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One Dimensional Modeling the Pseudoelastic Effect of Shape Memory Alloys

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***Abstract* – This work aims to develop a model to describe the macroscopic behavior of shape memory alloys (SMAs) under mechanical loading in isothermal conditions. To build the model we have made recourse to thermodynamics laws, followed by writing an expression of a thermodynamic potential with internal and control variables. We have used assumptions about the homogeneity and isotropy of the material. We have extracted constitutive equations and written the transformation criteria. To investigate the response of this model we simulated a tensile test performed on an alloy $Ni_{54.1}Ti_{45.9}$ and to validate the efficiency we compared the results with experimental data and there was a good consensus between the prediction model and experimental observations finally to give more credibility to this work we have implemented the model in Abaqus software.**

***Keywords* – Shape, Pseudoelasticity, Thermodynamic, Transformation.**

I. Introduction

The shape memory alloys (SMA) as they are called have a singular behavior, they can be largely deformed (about 10%) under an applied mechanical, a simple heating is sufficient to recover the previous form, that is why they are called that way. By varying controlled parameters (stress and temperature) these alloys can exhibit other properties like pseudoelasticity, two-way shape memory effect, one-way shape memory effect [1], [2], reorientation effect [3].

These properties have allowed an important number of applications in particularly biomedical and aerospace fields [4]

To describe the shape memory alloys behavior many models were developed [1], [5]. It should be noted that SMA properties derived from phases transformations i.e. higher temperature phase (austenite) to lower temperature phase (martensite) (Fig1.)

This paper aims to develop a simple phenomenological model to describe pseudoelasticity property and validate it numerically using a developed algorithm and as a last step to implement it in Abaqus software. In the first party we built the constitutive model using thermodynamic laws, in the last one we use data provided by (Ng et al) work to simulate the response of the model and compare it with experimental data.

II. Methods

2.1 Presentation of the subject

Pseudoelasticity is obtained with applying a thermomechanical loading heating cycle above a temperature $T^1 > A_f^0$ (Temperature of finish of austenite transformation) and applying a mechanical loading then the material undergoes a large deformation. When applied stress is canceled the alloy recovers its initial shape. (Fig3.). The significant deformation is due to the transformation of austenite to martensite.

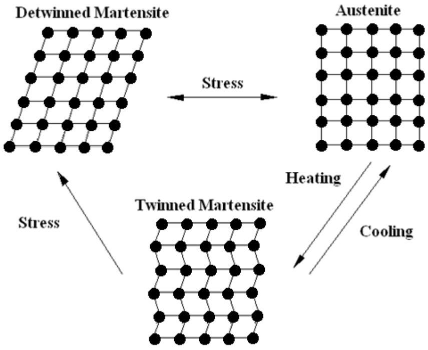

Fig.2. Phase change under thermomechanical loads.

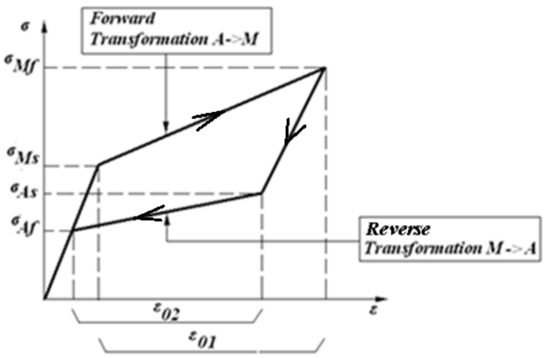

Fig.3. Pseudoelasticity effect

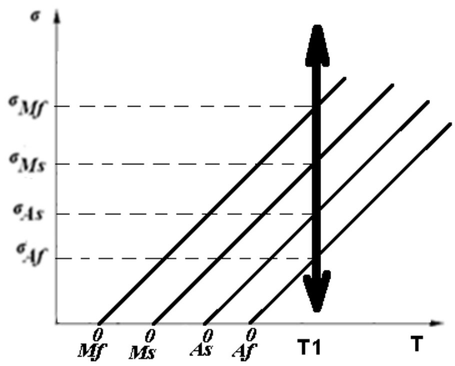

Fig.4. Loading Path

ε_{01} : Maximum deformation of direct transformation
ε_{02} : Maximum deformation of reverse transformation
σ_{Ms} : Stress of transformation start of Austenite to Martensite

