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Three Dimensional Modeling and a Simulation of the Shape Memory Effect

Belkacem Meddour[1)]
Zedira Hamma[2)]
Djebaili Hamid[2)]

The paper deals with modeling and simulating the shape memory effect , one of many behaviors of shape memory alloys. The effect was first divided into three stages. Every stage has its own thermodynamic potential and constitutive equations. The martensite fraction is the only internal variable to be considered: in the first stage, it represents the fraction of detwinned martensite; in the second stage, it represents the fraction of transformed martensite into austenite, and in the last stage, it represents the fraction of the produced martensite from the austenite transformation.

For every stage, we deduced the constitutive equations using the principles of thermodynamics and a simple formalism. When the model was defined, we simulated it using the experimental data obtained by analyzing a cube specimen subjected to triaxial traction and thermal load. The obtained results of this simulation reflect the behavior of this kind of materials when thermomechanical load is applied. The main finding of this paper is that the proposed constitutive model can be used to simulate the shape memory effect.

Key words: **martensite, thermomechanical load, modelling, fraction, shape memory effect, process simulation, experimental results.**

Introduction

IN the last decades, shape memory alloys (SMA) have occupied an important place in the world of advanced materials. They have a singular behavior comparable to conventional materials - they can be largely deformed (about 10%) (Kimiecik et al, 2013), (Zhong et al, 2012) under applied mechanical stress and simple heating is sufficient to recover their previous form. With varied controlled parameters (stress and temperature), these alloys can exhibit other properties such as pseudoelasticity, two-way shape memory effect, one-way shape memory effect (Arghavani et al, 2010), (Yutaka et al,2004), (Tonga et al, 2012) and reorientation effect **(**Pan et al, 2007). In addition to the previous properties, damping could be mentioned as an important property (Abdulridha et al, 2013).

These properties have allowed an important number of applications, particularly in biomedical and aerospace fields (Lagoudas et al, 2008), and some recent studies have been conducted to apply the damping property in seismic design (Abdulridha et al, 2013),(Eunsoo et al, 2013).

To describe the shape memory alloys behavior, many models have been developed (Arghavani et al, 2010), (Ng et al, 2006)**.** The shape memory effect is one of their most important properties. It requires three different stages:

1. Mechanical loading and unloading: at this stage, the structure is largely deformed after removing load because martensite is detwinned
2. Heating: the structure recovers its previous shape because martensite is transformed to austenite
3. Cooling: the structure undergoes only a phase change i.e. austenite is transformed to twinned martensite

The aim of this paper is to build a three dimensional constitutive model to describe the shape memory effect taking into account the three stages. In every stage we have proposed an expression of Gibbs free energy and, using the principles of thermodynamics, we have extracted the laws governing this behavior. Finally, we have performed a numerical simulation on a cubic Nitinol (NiTi) specimen (Ng et al, 2006).

Methods

The expression of Gibbs free energy is written as follows

$$G(\sigma,T,f) = -\sigma : S_M : \sigma - f\varepsilon_0\sigma R + fB\left(T - M_s^0\right) + Cf(1-f) \tag{1}$$

ε_0 : Uniaxial maximum deformation

f : Fraction of martensite $f \geq 0$ and $f \leq 1$

R : 2nd order tensor of the transformation given by:

$$R_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma : \sigma}} \tag{2}$$

S_M : 4th order complaisance tensor of martensite

B et C: Constants to be determined by a tensile test of pseudoelasticity.

a) Transformation criteria:

Assuming that transformation of austenite to martensite occurs with dissipation due to a phase change i.e. to the size of martensite (a fraction of martensite).

Then the driving force can be written:

1) University of Batna, Department of Mechanical Engineering, ALGERIA
2) University Abbas Laghrour, Labo LaSPI^{2}A Department of Mechanical Engineering, Khenchela, ALGERIA

$$F^{th} = -\frac{\partial G}{\partial f} = \varepsilon_0 \sigma : R - B\left(T - M_s^0\right) + C\left(2f - 1\right) \quad (3)$$

The chosen expression of the dissipative force will be:

$$F^{di} = Kf + H \quad (4)$$

The forward and reverse transformations will occur if the following conditions are satisfied:

$$\begin{cases} F^{th} = F^{di}; & \dot{f} > 0 \quad \text{Forward transformation} \\ F^{th} = -F^{di}; & \dot{f} < 0 \quad \text{Reverse transformation} \end{cases} \quad (5)$$

