NUMERICAL AND EXPERIMENTAL ANALYSIS OF THE SUPERELASTIC BEHAVIOR OF A Ni-Ti ORTHODONTIC WIRE

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Abstract. *In this work it was carried out the thermomechanical characterization of a superelastic Ni-Ti shape memory alloy (SMA) wire to subsequent simulation of the stress – strain behavior. For this one, it was used a Ni-Ti orthodontic wire which was tested in an electromechanical universal machine equipped with a heating chamber that ensures the maintenance of a constant temperature. A set of stress versus strain loops for different temperatures between 30 ºC and 90 ºC, were experimentally determined. From a limited amount of experimental data, simulations were performed by means of the finite element method (FEM) using the ANSYS software to compare the theoretical and experimental superelastic behavior of the Ni-Ti orthodontic wire. It was shown that the realization of three experiments is sufficient to simulate with good approximation the superelastic behavior of the orthodontic wire in a wide range of temperatures, minimizing the cost compared with a more extensive experimental analysis.*

Keywords*: Shape memory alloys, Orthodontic wires, Superelasticity, Ni-Ti alloys.*

1. INTRODUCTION

Shape memory alloys (SMA) are metallic materials that may undergo phase transformation in solid state as a result of the application of a thermo-mechanical loading. These special materials can recover deformations as high as 6%, or even develop considerable forces, after applying of temperature and/or stress fields. This phenomenon, known as Shape Memory Effect (SME), is closely associated with a thermoelastic reversible martensitic phase transition (Otsuka & Wayman, 1998). To observe the SME, the deformation is introduced in the low-temperature (martensite), and a simple heating takes material for high temperature phase (austenite), resulting in shape recovery. This phase transformation can also occur by application of mechanical loading in austenitic state. In this case, there will be the formation of martensite phase by mechanical stress, causing a major deformation (~ 6%) which is completely reversible upon unloading. This phenomenon is called superelasticity (SE). The SME and SE phenomena presented by SMA are used in various areas, from robotics to the medical and dental industry (Lagoudas, 2009).

Seeking a more precise analysis of the thermomechanical behavior of these materials, a series of mathematical models capable of describing them have been developed over the years, allowing explore their full potential. The SME and SE modeling has two distinct approaches: the first is a microscopic approach that takes into account the metallurgical aspects of the SMA and was discussed in several studies (Warlimont et al.1974; Levitas et al. 1998, Gall et al. 1999). The second approach, at the macroscopic scale, is based on the phenomenological aspects of the SMA behavior (Silvia et al. 2006).

In this context, the Auricchio model is a macroscopic approach initially proposed in a one-dimensional way and later extrapolated to a three-dimensional context (Auricchio et al 1997; Auricchio & Sacco, 1997). These models use the elastoplastic theory to describe the phase transformations associated with SME. The numerical implementation of these models is rather difficult; however a computational tool that uses the Finite Element Method (FEM), such as the ANSYS and ABAQUS software, allow obtaining complex responses of a system without the need for a high-level programming.

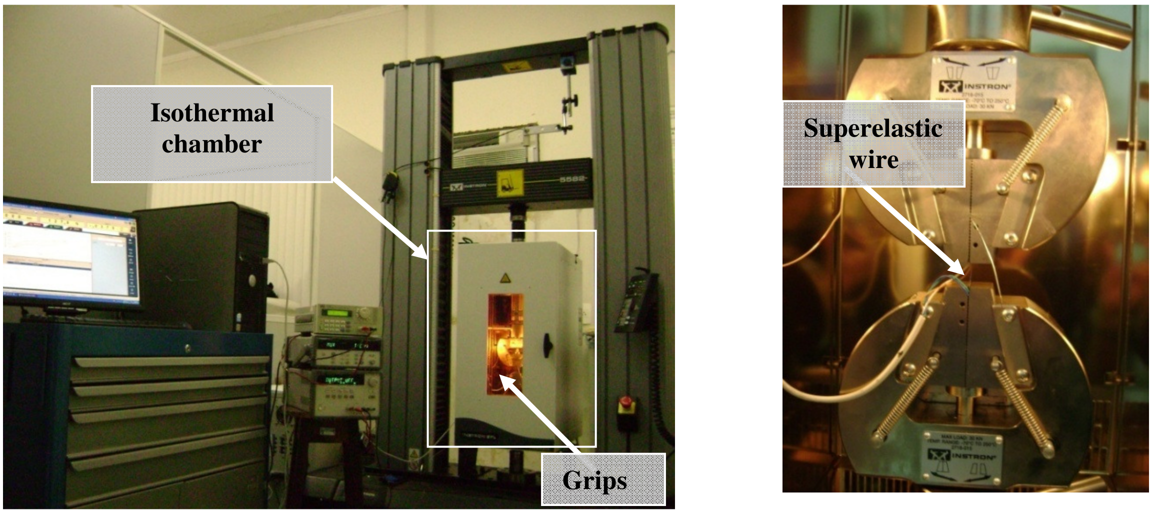
This work deals with the numerical simulation of superelastic behavior via FEM aiming to minimize the costs of thermomechanical characterization procedure, as well as, the time consumed in the experimental characterization of the SMA mechanical properties. In addition, this study aims to evaluate, reproduce and validate the superelastic behavior of a Ni-Ti superelastic orthodontic wire using the Auricchio model implemented in the ANSYS software, also regarding the potential and limitations of the material model. The numerical results were compared with experimental data from uniaxial tensile tests performed with the superelastic Ni-Ti orthodontic wire at different temperatures using a universal testing machine.

