ORIGINAL ARTICLE

Mechanical Deformation of Superelastic NiTi Wire at Different Deflections in an Orthodontic Bracket System

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ABSTRACT

Introduction: Most patients with malocclusion are given orthodontic leveling therapy with the aim of reducing the vertical discrepancy between teeth. This computational study aims to evaluate the degree of deformation of superelastic NiTi arch wire upon bending at different deflections in a bracket system. **Methods:** A three-dimensional finite-element model of a wire-bracket system was developed to simulate the bending behavior of superelastic NiTi arch wire in three-brackets configuration. A superelastic subroutine was integrated in the model to anticipate the superelastic behavior of the arch wire. The mid span of the arch wire was loaded to different extent of deflections, ranging from 1.0 to 4.0 mm. The mechanical deformation of the arch wires was accessed from three parameters, in specific the unloading force, the bending stress and the martensite fraction. **Results:** The superelastic wire deflected at 4.0 mm yielded smaller unloading force than the wire bent at 1.0 mm. The bending stress was highly localized at the wire curvature, with the stress magnitude increased from 465 MPa at 1.0 mm to 951 MPa at 4.0 mm deflection. The martensite volume consistently increased throughout the bending, with a fully transformed martensite was observed as early as 2.0 mm of deflection. The magnitude of bending stress and the volume of fully transformed martensite increased gradually in relation to the wire deflection. **Conclusion:** The wire-bracket system induced localize wire deformation, hindering complete utilization of superelasticity during orthodontic treatment.

Keywords: Orthodontic, Malocclusion, Bending stress, NiTi arch wire, Superelasticity

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INTRODUCTION

Orthodontic treatment is a process of improving dental appearance by moving poorly aligned teeth to a desirable position. Most orthodontic treatments are carried out using fixed appliance technique, as it promotes accurate tooth positioning (1). This technique requires the bonding of dental brackets on selected teeth, before an arch wire is installed by securing it within the bracket slot. In most cases, the installation process introduces few bends across the wire length, in which the degree of the bends dependent on the severity of patient's malocclusion.

NiTi arch wires are widely used during orthodontic treatment, especially during initial aligning and leveling, due to its superelastic behavior. Compared to the conventional alloy, superelastic behavior allows the NiTi wire to completely return to its preformed arch shape after severely bent in an irregular bracket system. This unique behavior is originated from the alloy ability to undergo reversible martensitic phase transformation (austenite-martensite) upon the application of stress, which is not found in any other conventional materials. On the load-deflection curve, this superelastic behavior is presented by a force plateau on the loading and unloading curve (2), which signifies constant force delivery for a considerable range of bending.

To date, several in-vitro bending models have been introduced to assess the flexural behavior of NiTi wires, ranging from cantilever bending (3), three-point bending (2) and bending in brackets system (4). Out of these three models, the latter bending system is reported to provide accurate representation of wire deformation intraorally, as it simulated the constraint bending condition of NiTi wires in the bracket slot. Recent in vitro bending studies have shown that NiTi wires yielded different force-deflection trend, depending on the configurations of the bending (4, 5). It is reported that in the bracket system, the classic unloading plateau of NiTi wire transformed into a slope trend as soon as the wire recovered from large deflection (3.0 mm and above). This slope plateau is associated to the variation of friction intensity at the wire-bracket interface, such claimed in (6).

During orthodontic treatment, it is a good practice to keep the wire deformation below the yield limit of elastic martensite. Any amount of deformation taken place over this superelastic threshold initiates plastic distortion, from which the wire cannot recover. Unfortunately, at present, the progress of flexural deformation and phase transformation underwent by NiTi wire upon its engagement in the bracket system, is lacking. Therefore, the aim of this study is to quantify the extent of NiTi arch wire deformation at different deflections by means of finite element analysis. This finding provides useful information in understanding the utilization of superelastic behavior of NiTi wire during the orthodontic treatment.

MATERIALS AND METHODS

A three-dimensional finite-element model of the wire-bracket system was developed by using Abaqus/CAE 6.12. The superelastic behavior of the NiTi wire was simulated through the employment of built-in user material subroutine for NiTi (UMAT/Nitinol). The material data needed by the subroutine are shown in Table I. These data were selected as it showed good agreement with the experimental result of uniaxial and bracket bending test (7).