Let us write the criteria function:

$$\varphi^{di}\left(\sigma, T, f\right) = F^{th} - F^{di}$$

Forward transformation:

$$\begin{aligned} &\varphi^{di}\left(\sigma, T, f\right) = \varepsilon_0 \sigma : R - B\left(T - M_s^0\right) + \\ &+ C\left(2f - 1\right) - Kf - H; \quad \dot{f} > 0 \end{aligned} \quad (6)$$

Reverse transformation

$$\begin{aligned} &\varphi^{re}\left(\sigma, T, f\right) = \varepsilon_0 \sigma : R - B\left(T - M_s^0\right) + \\ &+ C\left(2f - 1\right) + Kf + H; \quad \dot{f} < 0 \end{aligned} \quad (7)$$

The transformation occurs when:

$$\varphi^{di}\left(\sigma, T, f\right) = 0 \quad (8)$$

The consistency condition gives:

$$d\varphi^{di}\left(\sigma, T, f\right) = 0 \quad (9)$$

$$\frac{\partial \varphi^{di}}{\partial \sigma} d\sigma + \frac{\partial \varphi^{di}}{\partial T} dT + \frac{\partial \varphi^{di}}{\partial f} df = 0 \quad (10)$$

Equations (9) and (10) give the evolution of the martensite fraction:

$$df = \frac{\varepsilon_0 R : d\sigma - Bdt}{K - 2C}; \quad f > 0 \quad (11)$$

$$df = \frac{\varepsilon_0 R : d\sigma - BdT}{K + 2C}; \quad f < 0 \quad (12)$$

Strain can be obtained as follows:

$$\varepsilon = -\frac{\partial G}{\partial \sigma} \quad (13)$$

$$\varepsilon = S_M : \sigma + f \varepsilon_0 R \quad (14)$$

Total strain is composed of elastic and transformation strains:

$$\varepsilon = \varepsilon^e + \varepsilon^t \quad (15)$$

ε^e : Elastic strain

ε^t : Transformation strain

$$\varepsilon^e = S_M : \sigma \quad (16)$$

$$\varepsilon^t = f \varepsilon_0 R \quad (17)$$

$$d\varepsilon = d\varepsilon^e + d\varepsilon^t \quad (18)$$

$$d\varepsilon^t = df \varepsilon_0 R \quad (19)$$

Equations (10), (11) and (9) give:

$$d\varepsilon^t = -\frac{\varepsilon_0^2}{K - 2C} R \times R : d\sigma - \frac{\varepsilon_0 BR}{K - 2C} dT; \quad \dot{f} > 0 \quad (20)$$

$$d\varepsilon^t = -\frac{\varepsilon_0^2}{K + 2C} R \times R : d\sigma + \frac{\varepsilon_0 BR}{K + 2C} dT \quad (21)$$

($\times$) means tensor product.

Let us assign to every stage its free energy because of different interactions of the phases in the three cases:

b) Stage of orientation:

$$\begin{aligned} &G_1\left(\sigma, T, f\right) = -\sigma : S_M : \sigma - f\varepsilon_0 : R + \\ &+ fB\left(T - M_s^0\right) + Cf\left(1 - f\right) \end{aligned} \quad (22)$$

$$\begin{aligned} &\varphi_1\left(\sigma, T, f\right) = \varepsilon_0 \sigma : R - B\left(T - M_s^0\right) - \\ &- Cf\left(1 - 2f\right) - a_1 - a_1 f \end{aligned} \quad (23)$$

$$d\varepsilon^t = \frac{\varepsilon_0^2}{a_1 - 2C} R \times R : d\sigma \quad (24)$$

c) Stage of heating:

$$G_2\left(\sigma, T, f\right) = +fB\left(T - M_s^0\right) + Hf\left(1 - f\right) \quad (25)$$

$$\begin{aligned} &\varphi_2\left(\sigma, T, f\right) = \varepsilon_0 \sigma : R - B\left(T - M_s^0\right) - \\ &- H\left(1 - 2f\right) + a_2 f + b_2 \end{aligned} \quad (26)$$