2. EXPERIMENTAL PROCEDURE

The experimental superelastic stress-strain curves of the Ni-Ti orthodontic wire (trademark Neo Sentalloy) were obtained by uniaxial tensile tests. The wire has a rectangular cross-section of dimensions 0.65 mm in width and 0.48 mm in height while length was approximately 149 mm. This wire was tested with growing temperatures in the range of

25 to 100 ° C in a universal testing machine (Instron, model 5582) equipped with heating chamber, as shown in Fig. (1.a). The tests were performed for a usable length of 12 mm from the straight region of the Ni-Ti wire.

The details of the assembly of the Ni-Ti arch-wire in the grips of the testing machine are shown in Fig. (1.b). Whereas the Ni-Ti wire undergoes large deformations, a strain gauge was not used directly on the sample, and the deformations have been obtained based on the displacement of the mobile clamp of the test machine.



(a) (b)

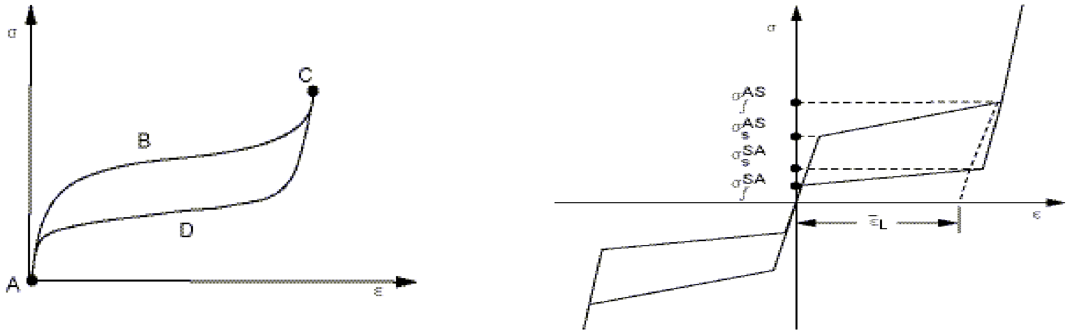
Figure 1. Experimental test bench to evaluate the superelastic behavior of the Ni-Ti orthodontic wire. (a) Instron 5582 universal testing machine . (b) Ni-Ti arch-wire installed in the grips.

The Ni-Ti arch-wire was initially subjected to a stabilization of the superelastic behavior through the completion of 30 cycles of stress - strain under a constant temperature of 50 ° C. In this temperature the structure of the Ni-Ti wire is fully austenitic.

In the test machine it was created a method for controlling displacement during the loading, limited to 5 % of deformation in the effective length of the Ni-Ti wire, using a displacement rate of 0.5 mm/min. Unloading was realized until approximately 3 N of residual force on the wire. After cyclic stabilization, a series of isothermal tests between 25 ºC and 80 °C in steps of 5 °C, were carried out.

3. NUMERICAL SIMULATION

The SMA material model implemented in ANSYS software (accessed with TB,SMA) is intended for modeling the superelastic behavior of Ni-Ti alloys, in which the material undergoes large-deformation without showing permanent deformation under isothermal conditions, as shown in Fig.(2). In the schematization of Fig. 2(a) the material is first loaded (ABC), showing a nonlinear behavior due to austenite to martensite transformation. When unloaded (CDA), the reverse transformation occurs. The ideal superelastic behavior is hysteretic with no permanent strain (Auricchio et al.1997).