Table I: Material properties and behaviors of NiTi arch wire

Parameter	Description	Value (unit)
E_A	Austenite elasticity	44 (GPa)
(ν_A)	Austenite Poisson's ratio	0.33
E_M	Martensite elasticity	23 (GPa)
(ν_M)	Martensite Poisson's ratio	0.33
(ε_L)	Transformation strain	0.06
$(\delta\sigma/\delta T)_L$	Stress rate during loading	6.7 (MPa/°C)
σ_{SL}	Start of transformation loading	377 (MPa)
σEL	End of transformation loading	430 (MPa)
T_0	Reference temperature	26 (°C)
$(\delta\sigma/\delta T)_U$	Stress rate during unloading	6.7 (MPa/°C)
$\sigma_S U$	Start of transformation unloading	200 (MPa)
σ_{EU}	End of transformation unloading	140 (MPa)
σ_{SCL}	Start of transformation stress in compression	452 (MPa)

In this study, the wire-bracket model was developed with reference to the standard case of leveling, where a highly displaced canine is to be leveled with the adjacent incisor and premolar tooth. Fig. 1 shows the assembly of 0.4 mm round NiTi wire inside the bracket slots. The distance from center-to-center of each bracket was set to 7.5 mm. The brackets were modeled following the actual geometry of commercial MTX Bracket-Roth, each with a 0.46 mm slot height and 2.80 mm slot width.

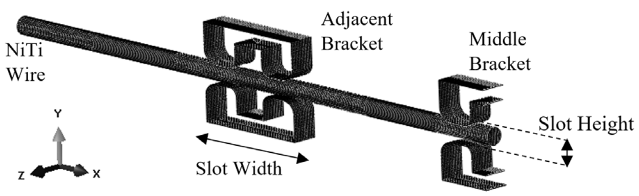

Figure 1: Finite element model for the wire-bracket system

The suitable number of elements for the wire model was determined from the mesh convergence test. As shown in Table II, five convergence runs were considered by globally seeding the element size of the wire model from 0.07 mm to 0.03 mm by increments of 0.01. A total of 72,144 linear hexahedral elements with reduced integration (C3D8R) was used to mesh the wire, as it capable of predicting the wire force at 4.0 mm with approximately 2% deviation from the experimental value. On the other hand, each bracket was meshed with 12,992 bilinear rigid quadrilateral element (R3D4).

Table II: Summary of mesh refinement model

Run	Element Size (mm)	No. Element	Force (N)	Deviation (%) from experiment	Computation period (h)
1	0.07	18,832	6.25	8.0	2.9
2	0.06	22,000	6.41	6.4	5.5
3	0.05	36,000	6.49	4.6	10.4
4	0.04	72,144	6.66	2.1	15.4
5	0.03	180,000	6.68	1.8	35.1

The bending test was assigned by allowing the vertical movement (Ux=Uz=0) of the middle bracket, at the same time, fixing the movement of the adjacent brackets in every direction (Ux=Uy=Uz=0). The bending was initiated by moving the middle bracket downwards (loading cycle) at a speed of 1.0 mm/min, before it returns to its original position by moving upward (unloading cycle) with the same speed. These loading and unloading cycles reflect the activation of the wire during installation and deactivation of the wire during tooth movement, respectively. All in all, the bending simulation were performed at four different deflections of 1.0, 2.0, 3.0 and 4.0 mm in a constant temperature of 36°C.

The interaction between the wire and the brackets was defined by surface-to-surface formulation, with the wire surface was assigned as the slave and the bracket surface as the master. A friction coefficient at the wire-bracket interfaces was set to 0.27; the common coefficient recorded when pairing stainless-steel bracket with NiTi wire (8). In this study, the mechanical deformation of the superelastic wire was accessed from three parameters, in specific the force-deflection curve, the martensite fraction and the bending stress. The first parameter was obtained from the vertical reaction force (RF2) acting at the middle bracket, the second parameter was acquired from the nodal output of the UMAT and the last parameters was analyzed from the field output of principal stress.

RESULTS

Fig. 2 shows the force-deflection curves of NiTi wire, prior to bending at different deflections in the bracket system. It is seen that the trend of the curve was