B and H are determined by a tensile test of pseudoelasticity [5].

a_1 and C are determined by a tensile test of orientation [5]:

$$df = \frac{BdT}{2H + a_2} \quad (27)$$

$$d\varepsilon^t = \frac{B\varepsilon_0}{2H + a_2} R \quad (28)$$

d) Stage of cooling:

$$G_\delta\left(\sigma, T, f\right) = fB\left(T - M_s^0\right) + Hf\left(1 - f\right) \quad (29)$$

$$\begin{aligned} &\varphi_2\left(\sigma, T, f\right) = -B\left(T - M_s^0\right) - \\ &- H\left(1 - 2f\right) - a_2 f - b_2 = 0 \end{aligned} \quad (30)$$

$$df = \frac{BdT}{2H - a_2} \quad (31)$$

$$d\varepsilon^t = 0 \quad (32)$$

The experimental data were provided by the performed tests of pseudoelasticity and orientation on an NiTi specimen [5].

Table 1. Experimental data [5]

M_s^0	279K	EA	25775MPa
M_f^0	240K	σ_s	70MPa
A_s^0	296K	σ_f	120MPa
A_f^0	330K	B	0.1874MPa.K^{-1}
E_M	18442MPa	C	3.4577MPa
a_1	10.118MPa	a_2	-22.388MPa
b_2	17.661MPa	H	8.0074MPa
a_3	23.232MPa	b_3	-8.0074MPa
ε_0	0.04064		

To perform a numerical simulation, we have considered an NiTi cubic specimen subjected to triaxial traction $\sigma_{11} = \sigma_{22} = \sigma_{33} = 400\,\text{MPa}$

Results and Discussion

a) Orientation

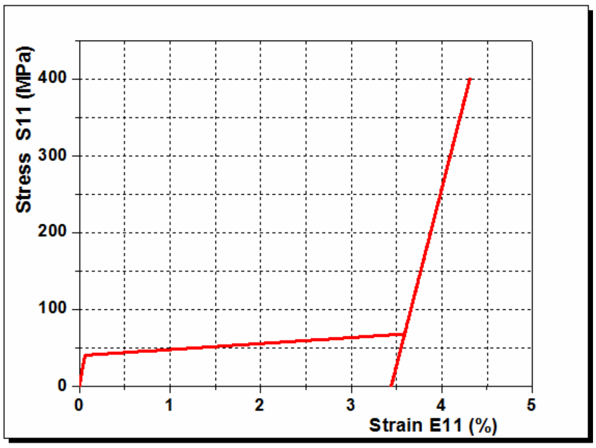

Figure 1. Plot $\varepsilon_{11} - \sigma_{11}$

Fig.1 shows the plot $\varepsilon_{11} - \sigma_{11}$ which begins with a small elastic deformation (0.07%) followed by a nonlinear deformation (3.5%) due to the transformation of twinned martensite to detwinned martensite, followed by an elastic deformation (0.56%) of martensite. When the mechanical load is removed, an elastic recovering is observed but a large deformation (3.4%) remains. This is the orientation of martensite. It should be noted that the stresses of the start and the finish of the transformation of twinned to detwinned martensite are lower than the values in the case of one dimensional traction due to the volume.

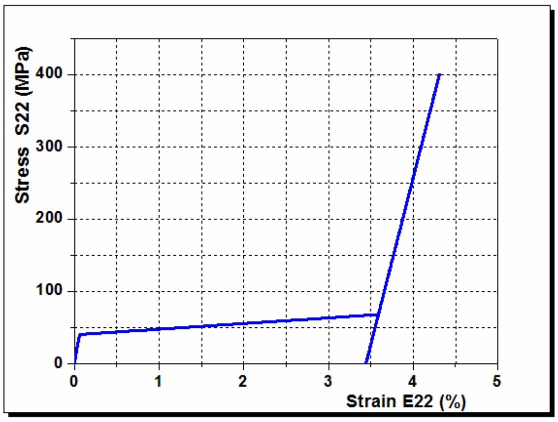

Figure 2. Plot $\varepsilon_{22} - \sigma_{22}$

Fig.2 shows the plot $\varepsilon_{22} - \sigma_{22}$ which begins with a small elastic deformation (0.07%) followed by a nonlinear deformation (3.5%) due to the transformation of twinned martensite to detwinned martensite, followed by an elastic deformation (0.56%) of martensite. When the mechanical load is removed, an elastic recovering is observed but a large deformation (3.4%) remains. This is the orientation of martensite. It should be noted that the stresses of the start and the finish of the transformation of twinned to detwinned martensite are lower than the values in the case of one dimensional traction due to the volume.