(a) (b)

Figure 2. Schematic illustration of the superelastic behavior in SMA. (a) Typical superelasticity (Auricchio et al., 1997). (b) Idealized stress-strain diagram for superelasticity.

The software ANSYS 8.0, widely used to perform static and dynamic simulations based on FEM, has a subroutine which allows analyzing the superlastic behavior of SMA using the model proposed by Auricchio et al (1997).

The phase transformation mechanisms involved in the superelastic behavior are: Austenite to Martensite (AS) and Martensite to Austenite (SA).

With the objective of limiting the dimension of the problem, the model of Auricchio et al (1997) not makes differentiate between different kinds of variants of martensie and assumes that the material is isotropic. In the subroutine SMA ANSYS 8.0, there are considered only the two phases above mentioned. Two internal variable are also introduced, the martensitic fraction, ξ_S, and the austenitic fraction, ξ_A. ξ_S is considered the independent variable, so that the relationship $\xi_S + \xi_A = 1$, is satisfied.

The pressure dependency of the phase transformation is modeled by introducing the Drucker-Prager criterion, represented by Eq.(1):

$$F = q + 3\alpha p \tag{1}$$

where α is a material parameter, σ is the stress vector, Tr is the trace operator, $p = \frac{Tr(\sigma)}{3}$, $q = \sqrt{\sigma : M : \sigma}$, M is a matrix defined by:

$$M = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

The evolution of the martensite fraction, ξ_S, is defined by Eqs. (2) and (3), where σ_f^{AS} and σ_f^{SA} are critical stresses as defined in Fig. (2.b):

$$\dot{\xi} = \begin{cases} -H^{AS}(1-\xi_S)\dfrac{\dot{F}}{F - R_f^{AS}}, \quad A \to S \quad \text{transformation, where } R_f^{AS} = \sigma_f^{AS}(1+\alpha) & (2) \\ H^{SA}\xi_S \dfrac{\dot{F}}{F - R_f^{SA}}, \quad S \to A \quad \text{transformation, where } R_f^{SA} = \sigma_f^{SA}(1+\alpha) & (3) \end{cases}$$

where the constants H^{SA}, H^{AS} are obtained using Eqs. (4) and (5):

$$H^{AS} = \begin{cases} 1 \quad if & \begin{cases} R_s^{AS} < F < R_f^{AS} \\ \dot{F} > 0 \end{cases} \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

$$H^{SA} = \begin{cases} 1 \quad if & \begin{cases} R_s^{SA} < F < R_f^{SA} \\ \dot{F} < 0 \end{cases} \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

The material parameter α, defined by Eq.(6), characterizes the material response in tension and compression. If tensile and compressive behaviors are the same, $\alpha = 0$. For a uniaxial tension - compression test, α can be related to the initial value of austenite to martensite phase transformation in tension, σ_c^{AS} and compression, σ_t^{AS}, as:

$$\alpha = \frac{\sigma_c^{AS} - \sigma_t^{AS}}{\sigma_c^{AS} + \sigma_t^{AS}} \tag{6}$$

The incremental stress-strain relations are defined by Eqs.(7) and (8):

$$\{\Delta\sigma\} = [D](\{\Delta\varepsilon\} - \{\Delta\varepsilon^{tr}\}) \tag{7}$$

$$\{\Delta\varepsilon^{tr}\} = \Delta\xi_S \bar{\varepsilon}_L \frac{\partial F}{\partial\{\sigma\}} \tag{8}$$

where: [D] is the stress-stain matrix, $\{\Delta\varepsilon^{tr}\}$ is the incremental transformation strain, $\bar{\varepsilon}_L$ is the superelastic deformation parameter shown in Fig.(2.b).

These variables are temperature-dependents and therefore, the temperature value at which these parameters were evaluated, should be informed. The software ANSYS allows the inclusion of up to 40 temperatures. These variables can be observed in Table 1.

Table 1. Input parameters for modeling the subroutine SMA ANSYS 8.0.