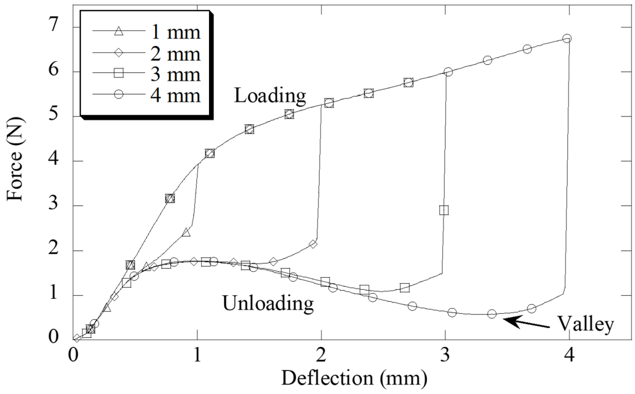

Figure 2: Force-deflection of NiTi wire at different magnitude of deflections

dependent on the magnitude of deflection applied on the wire during the loading. The wire deformed at 1.0 mm yielded about an elastic curve, signifying the elastic deformation of austenite structure. A brief force plateau starts to be observed during the unloading for the wire deflected to 2.0 mm. This plateau was corresponded to the reverse transformation of the wire phase from martensite to austenite.

For the case with wire deflection greater than 2.0 mm, the enhancement of binding at contact interface turned the loading and unloading curves into a positive and negative slope, respectively. As a result, a deeper valley depth was observed in the case of 3.0 and 4.0 mm. This delay in force magnitude (valley) denotes the reduction of considerable portion of the wire force against the strong sliding resistance created at the corners of the adjacent brackets.

Fig. 3 presents the evolution of NiTi wire's martensite fraction (SDV21) throughout the four-millimeter deflection in the bracket system. The value of 0.0 and 1.0 denotes the area with zero and complete martensite transformation, respectively. The area associated to any value within this range is in the state of partial phase transformation (i.e. phase transformation has started, but not yet been completed). From Fig 3(a), it is observed that there is no complete martensite induced during the deformation of the wire at 1.0 mm deflection. This observation highlights that the superelastic NiTi wire was only stressed within its elastic domain upon use in a minor malocclusion case (tooth discrepancy of 1.0 mm and below). The area corresponding to a complete martensite (red contour) starts to be perceived at 2.0 mm, and this area gradually expanded as the deflection continues from 2.0 mm (Fig 3b) to 4.0 mm (Fig 3d).

From Fig. 3 inset, it is seen that the wire length evolved into three different zones during the bending. The first zone denotes the fully transformed martensite (M), situated at the outer portion of the wire curvature. The second zone reflects the partially transformed martensite (A-M) that surround the first zone. The last and largest zone belongs to the austenite (A), which located at

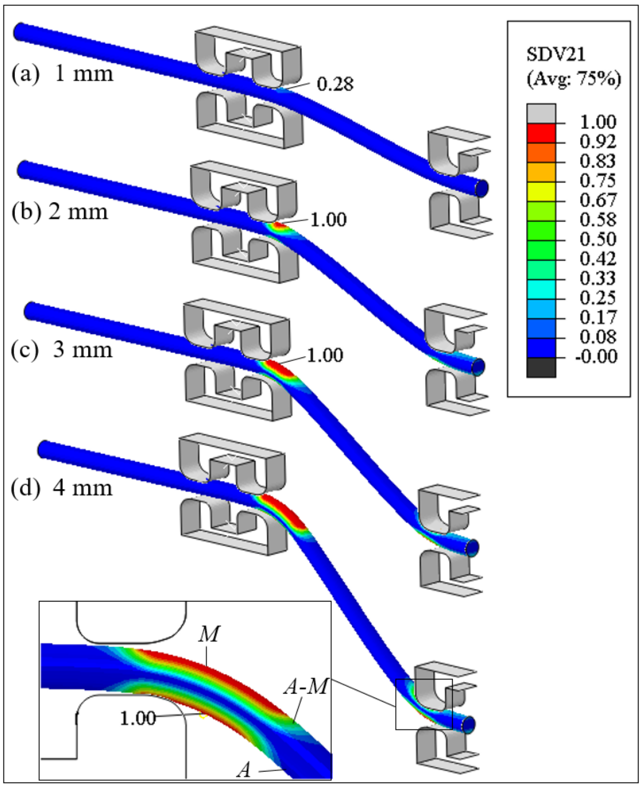

Figure 3: Evolution of NiTi wireâ•Žs martensite fraction upon bending to 4.0 mm deflection

the core and the remaining length of the wire. In brief, the deformation of NiTi wire in bracket system was highly localized near the bracket curvatures, leaving the rest of the length essentially untransformed (dark blue contour). This localized deformation highlighted that the superelastic behavior of NiTi wire is minimally exploited in the current wire-bracket system.