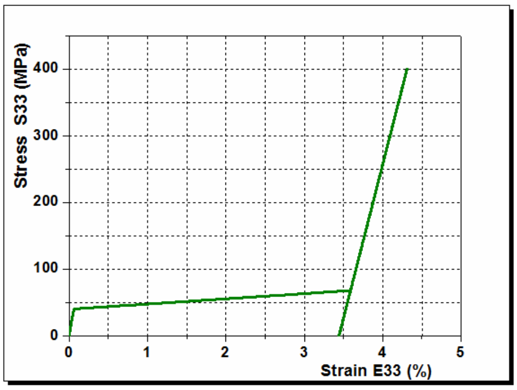

Figure 3. Plot $\varepsilon_{33} - \sigma_{33}$

Fig.3 shows the plot $\varepsilon_{33} - \sigma_{33}$ as the previous plot begins with a small elastic deformation (0.07%) followed by a nonlinear deformation (3.5%) due to the transformation of twinned martensite to detwinned martensite, followed by an elastic deformation (0.56%) of martensite. When the mechanical load is removed, an elastic recovering is observed but a large deformation (3.4%) remains. This is the orientation of martensite. It should be noted that the stresses of the start and the finish of the transformation of twinned to detwinned martensite are lower than the values in the case of one dimensional traction due to the volume.

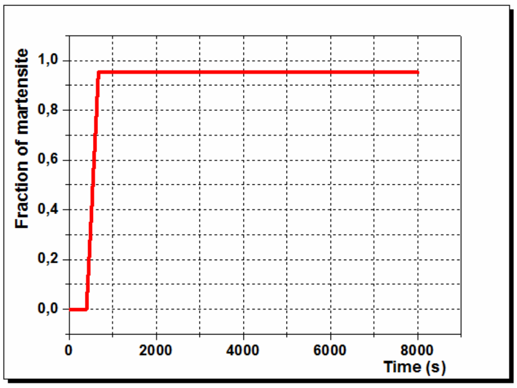

Figure 4. Evolution of the fraction of martensite

Fig.4 shows the evolution of the fraction of detwinned martensite. It appears compatible with the figures (Figures 1-3) i.e. before the transformation, there is an elastic deformation (f=0); after the elastic deformation, the transformation begins and ($0 < f <= 1$) on the plot the fraction attains the ultimate value of 0.95. After the transformation, the fraction of detwinned martensite remains invariable until the start of cooling when the fraction f will define the remaining amount of martensite.

b) Heating

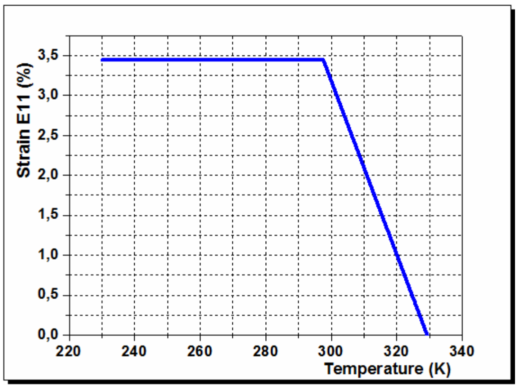

Figure 5. Plot $T - \varepsilon_{11}$

Fig.5 is characterized by a dependence between temperature and strain because at this stage (heating) the transformation of martensite to austenite is controlled by temperature. At the beginning of the evolution of the strain ε_{11}, there is no transformation of martensite until temperature reaches $A_s^0 = 295K$ (the temperature of the start of the transformation of austenite). The transformation continues and the strain also increases until the temperature reaches $A_f^0 = 330K$ (the temperature of the finish of the transformation of austenite). It is at this temperature that the deformation will be recovered, i.e. the specimen finds its previous original shape.