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σ_{Mf} : Stress of transformation finish of Austenite to Martensite

σ_{As} : Stress of transformation start of Martensite to Austenite

σ_{Af} : Stress of transformation finish of Martensite to Austenite

2.2 Constitutive equations

We consider a representative elementary volume REV of austenite with sufficient size to have a fraction of martensite when the transformation occurs. **(Fig4.)**

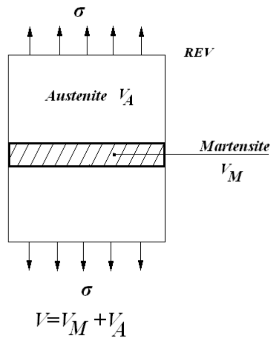

Fig.4. The representative elementary volume (REV).

Fraction of Martensite $f = \frac{V_M}{V}$

The macroscopic strain:

$$\mathrm{E} = \mathrm{E}^e + \varepsilon^t \quad (1)$$

ε^t: Deformation due to transformation Austenite to Martensite directly related to the formation of Martensite:

$$\varepsilon^t = f.\varepsilon_0 \quad (2)$$

ε_0: Maximum strain of transformation

$$\varepsilon_0 = \begin{cases} \varepsilon_{01} & forward\ transformation \\ \varepsilon_{02} & reverse\ transformation \end{cases}$$

E^e: Overall elastic deformation:

$$\mathrm{E}^e = f.\varepsilon_M^e + (1-f).\varepsilon_A^e \quad (3)$$

ε_M^e; ε_A^e : Respectively elastic deformation of formed Martensite and elastic deformation of remaining Austenite

$$\varepsilon_M^e = \frac{\sigma}{E_M} \quad (4)$$

$$\varepsilon_A^e = \frac{\sigma}{E_A} \quad (5)$$

E_M, E_A : Respectively Young modulus of Martensite and Austenite

The thermodynamic potential is Gibbs free energy:

$$\Psi(\sigma, T, f) = W_m + W_{ch} + W_{int} \quad (6)$$

- W_m: Mechanical energy:

$$W_m = -\sigma.E \quad (7)$$

Using equations (1) ,(2),(3),(4) W_e can be written

$$W_m = -\frac{\sigma^2}{2}\left(\frac{1-f}{E_A} + \frac{f}{E_M}\right) - \sigma.f.\varepsilon_0 \quad (8)$$

- W_{ch} : Chemical free energy due to phase change

$$W_{ch} = f.B.(T - T_0) \quad (9)$$

T_0 : Reference temperature; $T_0 = M_s^0$ (M_s^0 temperature of transformation start of Martensite)

- W_{int} : Interaction energy which is a function of the fraction of Martensite

We can choose the expression:

$$W_{int} = C.f.(f-1) \quad (10)$$

Gibbs free energy can be written:

$$\Psi(\sigma, T, f) = \frac{\sigma^2}{2}\left(\frac{1-f}{E_A} + \frac{f}{E_M}\right) - \sigma.f.\varepsilon_0 + f.B.(T - T_0) + C.f.(f-1) \quad (11)$$

B and *C:* coefficients to be determined

E_A; E_M: Young modulus respectively of Austenite and Martensite

The second principle of thermodynamic expressed by Clausius inequality gives:

$$-\frac{d\Psi}{df}.\dot{f} \geq 0 \quad (12)$$

We can write:

$$F^{th} = -\frac{\partial\Psi}{\partial f} \quad (13)$$

F^{th}: The driving force is deriving from the potential $\Psi(\sigma, T, f)$

Clausius inequality becomes:

$$F^{th}.\dot{f} \geq 0 \quad (14)$$

$$F^{th} = \frac{\sigma^2}{2}\left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \sigma.\varepsilon_0 - B.(T - T_0) - C.(2f - 1) \quad (15)$$

