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Finite element modeling of superelastic nickel–titanium orthodontic wires☆

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ABSTRACT

Thanks to its good corrosion resistance and biocompatibility, superelastic Ni–Ti wire alloys have been successfully used in orthodontic treatment. Therefore, it is important to quantify and evaluate the level of orthodontic force applied to the bracket and teeth in order to achieve tooth movement. In this study, three dimensional finite element models with a Gibbs-potential-based-formulation and thermodynamic principles were used. The aim was to evaluate the influence of possible intraoral temperature differences on the forces exerted by NiTi orthodontic arch wires with different cross sectional shapes and sizes. The prediction made by this phenomenological model, for superelastic tensile and bending tests, shows good agreement with the experimental data. A bending test is simulated to study the force variation of an orthodontic NiTi arch wire when it loaded up to the deflection of 3 mm, for this task one half of the arch wire and the 3 adjacent brackets were modeled. The results showed that the stress required for the martensite transformation increases with the increase of cross-sectional dimensions and temperature. Associated with this increase in stress, the plateau of this transformation becomes steeper. In addition, the area of the mechanical hysteresis, measured as the difference between the forces of the upper and lower plateau, increases.

1. Introduction

Superelastic (SE), nickel–titanium-alloy (NiTi) wires have become the wires of choice for orthodontic aligning and leveling mechanics due to their good mechanical properties, biocompatibility and resistance to corrosion, greater strength and lower elastic modulus compared with stainless steel alloys. These wires readily sustain large deflections without exceeding the elastic limit of the alloy (Es-Souni and Brandies., 2001). As an SE NiTi wire is deflected, it is firstly deformed in an elastic manner in the austenitic state. As the stress induced in the wire increases, a phase transformation begins from austenitic toward martensitic phase. In practice, the transformation is likely incomplete at wire engagement, when the wire is allowed to unload, hysteresis occurs, thus causing the alloy to return to its austenite phase by delivering light continuous forces over a wider range of deformation which is claimed to allow dental displacements.

In orthodontics, the normal force is the component which acts perpendicularly to the direction of the desired movement. Two categories of normal force are present in orthodontic leveling. Firstly, slot-wire contact(s) exist due to wire-curvatures at/through the slot. Secondly, the ligation securing the wire in the slot can create normal force (Trenton, 2008). It has been demonstrated that elastomeric ligation produces the highest normal force, followed by stainless steel ties and self-ligating mechanisms (Khambay et al., 2005). For this reason, manufacturers continue to develop self-ligating designs to decrease the normal force exerted on the arch wire in order to reduce friction at the bracket arch wire interface that might prevent attaining optimal orthodontic force levels in the supporting tissues (Krishnan et al., 2009). Normal force induced by wire curvatures is responsible for correcting malpositioned teeth and simultaneously exerts pressure on anchorage teeth. Actually, it can be directly related to the stiffness of the activated arch wire. As the flexural stiffness(es) of a wire increase(s), the amplitude(s) of normal forces which press

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against the walls increase(s), it is/they are also influenced by interbracket distance and cross-sectional shape and size (Queiroz et al., 2012).

During recent years, the area of constitutive modeling of shape memory alloys (SMA) has been the point of interest of many researchers (Arghavani, 2010; Auricchio et al., 1997; Dumoulin and Cochelin, 2000; Etave et al., 2001; Huang et al., 2000; Gao and Brinson, 2002; Marketz and Fischer, 1996; Majo et al., 2004). The main difficulty is the modeling of the temperature–stress dependence and a nonlinear behavior of SMA alloy. Therefore, it is necessary to adopt constitutive laws able to be implemented in commercial Finite Element codes and to predict the SMAs response.

In this study, one of the famous phenomenological constitutive models of shape memory alloys based on Boyd and Lagoudas (1996) formulation is proposed and implemented as a user defined subroutine using the finite element analysis software, ABAQUS (Abaqus, Analysis User's Manual, 2009). The aims were to compare and evaluate the level of the normal force generated by SE NiTi orthodontics wires subjected to 3-mm deflection with different cross-sectional shapes, sizes and temperatures.

2. Methods

2.1. Shape memory alloy constitutive model

The constitutive model used in this paper is based on the formulation proposed by Boyd and Lagoudas (1996). In this section, a brief description of this model is proposed. In fact, it is a three-dimensional model based on small deformation assumptions. Besides, it is a thermodynamic model based upon the expression of the Gibbs free energy which is defined as the portion of enthalpy available for doing work at constant temperature (Lagoudas and Bo, 1999). Moreover, such potential considers the martensitic volume fraction (ξ) and the transformation strain (ε) as the internal state variables since both of them play an important role in characterizing the phase transformation and the observable thermomechanical response of SMAs.