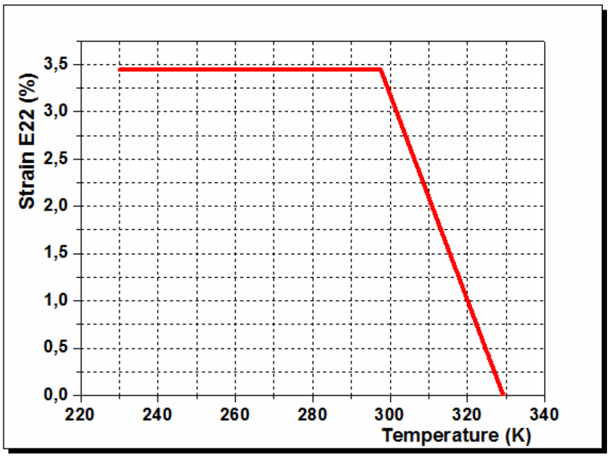

Figure 6. Plot $T-\varepsilon_{22}$

Fig.6 is also characterized by a dependence between temperature and strain because at this stage (heating) the transformation of martensite to austenite is controlled by temperature. At the beginning of the evolution of the strain ε_{22}, there is no transformation of martensite until the temperature reaches $A_s^0 = 296K$ (the temperature of the start of the transformation of austenite). The transformation continues and the strain also increases until the temperature reaches $A_f^0 = 330K$ (the temperature of the finish of the transformation of austenite). It is at this temperature that the deformation will be recovered, i.e. the specimen finds its previous original shape.

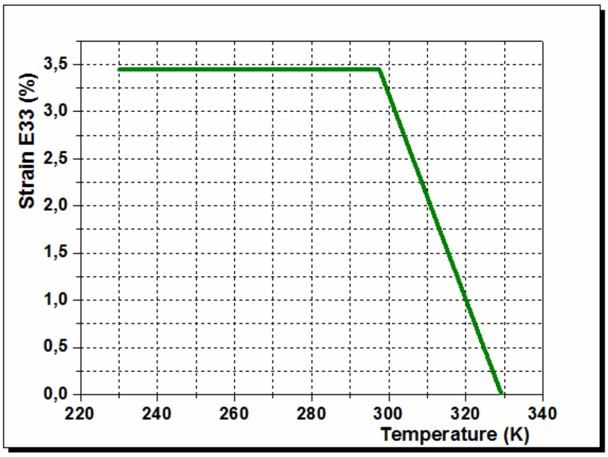

Figure7. Plot $T-\varepsilon_{33}$

As the previous Figures, Fig.7 is also characterized by a dependence between temperature and strain because at this stage (heating) the transformation of martensite to austenite is controlled by temperature. At the beginning of the evolution of the strain ε_{11}, there is no transformation of martensite until the temperature reaches $A_s^0 = 296K$ (the temperature of the start of the transformation of austenite). The transformation continues and the strain also increases until the temperature reaches $A_f^0 = 330K$ (the temperature of the finish of the transformation of austenite). It is at this temperature that the deformation will be recovered, i.e. the specimen finds its previous original shape.

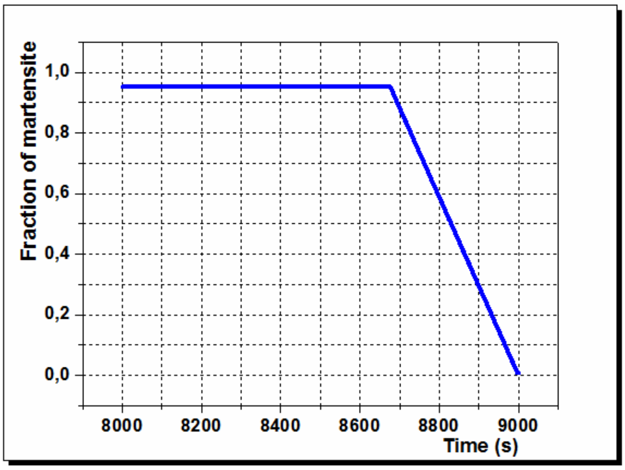

Figure 8. Evolution of the fraction of martensite

Fig.8 shows the evolution of the fraction of martensite (It corresponds to a reverse transformation in a pseudoelastic test) as it was detailed previously but in this stage it should be noted that the value of the fraction decreases to 0 corresponding to the end of the transformation. The evolution of the fraction of martensite is in accordance with the shapes of the three plots (Figs. 5-7)

