this sigma stress is a function of all the state variables epsilon psi and t.

So, in the rate form we can say that the rate of change of sigma with time sigma dot is equal to del sigma by del epsilon multiplied by epsilon dot plus del sigma by del xi multiplied by xi dot plus del sigma by del T multiplied by T dot. And again using this definition we can write it is equal to rho 0 multiplied by del 2 psi by del epsilon 2 multiplied by epsilon dot plus rho 0 multiplied by del 2 psi by del epsilon del xi multiplied by xi dot plus rho 0 multiplied by del 2 epsilon by del xi del 2 psi by del epsilon del T multiplied by T dot. Now this quantity gives a material constant E. So, we write it E multiplied by epsilon dot this quantity gives a term omega. So, we write omega multiplied by xi dot and then this quantity gives a term maybe we can use capital phi.

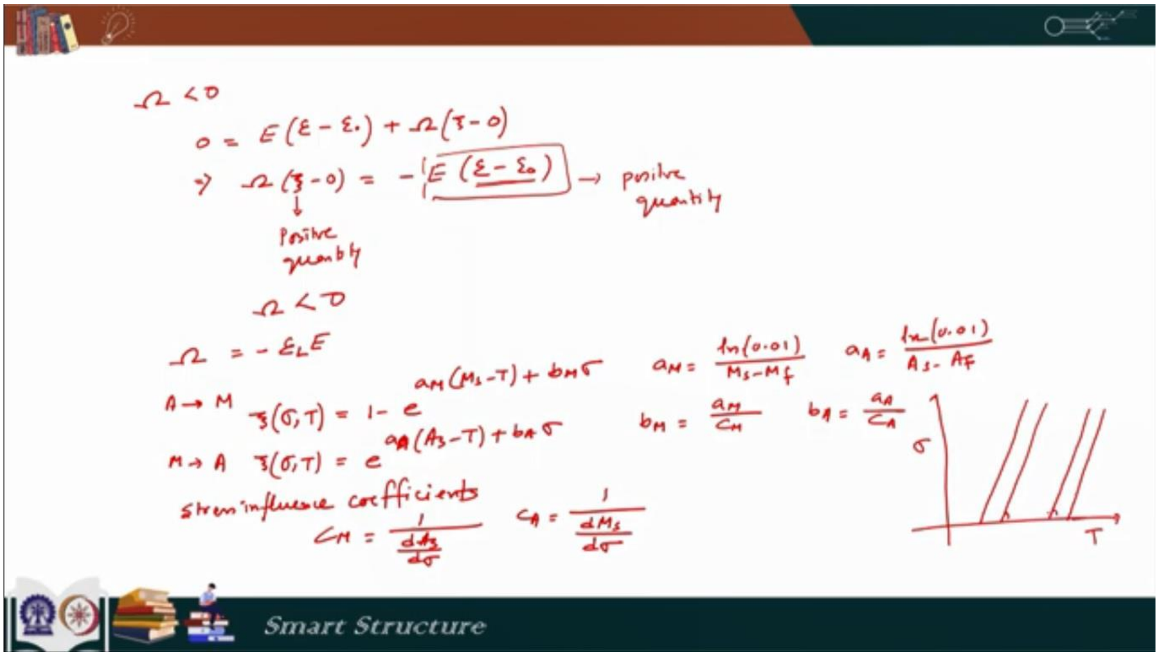
So, capital phi multiplied by T dot. So, this is Young's modulus if the material is linearly elastic we can call it Young's modulus. So, it just says if my strain changes what is the corresponding change in the stress this is a phase transformation constant and this is thermo elastic constant. Now if we integrate both side suppose the the stress is we are taking 2 time steps initial time step maybe ti the present time step tf and in between these 2 time step sigma is changing epsilon is changing xi is changing t is changing. So, it is changing from sigma 0 to sigma epsilon 0 to epsilon xi 0 to xi t 0 to t.

So, we can say sigma minus sigma 0 change in sigma equal to E multiplied by epsilon minus epsilon 0 plus omega multiplied by xi xi minus xi 0 plus capital phi multiplied by T Minus T 0. Now these constants E is in general a function of xi because we know that E has different values when the material is martensite and when it is austenite. So, when it is austenite xi is equal to 0 it has certain value of E and when it is martensite it xi is equal to 1 and it has a certain value of E. So, we can say E as a function of xi is E A which means E at the austenite phase plus xi multiplied by E M Minus E A. So, we are using a rule of mixture here.

So, at any point of time the material can be a can have certain martensite fraction. So, based on the martensite fraction the effective E is this where E A is E E for austenite phase and E M is E for martensite phase. Accordingly, even phi can also be defined as a function of xi using the rule of mixture. So, phi can be different for austenite and martensite phase and accordingly the rule of mixture gives phi as a function of xi as this. Now although E is a function of xi, but in many cases specially in these models we will in some cases we will assume them to be constant to derive few relations.