Fig. 4 presents the advancement of NiTi wire's principal stress throughout the 4.0 mm bending. The region of interest was located on the bending curvature, near the bracket corner, where the wire's outer elements were highly stressed in both tension and compression modes. The principal stress values of elements in tension keep increasing in relation to the applied deflection, with the stress ranging from 467 MPa at 1.0 mm to 951 MPa at 4.0 mm. These stress magnitudes are comparable to the finite element analysis conducted in (9), who predicted the maximum principal value of the arch wire at 3.0 mm deflection to be around 877 MPa. Additionally, note that the compressive stress peak is about 1109 MPa, which is much higher than the tensile stress peak (951 MPa). This observation is due to the greater critical stress for compression (σ_c^{As}), set for the material data (7).

DISCUSSION

In this study, the mechanical deformation of NiTi arch wire during bending was simulated by three-dimensional numerical modeling. The bending test considered the combination of 0.4 mm round NiTi arch wire with the

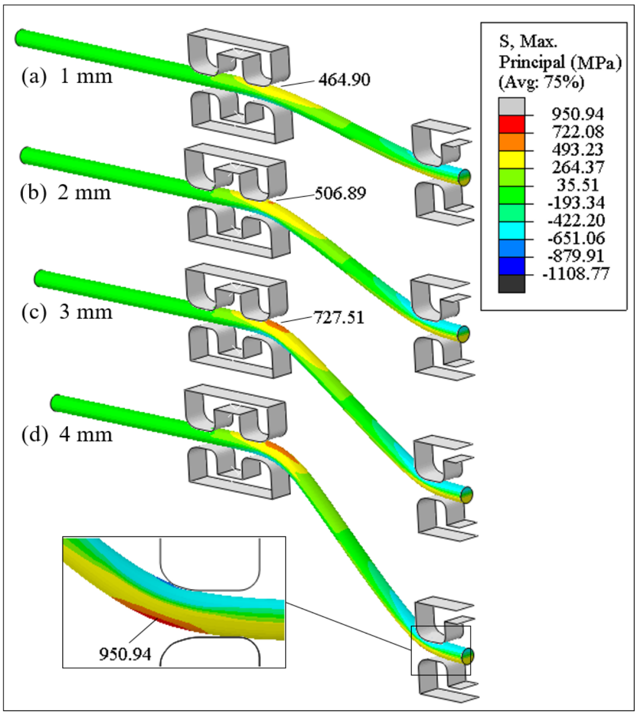

Figure 4: Progress of principal stress along the superelastic NiTi wire towards 4.0 mm bending

0.46 mm-slot bracket, which represents the normal wire-bracket combination used during leveling therapy. The bending deformation of the arch wire in relation to the displacement of the central bracket was evaluated from the change of its bending stress and martensite fraction. The numerical visualization acquired from this study offers a clear insight to what extend the superelastic NiTi arch wire is deformed in the bracket system during orthodontic treatment.

The most important question the result from Fig. 4 can answer is whether or not the principal stress recorded during the bending exceeds the martensite's yield stress. This is because, if the loading stress surpasses the elastic limit, the wire is expected to exhibit some permanent distortion, hence slightly producing deflection residual at the end of the unloading. At this juncture, we know that the critically tensioned part of the wire was stressed up to 951 MPa, and this value is approaching the yield stress of elastic martensite, which measured to be around 980 MPa during the uniaxial test (unpublished work). This preliminary result suggested that the current practice of engaging NiTi wire to a highly displace bracket (4.0 mm and above) deformed the wire way beyond its superelastic plateau range, thus introducing small portion of plastic deformation.

While interpreting the present results, it should be noted that the stress and material phase data reported in this study presented the mechanical deformation of the NiTi arch wire only for the current bending setting. If the same wire size is bent in a critical bending condition, for example, in a narrower inter-bracket distance and larger bracket displacement, greater bending stress can be anticipated from the curvature region of the arch wire. Additionally, since the thermomechanical behavior of NiTi wire is very sensitive to temperature (1), the shift in oral temperature following the consumption of warm and cold intakes also will cause sudden change in the magnitude of bending stress of the respective wire curvature

CONCLUSION

The NiTi wire yielded different force-deflection curve upon recovered from different magnitude of deflections, with lower unloading force was registered for the wire loaded at greater deflection. During the bend, the deformation of the wire chiefly commenced at the region near the bracket corners, with the magnitude of principal stress and the volume of fully transformed martensite increased gradually in relation to the applied deflection. At 4.0 mm deflection, the wire was deformed close to the yield stress of elastic martensite. This finding suggests dentist to put more caution when levelling tooth with discrepancy more than 4.0 mm, as the wire may breaks during the treatment.

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