In this constitutive model, the total specific Gibbs free energy, of a polycrystalline SMA is assumed to be equal to the mass weighted sum of the free energy of each phase (martensitic and austenitic) plus the free energy of mixing (Boyd and Lagoudas, 1996).

$$G(\sigma,T,\xi,\varepsilon^t) = -\frac{1}{2}\frac{1}{\rho}\sigma : S : \sigma - \frac{1}{\rho}\sigma : \left[\alpha(T-T_0)+\varepsilon^t\right] + c\left[(T-T_0) - T\,In\left(\frac{T}{T_0}\right)\right] - s_0T + \upsilon_0 + f(\xi), \tag{1}$$

where σ, ξ, ε^t, T and T_0 are defined as the Cauchy stress tensor, martensitic volume fraction, transformation strain tensor, current temperature and reference temperature, respectively. Other material constants α, S, ρ, c, u_0 and S_0 are the effective thermal expansion tensor, effective compliance tensor, density, effective specific heat, and effective specific internal energy at reference state and effective entropy at reference state.

In (1), the hardening function $f(\xi)$, is responsible for the transformation induced strain hardening in the SMA material. This function is given by

$$f(\xi) = \begin{cases} \frac{1}{2}\rho b^M \xi^2 + (\mu_1+\mu_2)\xi, \dot{\xi} > 0, \\ \frac{1}{2}\rho b^A \xi^2 + (\mu_1-\mu_2)\xi, \dot{\xi} > 0. \end{cases} \tag{2}$$

where ρb^A, ρb^M, μ_1 and μ_2 are material constants for transformation strain hardening. The first condition in (2) represents the forward phase transformation (A→M) and the second one represents the reverse phase transformation (M→A). The constitutive relation of a shape memory material can be obtained by the total

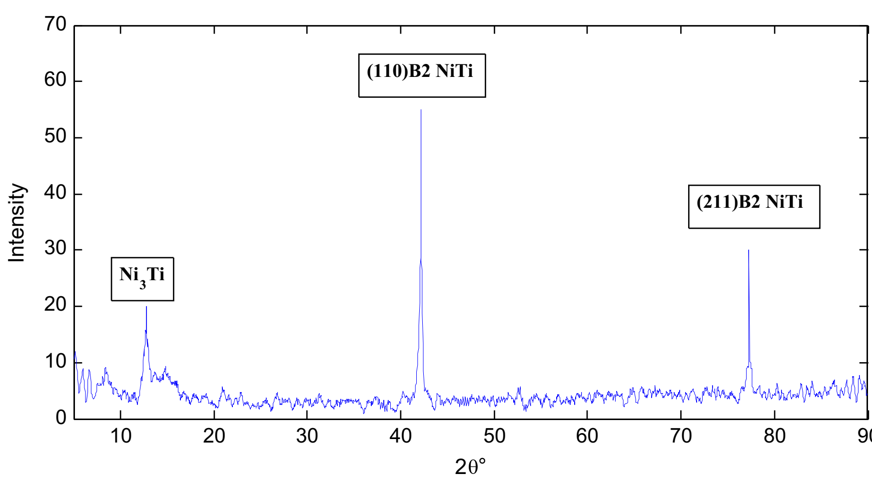

Fig. 1. XRD pattern measured at room temperature on the surface of 0.46*0.64 mm^2 orthodontic wire.

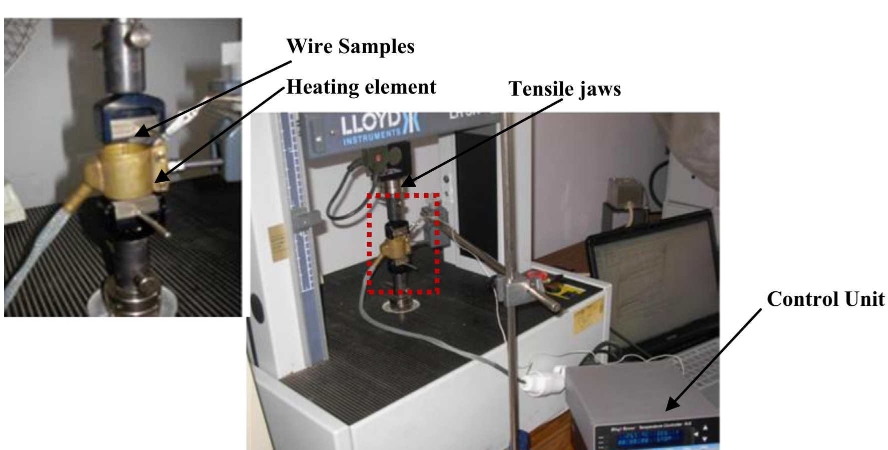

Fig. 2. Tensile test setup machine for superelastic NiTi wire.