c) Cooling

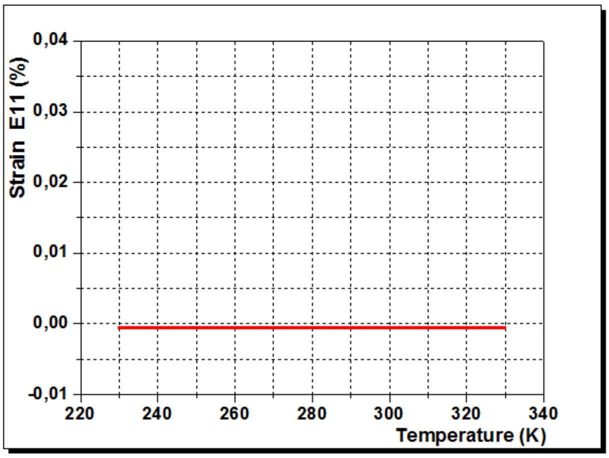

Figure 9. Plot $T-\varepsilon_{11}$

Fig.9 shows that there is no deformation controlled by temperature $(\varepsilon_{11} = 0)$ during this period because at this stage the structure has recovered the previous nonlinear deformation and no mechanical work occurs but the chemical work of the phase change (austenite to martensite). The martensite is obtained at $M_s^0 = 279K$ and the transformation is finished at $M_s^0 = 240K$.

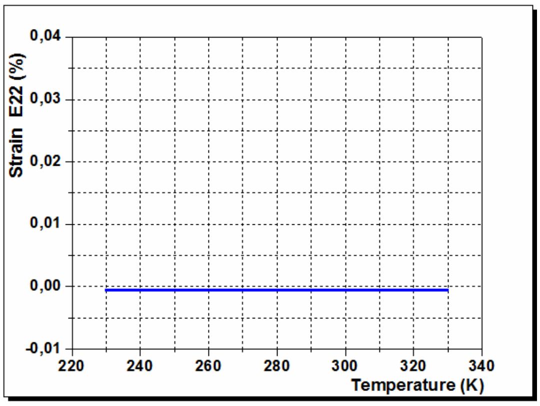

Figure 10. Plot $T-\varepsilon_{22}$

As the previous plot, Fig.10 shows that there is no deformation controlled by temperature $(\varepsilon_{22}=0)$ during this period because at this stage the structure has recovered the previous nonlinear deformation and no mechanical work occurs but the chemical work of the phase change (austenite to martensite). The martensite is obtained at $M_s^0=279K$ and the transformation is finished at $M_s^0=240K$.

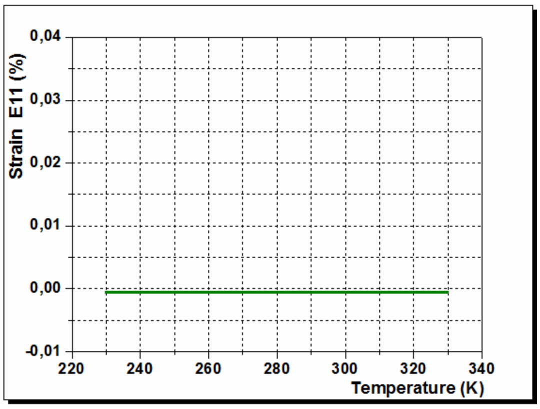

Figure11. Plot $T-\varepsilon_{33}$

Fig.11 also shows that there is no deformation controlled by temperature $(\varepsilon_{33}=0)$ () during this period because at this stage the structure has recovered the previous nonlinear deformation and no mechanical work occurs but the chemical work of the phase change (austenite to martensite). The martensite is obtained at $M_s^0=279K$ and the transformation is finished at $M_s^0=240K$.