Constants	Symbolic	Description
SIG-SAS (C1)	σ_S^{AM}	Stress value for the start of martensitic transformation.
SIG-FAS(C2)	σ_f^{AM}	Stress value for the finishingof martensitic transformation.
SIG-SSA(C3)	σ_S^{MA}	Stress value for the start of austenitic transformation.
SIG-FSA(C4)	σ_f^{MA}	Stress value for the finishing of austenitic transformation.
EPSILON(C5)	e_L^{-}	Maximum residual strain
ALPHA(C6)	α	Parameter proportional to the difference between the response of material in tension and compression.
TEMPERATURE	T	Temperature assessment of the properties.

The SMA subroutine that is used to model the superelastic behavior uses a command named MP (Material Property), which defines the linear behavior of the austenitic phase, a command named TB SMA, to enter the transition behavior of martensitic phase and a command TBDATA used to enter parameters associated with each temperature. The SMA model via ANSYS can be used with the following elements: PLANE182, PLANE283, SOLID185, SOLID186 and SOLID187. In this work, it was used the element SOLID185 for meeting the needs of the simulation. This element is used for tridimensional modeling of solid structures. It is defined by eight nodes having three degrees of freedom at each node: translations in the nodal x, y, and z directions. The element has plasticity, hyperelasticity, stress stiffening, creep, large deflection, and large strain capabilities. It also has mixed formulation capability for simulating deformations of nearly incompressible elastoplastic materials, and fully incompressible hyperelastic materials.

The properties between the temperature values are interpolated linearly by ANSYS. The expressed variable independent of temperature is the deformation level of the SMA specimen. According to the model of Auricchio et al (1997) in the ANSYS program, deformation can reach 8%.

The ANSYS tool can be used to perform analysis of thermomechanical requests of various systems and types of devices. Within this research line, the subroutine SMA ANSYS 8.0 can be used to simulate the behavior of superelastic orthodontic wires under tensile load. For the simulations of the superelastic effect in ANSYS 8.0, the results obtained in experiments were evaluated and included in the database of the subroutine SMA ANSYS. For these simulations were initially used two results of different test temperatures, with their respective parameters, aiming that simulations reproduce the experimental results for other temperatures. To compare the experimental and numerical results, the data were manipulated in the program ORIGIN and compared graphically.

4. RESULTS AND DISCUSSION

4.1. Stabilization of the superelastic Ni-Ti SMA wire

Initially, tests were carried out to stabilize the superelastic behavior of Ni-Ti wire through cycles of stress - strain. Figure (3) shows that after about 10 cycles of loading and unloading, the stress - strain behavior tends to stabilize because of an accumulation of plastic strain which reaches approximately 1.7% after 30 cycles. Associated with this accumulation of plastic deformation there is a decrease in the critical stress for inducing martensite phase, which decreases from 350 MPa to about 200 MPa. This behavior confirms that the Ni-Ti orthodontic wire is supplied without any stabilization treatment, so that their behavior of force in the teeth may change during use by patient.

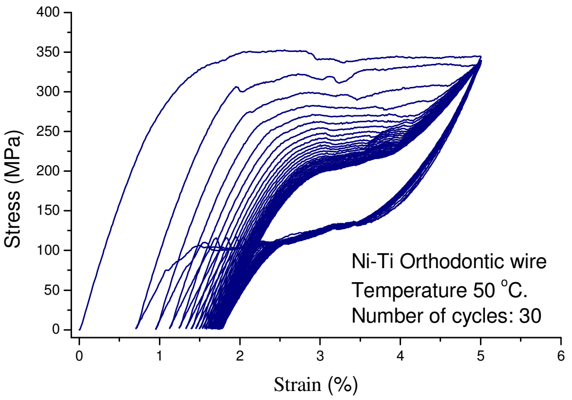


Figure 3. Cyclic behavior of the studied superelastic Ni-Ti wire at 50 °C.

4.2. Thermomechanical behavior at different temperatures

After the stabilization process shown in Fig. (3), isothermal tests were started for different temperatures. Figure (4) show a lot of stress – strain behaviors for temperatures of 30, 40, 50 and 60 °C, respectively. It can be observed a gradual increase of critical stress to start the austenite to martensite phase transformation (σ_s^{AS} in Fig. 2) as well as in the elastic module with temperature test. A residual plastic strain of less than 0.3 % was verified for all temperatures.