It should be important to observe the hysteresis appearing when the inverse transformation happens, dissipation takes place. The dissipative force F^{di} will oppose the driving force F^{th} :

$$F^{th} = F^{di} \quad (16)$$

F^{di} Can be given as following:

$$F^{di} = Gf + H \quad (17)$$

G and H are coefficients to be determined

Considering conditions of direct and reverse transformations we can write the following:

$$\begin{cases} F^{th} = F^{di};\ \dot{f} > 0 & Forward\ transformation \\ F^{th} = -F^{di};\ \dot{f} < 0 & Reverse\ transformation \end{cases} \quad (18)$$

a) Forward transformation

From equation (16) we obtain:

$$F^{th} - F^{di} = 0 \quad (19)$$

Using consistency conditions we obtain:

$$\dot{F}^{th} - \dot{F}^{di} = 0 \quad (20)$$

Finally:

$$\frac{\sigma^2}{2}\left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \sigma.\varepsilon_{01} - B.(T - T_0) - C.(2f - 1) - Gf - H = 0 \quad (21)$$

Let us write:

$$\frac{\sigma^2}{2}\left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \sigma.\varepsilon_{01} - B.(T - T_0) - C.(2f - 1) - Gf - H = \varphi^1(\sigma, T, f) \quad (22)$$

$$\frac{\partial\varphi^1(\sigma, T, f)}{\partial t} = \frac{\partial\varphi^1}{\partial\sigma}\frac{d\sigma}{dt} + \frac{\partial\varphi^1}{\partial T}\frac{dT}{dt} + \frac{\partial\varphi^1}{\partial f}\frac{df}{dt} = 0 \quad (23)$$

Equation (20) gives:

$$\left[\sigma\left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \varepsilon_{01}\right]\dot{\sigma} - B.\dot{T} - (2C + G);\dot{f} > 0 \quad (24)$$

$$\dot{f} = \frac{1}{(2C+G)}\left[\left[\sigma\left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \varepsilon_{01}\right]\dot{\sigma} - B.\dot{T}\right] \quad (25)$$

Equation (25) determines the evolution of the transformation

In our case the transformation is isothermal: $\dot{T} = 0$

$$\dot{f} = \frac{1}{(2C+G)}\left[\sigma\left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \varepsilon_{01}\right]\dot{\sigma} \quad (26)$$

b) Reverse transformation

Doing the same as previously:

$$\frac{\sigma^2}{2}\left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \sigma.\varepsilon_{02} - B.(T - T_0) - C.(2f - 1) + Gf + H = 0 \quad (27)$$

$$\frac{\sigma^2}{2}\left(\frac{1}{E_M}-\frac{1}{E_A}\right)+\sigma.\varepsilon_{01}-B.(T-T_0)-C.(2f-1)+Gf+H=\varphi^2(\sigma,T,f) \quad (28)$$

$$\left[\sigma\left(\frac{1}{E_M}-\frac{1}{E_A}\right)+\varepsilon_{02}\right]\dot{\sigma}-B.\dot{T}-(2C-G);\dot{f}<0 \quad (29)$$

$$\dot{f}=\frac{1}{(2C-G)}\left[\sigma\left(\frac{1}{E_M}-\frac{1}{E_A}\right)+\varepsilon_{01}\right]\dot{\sigma}-B.\dot{T};\dot{f}<0 \quad (30)$$

As previous the transformation is isothermal: $\dot{T}=0$

$$\dot{f}=\frac{1}{(2C+G)}\left[\sigma\left(\frac{1}{E_M}-\frac{1}{E_A}\right)+\varepsilon_{01}\right]\dot{\sigma} \quad (31)$$

Behavior law can be obtained from:

$$\varepsilon=-\frac{\partial\Psi}{\partial\sigma} \quad (32)$$

$$\varepsilon=\sigma\left(\frac{1}{E_M}-\frac{1}{E_A}\right)+f.\varepsilon_0 \quad (33)$$

2.3. Transformation Criteria

2.3.1. Before transformation (elastic deformation):

$$\varphi^1(\sigma,T=T_1,f=0)=\frac{\sigma^2}{2}\left(\frac{1}{E_M}-\frac{1}{E_A}\right)+\sigma.\varepsilon_{01}-B.(T_1-T_0)+C-H \quad (34)$$