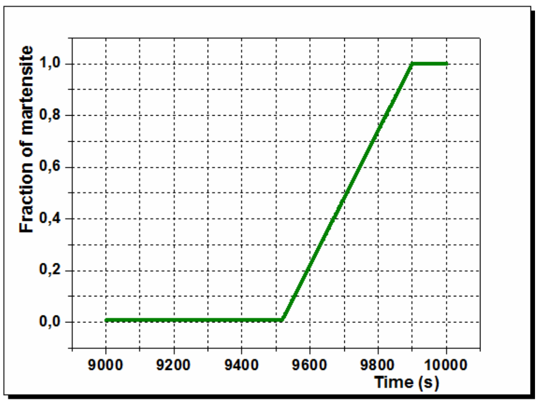

Figure 12. Evolution of the fraction of martensite

The figure (Fig.12) shows the evolution of the increasing fraction of martensite according to the chemical work of the phase change. It is in agreement with no mechanical work $(\varepsilon_{11}=\varepsilon_{22}=\varepsilon_{33}=0)$.

d) 3D Representation

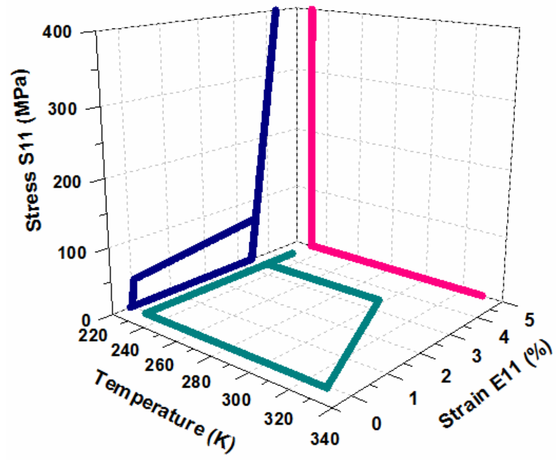

Figure 13. Space $T-\varepsilon_{11}-\sigma_1$

Fig.13 shows a plot of the shape memory effect in three dimensions $(T-\varepsilon-\sigma)$. It illustrates the beginning of the deformation and the recovering of the shape at the last stage.

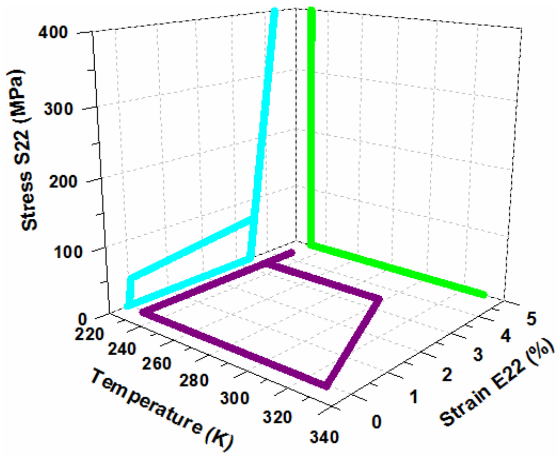

Figure 14. Space $T-\varepsilon_{22}-\sigma_{22}$

In the same manner, Fig.14 shows a plot of the shape memory effect in three dimensions $(T-\varepsilon-\sigma)$. It illustrates the beginning of the deformation and the recovering of the shape at the last stage.

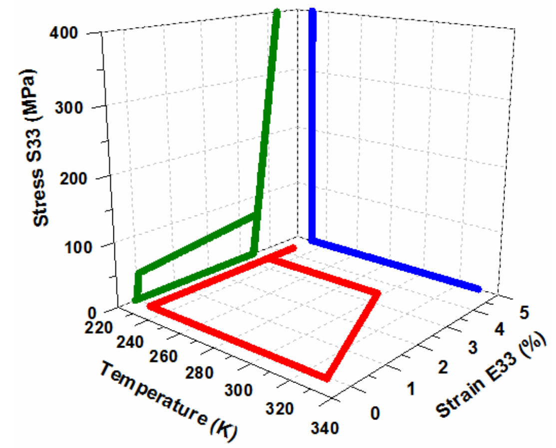

Figure 15. Space $T-\varepsilon_{33}-\sigma_{22}$

Fig.15 also shows a plot of the shape memory effect in three dimensions $(T-\varepsilon-\sigma)$. It illustrates the beginning of the deformation and the recovering of the shape at the last stage.

Conclusion

In this paper, we have considered the shape memory effect as a behavior of shape memory alloys. After dividing the behavior to three periods, we have considered the free energy and the constitutive equations for each period.

To simulate the response of the built model, we have used experimental data and a Nititnol cubic specimen subjected to triaxial traction.