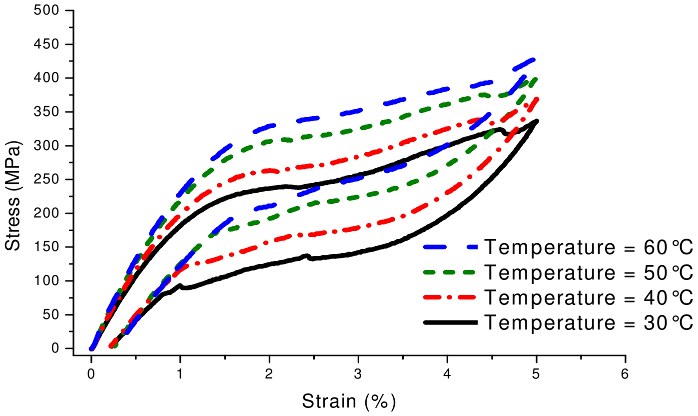


Figure 4 - Evolution of the superelastic stress - strain curves for the Ni-Ti wire.

From the results obtained during the isothermal tests at various temperatures, critical stress as defined in Fig. (2) were determined. Figure (5) shows the behavior of critical stresses as a function of temperature. It can be verified the linear relationship between stress and temperature. This behavior allows us to estimate the temperatures of phase transformation in the state free of stress (0 MPa) through an extrapolation to the axis of temperature. The transformation temperatures obtained in this extrapolation were: M_s = - 10.0 °C, M_f = - 56.0 °C, A_s = - 3.9 °C and A_f = 5.3 ° C.

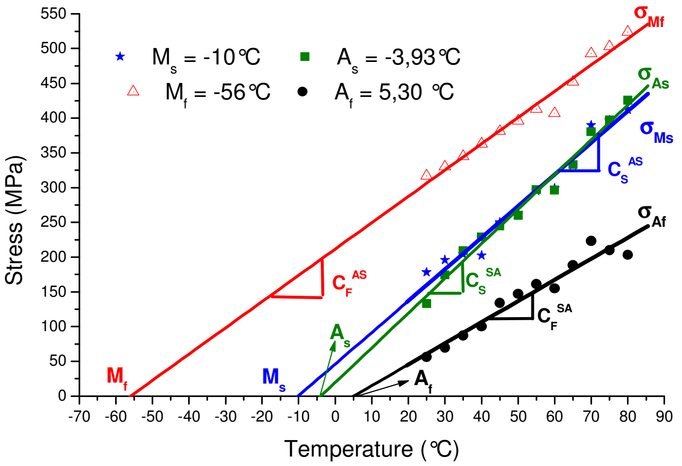


Figure 5. Relationship between the stresses transformation critical and test- temperature.

According to the model of Auricchio et al. (1997), for a uniaxial stress state in a range of application of tension - temperature, the region where the phase transformation can occur linear with good approximation is associated with inclination between 2.5 MPa/°C and 15 MPa/°C. From the treatment of the data shown in Fig. (5), the following slopes for the C^{AS} and C^{SA} coefficients are determined: C_s^{AS} = 4.6 MPa/°C, C_f^{AS} = 3.8 MPa/°C, C_s^{SA} = 5.0 MPa/°C and C_s^{SA} = 3.0 MPa/°C. The Auricchio model in ANSYS 8.0 considers the parallelism between coefficients $C_s^{AS} // C_f^{AS}$ and $C_s^{SA} // C_f^{SA}$. This coefficient is provided by the user of ANSYS 8.0 indirectly, i.e. the software makes use of the critical stresses for phase transformation, provided to characterize the material to determine these coefficients and thus simulate the superelastic effect for other temperatures and loading levels.

4.3. Simulation of superelastic behavior

To simulate the superelastic behavior of the orthodontic Ni-Ti SMA wire, was used the model developed by Auricchio *et al* (1997) which was incorporated into the ANSYS program. The importance of this step is to show that the model is capable of predict the superelastic behavior of SMA at any temperature, starting from a limited collection of experimental data at different temperatures. Therefore, it was analyzed the possibilities of comparing a lot of simulations using experimental data obtained from only two or three test temperatures. Figure (6) show the stress – strain curves for 30 °C, 65 °C e 74 °C used for model calibration.