Let us derive $\varphi^1(\sigma)$:

$$\frac{d\varphi^1}{d\sigma}=\sigma\left(\frac{1}{E_M}-\frac{1}{E_A}\right)+\varepsilon_{01} \quad (35)$$

It is noted that the austenite is more rigid than the martensite $\left(\frac{1}{E_M}-\frac{1}{E_A}\right)>0$ and $\sigma>0$; $\varepsilon_{01}>0$ gives:

$$\frac{d\varphi^1}{d\sigma}>0 \quad (36)$$

We deduce: $\varphi^1(\sigma)$ is an increasing function:

$$\varphi^1(\sigma,T=T_1,f=0)<0 \;;f=0;\dot{f}=0 \quad (37)$$

2.3.2. Transformation is occurring

$$\varphi^1(\sigma,T=T_1,f)=0 \quad (38)$$

$0\le f\le 1$ and $\dot{f}>0$

2.4.3. After transformation (elastic deformation)

Doing the same as for section 2.3.1 we obtain:

$$\varphi^1(\sigma,T=T_1,f=0)>0;f=1;\dot{f}=0 \quad (39)$$

2.4. Determination of coefficients B, C, G, H

2.4.1 Forward transformation

We use:

$$\varphi^1(\sigma,T,f)=0;\sigma=\sigma_{Ms}\;;f=0 \quad (40)$$

$$\varphi^1(\sigma,T,f)=0;\sigma=\sigma_{Mf}\;;f=1 \quad (41)$$

2.4.2. Reverse transformation

We use:

$$\varphi^2(\sigma,T,f)=0;\sigma=\sigma_{As}\;;f=1 \quad (42)$$

$$\varphi^2(\sigma,T,f)=0;\sigma=\sigma_{Af}\;;f=0 \quad (43)$$

2.5. Model parameters and simulation

σ_{Ms} ; σ_{Mf} ; σ_{As} ; σ_{Af} ; E_A; E_M; ε_{01}; ε_{02} are parameters to be determined from a test of tensile performed on a tube of NiTi at T=70°C and a mechanical loading $\sigma=400MPa$ (Table1.), [5]

To simulate the model response using experimental data, we have used a Fortran program and finite elements software which Abaqus

Table 1: Parameters of the model

σ_{Ms} (MPa)	300
σ_{Mf} (MPa)	305
σ_{As} (MPa)	100
σ_{Af} (MPa)	50
E_A (MPa)	25775
E_M (MPa)	18442
M_s^0 (K)	279
M_f^0 (K)	240
A_s^0 (K)	297
A_f^0 (K)	330
ε_{01}	0.06106
ε_{02}	0.05903
B (MPa.K^{-1})	1.788898E-01
C (MPa)	8.141997E-01
G (MPa)	-1.323100
H (MPa)	7.683250

The used specimen is a wire NiTi 100 mm length and having a box profile 10 x10 mm^2

III. RESULTS

The results are presented below.

3.1. Using Fortran program:

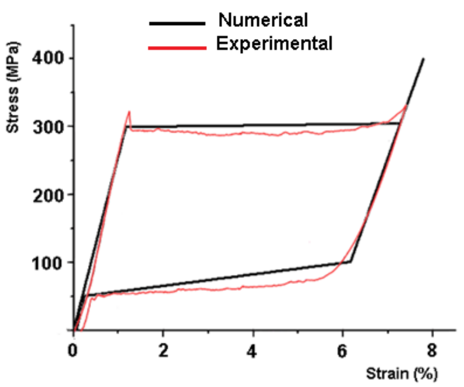

Fig.5. Model response (T=70°C, σ=400MPa) (with Fortran program)