Now comes omega now comes omega is less than 0 and this can be proved also using some simple logic. Let us say that it is transforming from austenite to martensite. Now during this transformation the stress is constant we are keeping the material free. So, there is no stress involved it is a purely temperature driven transformation. So, if you write the equation constitutive relation sigma minus sigma 0 is equal to 0 and during this transformation stress changes sorry strain changes.

(Refer slide time: 25:38)



$$\Omega < 0$$

$$0 = E(\varepsilon - \varepsilon_0) + \Omega(\xi - 0)$$

$$\Rightarrow \underset{\text{Positive quantity}}{\Omega(\xi - 0)} = -\boxed{E(\varepsilon - \varepsilon_0)} \rightarrow \text{positive quantity}$$

$$\Omega < 0$$

$$\Omega = -\varepsilon_L E$$

$$A \rightarrow M \quad \xi(\sigma, T) = 1 - e^{a_M(M_s - T) + b_M\sigma} \qquad a_M = \frac{\ln(0.01)}{M_s - M_f} \qquad a_A = \frac{\ln(0.01)}{A_s - A_f}$$

$$M \rightarrow A \quad \xi(\sigma, T) = e^{a_A(A_s - T) + b_A\sigma} \qquad b_M = \frac{a_M}{c_M} \qquad b_A = \frac{a_A}{c_A}$$

stress influence coefficients

$$c_M = \frac{1}{\frac{dA_s}{d\sigma}} \qquad c_A = \frac{1}{\frac{dM_s}{d\sigma}}$$

$$\Omega < 0$$

$$0 = E(\varepsilon - \varepsilon_0) + \Omega(\xi - 0) \Rightarrow \Omega(\xi - 0) = -E(\varepsilon - \varepsilon_0)$$

$$\Omega = -\varepsilon_L E$$

$$\xi(\sigma, T) = 1 - e^{a_M(M_S - T) + b_M\sigma}, a_M = \frac{ln(0.01)}{M_s - M_f}, a_A = \frac{ln(0.01)}{A_s - A_f}$$

$$\xi(\sigma, T) = e^{a_A(A_s - T) + b_A\sigma}, b_M = \frac{a_M}{c_M}, b_A = \frac{a_A}{c_A}$$

$$c_M = \frac{1}{\frac{dA_S}{d\sigma}}, c_A = \frac{1}{\frac{dM_S}{d\sigma}}$$

So, that is epsilon minus epsilon 0 epsilon 0 may be a initial strain during the marten austenite phase it can be 0 also and then plus omega multiplied by xi minus 0 because initially in the austenite phase omega was xi was 0 during transformation at some point of time we have xi when transformation completes it becomes 1 and plus we have the phi term. Now the effect of that phi term is generally much less than the effect of these two terms. So, the strain due to the temperature much is generally much less than the I mean stress due to the temperature is generally much less than due to the other quantities. So, we can we are not writing that and even if you write that. So, whatever the expansion whatever the contraction is there due to reduction in temperature that is much less than the expansion due to the phase transformation.

So, we are not writing that. So, we can write this same quantity as minus of xi 0. Now temperature is reducing it is becoming martensite. Now when it becomes martensite it strains. So,   it expands. So, this means that this quantity is a positive quantity and E is also a positive quantity.

So, it is a positive quantity xi is a positive quantity. So, that tells me that omega is a negative quantity. So, omega is negative and also omega is related to the Young's modulus using this equation. Now this we are not going to discuss in details here later on when we talk about the Liang and Rogers model we will talk about this relation in more details because that is written in the paper by Liang and Rogers. So, this was the first part of the constitutive relation where we related stress change with strain change.

So, now, we already have a relation that relates strain change with strain change martensite fraction change at temperature change. Now we will need one more relation which relates the evolution of xi the change of xi with stress and temperature. Now in the last week we already worked on that and we derived some relations based on some cosine functions, but that is not used in Tanaka model. In Tanaka model change in xi is related using exponential formulation. So, for austenite to martensite transformation as per Tanaka model xi is xi as a function of sigma and T is 1 minus a M multiplied by M s minus T plus b M sigma and for martensite to austenite transformation xi as a function of sigma and T is e to the power a A multiplied by a Ss minus T plus b A sigma.

Now these quantities a M are defined as natural log of 0.01 divided by M s minus M f and we have a A that is natural log of 0.01 divided by A s minus A f and then we have and then we have b M that is equal to a M by c M and then we have b A and that is equal to A a by C A and this C A and C M are stress influence coefficients and they are defined as C M equal to 1 by d of A s by d sigma and C A equal to 1 by d of M s by d sigma. So, if you look at the phase transformation diagram that we drew before in the sigma T plane this is T and this is sigma and we have the slope of these lines A s and m s. So, d A s by d sigma is just the slope of this line and d m s by d sigma is just the slope of this line.