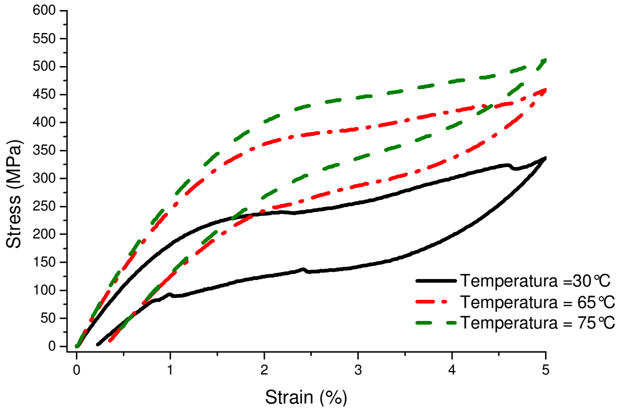


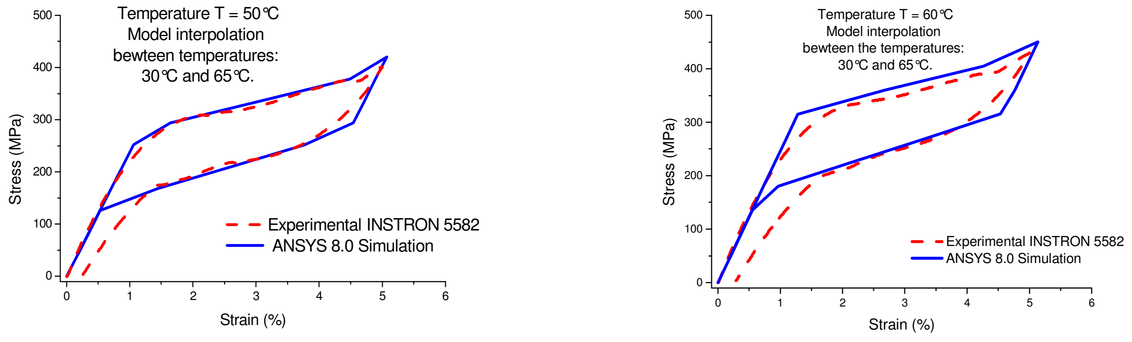
Figure 6. Superelastic experimental stress - strain behavior for the Ni-Ti wire.

From these results, the parameters needed to calibrate the model, as defined in Fig. (2), were obtained for each temperature as shown in Tab. (2).

Table 2. Parameters associated with the temperature for the model fit.

Parameters / **Temperature**	σ_S^{AS} (MPa)	σ_f^{AS} (MPa)	σ_S^{SA} (MPa)	σ_f^{SA} (MPa)	$\bar{e}_L$ (%)	α	Elastic Moduls (MPa)
30ºC	199	320	195	366	3,3	0	$22x10^3$
65ºC	351.51	440.13	366	189.24	3,2	0	$23x10^3$
75ºC	407.51	504.13	425	223.24	3,0	0	$25.5\ x10^3$

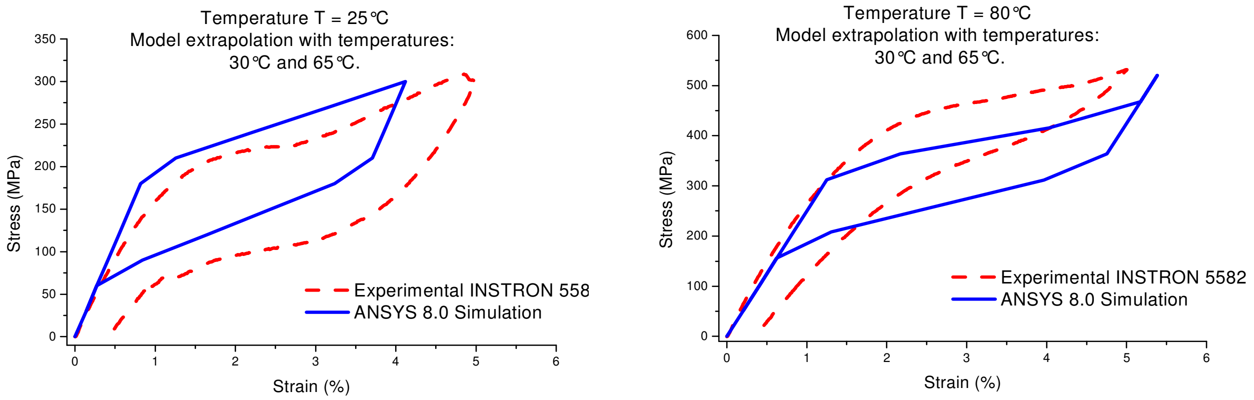
Figures (7) and (8) present the results of simulations for the powered model with the parameters of only two temperatures (30 ºC and 65 ºC) (Table 2). Figure (7) show the comparisons between the experimental and numerical results for superelastic behavior at 50 °C and 60 °C. The result can be considered quite satisfactory, except for the residual plastic deformation that the model cannot predict. Anyway, the results attest to the ability of the model to describe the superelastic phenomenon.