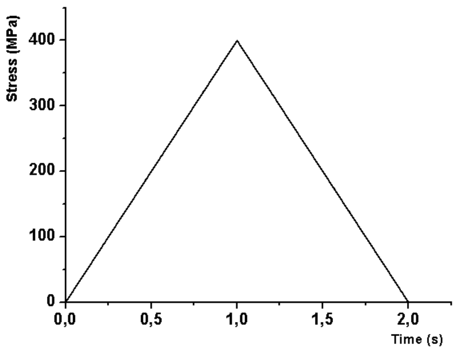

Fig.6. Loading history

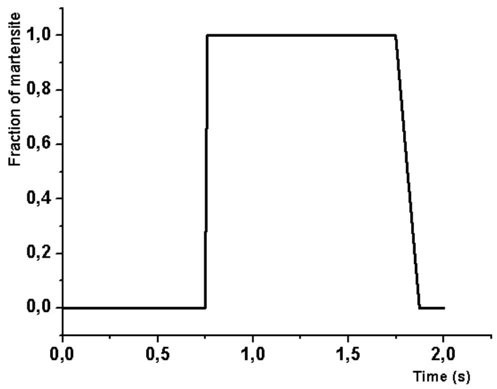

Fig.7. Fraction of martensite history

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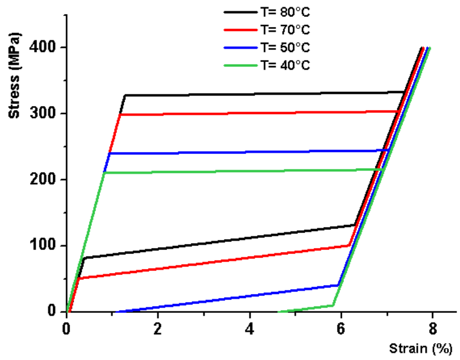

Fig.8. Response of the model at different temperatures

3.2. Using Abaqus UMAT

In addition to predefined laws of behaviour embedded, Abaqus is configured to include personalized constitutive models by using UMAT subroutine.

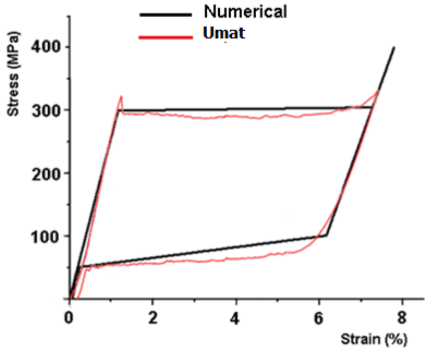

Fig.9. Model response (T=70°C, σ=400MPa) (with Abaqus UMAT)

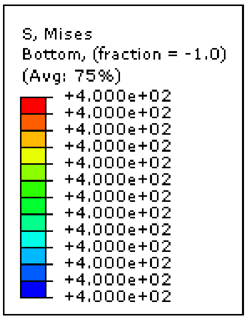

Fig.10. Stress Von Mises at the end of loading step

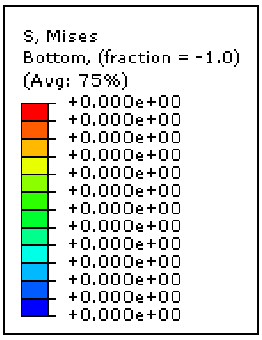

Fig.11. Stress Von Mises at the end of unloading step

IV. Discussions

By analyzing the figures (Fig5.) and (Fig9.) show a good agreement with experimental data especially (Fig5.) because of accuracy of the program but the (Fig9.) show an offset of approximately 0.0024 which means 2% in terms of precision. The figure (Fig7.) shows the evolution of martensite fraction according to macroscopic strain when the transformation occurs. The results shown by (Fig8.) imply the ability of the model to respond at different temperatures according the linear relationship between stress and temperature when transformation occurs.

The model was implemented in Abaqus so the figures (Fig10.; Fig11.) show Von Mises stress at the end of analysis of the steps of loading and unloading

We think that these results obtained by developed program and UMAT are satisfactory.

Conclusion

The behavior of shape memory alloys has several forms, among them we focused on the pseudoelasticity which is a property very required in industrial applications and despite the multitude of models developed we have built a constitutive model which seems very simple in terms of formulation.

First we have used thermodynamics principle to write constitutive equations and deduce transformation criteria, taking into account the kinetics of the transformation.

Using experimental data provided by tensile test, has allowed defining parameters of the model. The simulation was performed using a personal program and Abaqus Umat, the results were satisfactory according to experimental data and the model seems to respond well at different temperatures.

The developed model with its simplicity can be used to describe the effect of pseudoelasticity and can be used in engineering areas.

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