The results are in good agreement with the definition of the shape memory effect and we think that this model can be used in engineering to simulate 3D structures.

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Trodimenzionalno modelovanje i simulacija efekta memorije (pamćenja) oblika

Ovaj rad se bavi modelovanjem i simulacijom efekta memorije oblika koji predstavlja jedno od mnogih ponašanja legura memorije oblika (shape memory). Efekat je prvo podeljen u tri faze. Svaka faza ima svoj termodinamički potencijal i konstitutivnu jednačinu. Udeo martenzita je jedina interna promenljiva koja treba da se razmatra. U prvoj fazi predstavlja frakciju rasparnog martenzita, u drugoj fazi predstavlja frakciju transformisanog martenzita u austenit, a u poslednjoj fazi predstavlja frakciju proizvedenog martenzita iz transformacije austenita.
Za svaku fazu smo izveli konstitutivnu jednačinu koristeći principe termodinamike i jednostavni formalizam. Kada je definisan teoretski model, njegova valjanost je proverena simulacijom procesa uz pomoć eksperimentalnih podataka koji su dobijeni troosnim istezanjem i termičkim opterećenjem kocke. Dobijeni rezultati ove simulacije odražavaju ponašanje ove vrste materijala kada su izloženi termomehaničkom opterećenju. Suštinski, glavni zaključak ovog rada je da se ovaj predloženi model može koristiti za simulaciju efekta memorije oblika.

Ključne reči: **martenzit, termomehaničko opterećenje, modelovanje, frakcija, efekat pamćenja oblika, simulacija procesa, eksperimentalni rezultati.**

Трёхмерное моделирование и моделирование эффекта памяти (запоминания) формы

Данная работа посвящена моделированию и симуляции эффекта памяти формы, который является одним из многих поведений сплава с памятью формы (shape memory). Эффект впервые разделён на три этапа. Каждый этап имеет свой термодинамический потенциал и материальное уравнение. Доля мартенсита является единственной внутренней переменной, которая должна быть рассмотрена. На первом этапе представляет собой часть несоответствующего мартенсита, на второй стадии он представляет собой часть преобразованного мартенсита в аустенит, а на последнем этапе представляет собой фракцию произведённого мартенсита путём превращения аустенита.
Для каждой фазы мы провели материальное уравнение, используя принципы термодинамики и простой формализм. Когда определяется теоретическая модель, её достоверность проходит проверку моделирования процесса с помощью экспериментальных данных, полученных трёхосным растяжением и тепловой нагрузкой кубика. Результаты полученны этим моделированием отражают поведение этих типов материалов при воздействии на них термомеханической нагрузки. По сути, основным выводом данного исследования является то, что предложенная модель может быть использована для симуляции эффекта памяти формы.

Ключевые слова: **мартенсит, термомеханическая нагрузка, моделирование, фракция, эффект памяти формы, моделирование процесса, экспериментальные результаты.**

Modélisation 3D et simulation de l'effet de mémoire de forme

Le présent article est destiné à la modélisation et la simulation de l'effet de mémoire de forme qui est l'un des nombreux comportement des alliages à mémoire de forme. Pour ce faire premièrement nous avons divisé l'effet en trois étapes. Chaque étape à son propre potentiel thermodynamique et ses équations constitutives. La fraction de martensite est la seule variable interne à prendre en considération . Dans la première étape elle représente la fraction de martensite orientée et dans la deuxième étape elle représente la fraction de martensite transformée en austénite. Dans la dernière étape elle va représenter la fraction de martensite produite à partir de la transformation de l'austénite. Pour chaque étape nous avons déduit des équations constitutives en utilisant les principes de la thermodynamique et un formalisme simple. Lorsque le modèle semble être construit nous avons utilisé des données expérimentales pour simuler le modèle de considérer comme éprouvette en cube soumis à la traction triaxiale et un chargement thermique . Les résultats obtenus de cette simulation reflètent le comportement de ce type de matériaux thermomécanique lorsqu'une charge est appliquée. La principale conclusion de cette étude est que le modèle constitutif proposé peut être utilisé pour simuler l'effet de mémoire de forme.

Mots clés: **martensite, chargement thermique, modélisation, fraction, effet de mémoire de forme, simulation de processus, résultats expérimentaux.**