(a) (b)

Figure 7. Numerical-experimental comparison. (a) T = 50 °C. (b) T = 60 °C.

All results shown previously were obtained by interpolation between two temperatures, 30 °C and 65 °C, taken as input into the model. However, extrapolation is still limited because the amount of data is insufficient to adapt the model for all tests, as can be observed in Fig. (8).



(a) (b)

Figure 8. Numerical-experimental comparison. (a) T = 25 °C. (b) T = 80 °C.

Figures (9) and (10) show the results for the simulations with experimental data for three temperatures (30 ºC, 65 °C and 75 °C, Tab. 2) used as input data for calibration of model. These figures show comparisons between the simulations and the experimental superelastic stress - strain curves. The results show that the model is able to satisfactorily reproduce the superelastic effect and presents a better approximation for the extrapolations obtained in the previous case with calibrated two temperatures.

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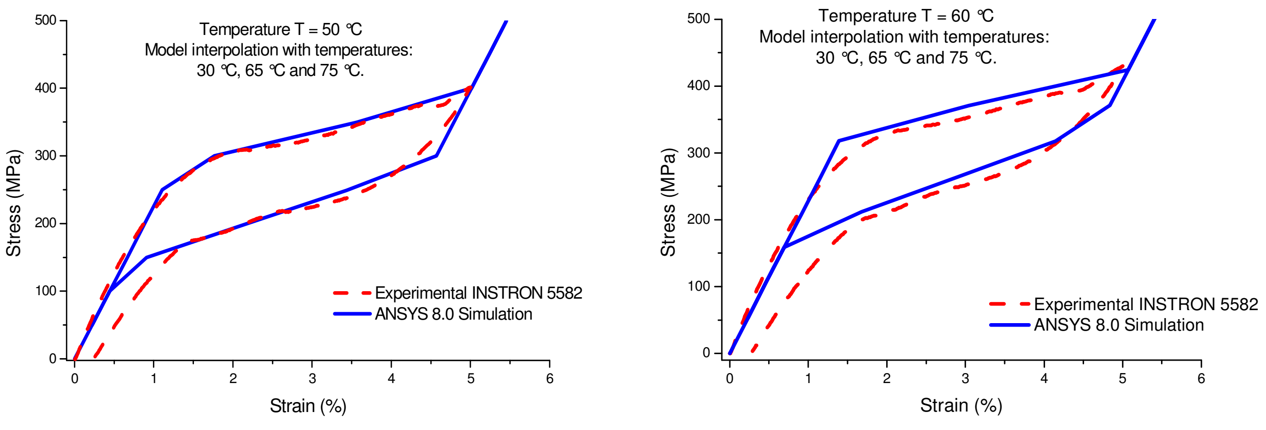
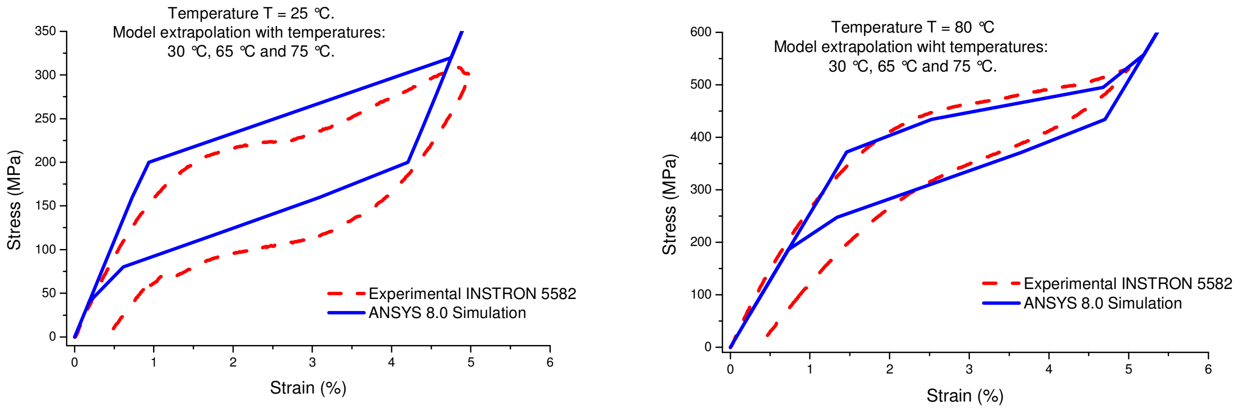