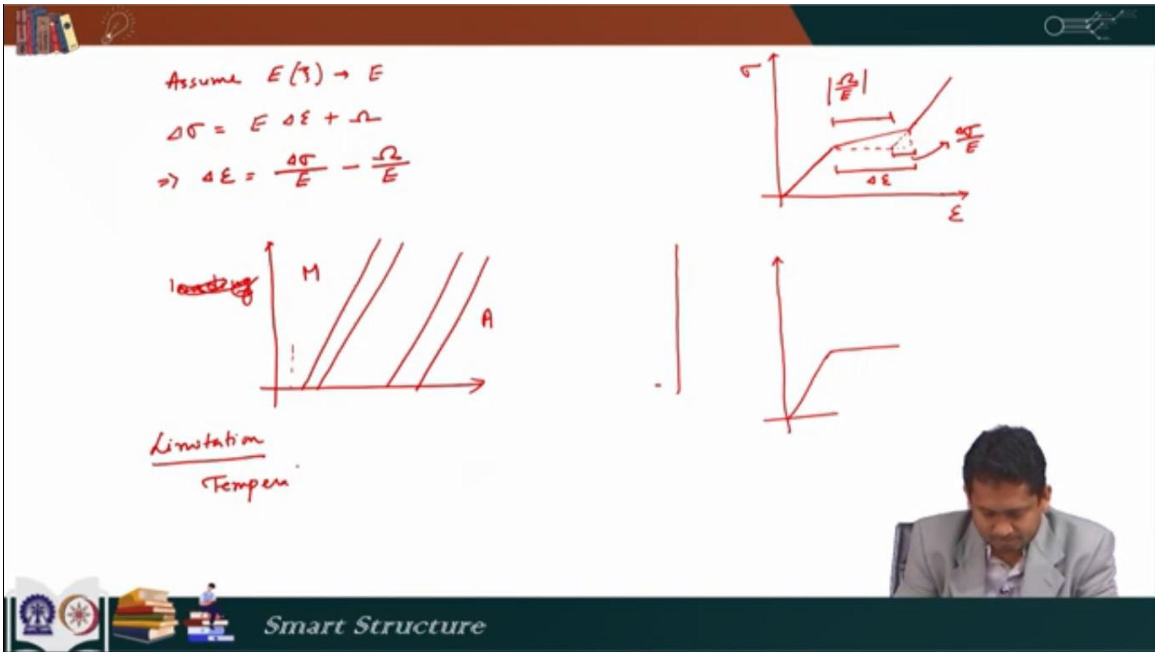
Now we will look into a very look into a phenomenon with some simplistic point of view. So, let us assume E is independent of psi. So, is constant that is a big assumption because we know that E m and E a are quite different however, sometimes these assumptions help to derive few things and these assumptions you will find in the paper by Tanaka in the second one that that we listed at the beginning. So, if we assume that the material is austenite at the beginning and then gradually we are increasing the gradually it is being loaded. So, stress strain curve is following a linear fashion when the transformation starts the slope changes and then after the transformation after it is fully martensite it again follows the same thing.

Now from here if we write if taking this as the starting position if we write the constitutive relation here we can write delta of sigma is equal to E multiplied by delta of epsilon plus omega that we are writing when the transformation has finished. So, xi has become 1. So, from here to here the change in sigma is sigma minus sigma 0 which is delta sigma from here to here change in strain is delta epsilon and from here to here change in xi is 1 because here transformation just started. So, xi was 0 here transformation finish.

So, xi is 1. So, that is the relation. So, we can write delta of epsilon equal to delta of sigma divided by E minus omega divided by E. So, graphically this quantity is my change in strain. So, that is delta of epsilon and if we draw the line and extend it and it intersects here. So, we can show it here may be. So, this quantity and we have two different quantities this quantity and this one.

Now this quantity is omega by E and it is modulus and this quantity is my delta sigma by. So, we will look into these things in more details when we talk about the next model that is the Liang and Rogers model. Now again to summarize this model started from a thermodynamic potential which is Helmer's potential and then using the second law of thermodynamics with other conservation laws we got the constitutive relation. And in this entire we have two relations one is the relation that is between the change in stress with change in strain change in martensite fraction and change in temperature and there is another relation that shows the evolution of xi with sigma and T. With those we can solve the problems and related to shape memory alloys.

(Refer slide time: 30:49)


Assume $E(\xi) \to E$

$\Delta\sigma = E\,\Delta\varepsilon + \Omega$

$\Rightarrow \Delta\varepsilon = \frac{\Delta\sigma}{E} - \frac{\Omega}{E}$

Limitation

Temper

$$E(\xi) \to E$$

$$\Delta\sigma = E\Delta\varepsilon + \Omega \Rightarrow \Delta\varepsilon = \frac{\Delta\sigma}{E} - \frac{\Omega}{E}$$

Now here one big thing that is missing in the model is it does not take care of the stress and temperature induced martensite separately. So, in the phase diagram we had this as we know this is austenite zone this is martensite zone, but in the martensite zone as we increase the stress the material is supposed to de twin. So, it is supposed to transform from temperature to martensite stress induced martensite, but those things are not in count taken care of in this model. So, that is a limitation. So, the limitation is temperature and stress induced martensite are not treated separately or differentiated.

So, later on when we see the Brinson's model we see that there is an effort to overcome this limitation. So, with this I would like to conclude this lecture here.

Thank you.