(a) (b)

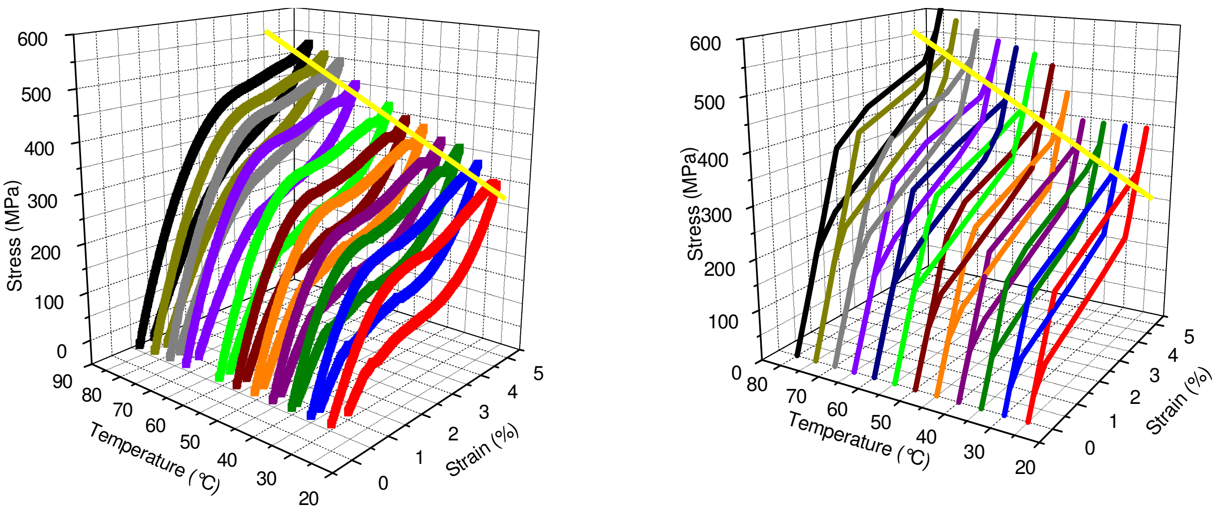
Figure 9. Numerical-experimental comparison. (a) T = 50 °C. (b) T = 60 °C .



(a) (b)

Figure 10. Numerical-experimental comparison. (a) T = 25 °C. (b) T = 80 °C

Figure (11) shows the totality of the stress - strain curves, experimental (a) and simulated (b) in a three-dimensional arrangement. From the Figure (11a) it can be observed a linear increase in the level of mechanical stress that is needed to convert the austenitic structure into martensite. This behavior is also observed in the Fig. (11b) where the simulation shows the same linear behavior observed in experimental curves.



(a) (b)

Figure 11. Three-dimensional stress - strain behavior of superelastic Ni-Ti wire. (a) Experimental. (b) Simulation.

5. CONCLUSIONS

All results presented here show the versatility of the superelastic model available in ANSYS, and its ability to reproduce the phenomenon in an orthodontic Ni-Ti archwire at several temperatures. The experimental determination of the parameters that directly influence the phenomenon is of fundamental importance for model adequacy. The utilization of experimental data from two or three temperatures for the calibration of the model shows that the more information is provided, the more the simulation will converge to the experimental results. The simplicity of the model has its limitations, here observed as the residual strain not contemplated, and its utilization to perform simulations at temperatures where the crystalline structure is fully martensitic, in which the same did not provide reliable results.

The vast majority of literature makes its own mathematical model, can be implemented in ANSYS or any other software that uses FEM for the same purpose. However, the SMA ANSYS subroutine shows that the results meet the expectations generated for the superelastic phenomenon studied. Therefore, in general, one can conclude that the model built by ANSYS can simulate with good approximation the experimental results and can be used to predict with accuracy the behavior of orthodontic Ni-Ti wires under uniaxial tensile load.

6. ACKNOWLEDGEMENTS

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