Modeling of Propagation of Phase Transformation Fronts in NiTi Under Uniaxial

by

Dongjie Jiang, Stelios Kyriakides¹, Chad M. Landis, Karlos Kazinakis

1 Corresponding author
e-mail: skk@mail.utexas.edu
Tel. 512-471-4167

Key Words:

Tensile test, NiTi strip, Pseudoelasticity, Inhomogeneous deformation, Modeling

Revised January 17, 2017

Research Center for Mechanics of Solids, Structures & Materials
WRW 110, The University of Texas at Austin
Austin, Texas 78712, USA

Abstract

Tension induced solid-state transformation in a nearly equiatomic NiTi results in inhomogeneous deformation with transformed and untransformed material coexisting. Strains of the order of 7% are recovered on unloading with the material reverting to its original phase. In a thin strip the two coexisting phases and deformation regimes are separated by inclined fronts monitored with digital image correlation. The fronts propagate along the strip until the transformation is completed with the stress remaining nearly unchanged. A recently developed constitutive model for the pseudoelastic behavior of NiTi is implemented in a finite element analysis used to simulate the strip experiment. The model is capable of addressing the tension/compression asymmetry by incorporating both the tensile and compressive responses of the material. Softening moduli are introduced over the extents of the plateaus of the tensile response at approximately the Maxwell stress levels. The numerical solution reproduced the closed hysteresis with the correct stress plateau levels and extents. Localized deformation initiates in a single narrow band of higher strain inclined to the axis of the strip. The high strain zone propagates initially with inclined fronts and subsequently with a crisscross pattern with the stress remaining essentially unchanged. The details of the front propagation are influenced by in-plane moment caused by secondary kinking of the strip. The strip unloads by tracing a lower stress plateau developing a similar propagation of localization patterns. Overall, the numerical simulation captures the main features of the response and the associated localization configurations. The sensitivity of the solution to the mesh, the boundary conditions, and the softening moduli are discussed.

1. INTRODUCTION

The pseudoelastic behavior of nearly equiatomic NiTi is a unique characteristic where the material develops strain of several percent that is fully recovered on unloading. This property is associated with diffusionless transformation from a B2 cubic lattice (*austenite*) to a monoclinic one (*martensite*) causing macroscopic deformation. It is well documented that under tensile stress states the nucleation and evolution of transformation leads to inhomogeneous deformation (e.g., see [Shaw and Kyriakides \[1995, 1997\]](#), [Li and Sun \[2002\]](#), and [Abeyaratne and Knowles \[2006\]](#), [Bechle and Kyriakides \[2016\]](#)). By contrast, under compression the transformation stress is significantly higher, the induced strain is lower, and deformation is essentially homogeneous (e.g., [Jacobus *et al.* \[1996\]](#), [Gall and Sehitoglu \[1999\]](#), [Gall *et al.* \[1999\]](#), [Mao *et al.* \[2010\]](#), [Bechle and Kyriakides \[2014\]](#), [Reedlunn *et al.* \[2014\]](#)).

As part of ongoing efforts to investigate the effects of these material nonlinearities on SMA structures, [Jiang *et al.* \[2016a, 2016b\]](#) (see also [Jiang and Landis, 2016](#)) presented a constitutive model framework for the pseudoelastic behavior of NiTi based on a J_2 -type nonlinear kinematic hardening model with the back stress represented through a potential. This phenomenological model addresses the tension/compression asymmetry by introducing a weighted mix of two potentials for the back stress that are calibrated to the tensile and compressive stress-strain responses of the material. The model was used to successfully simulate the axial buckling and recovery of a NiTi tube. In this problem the inhomogeneity of deformation under tension played a minor role and was not modeled.

In the present study we evaluate the performance of the model in a tensile test on a pseudoelastic NiTi strip that develops inhomogeneous deformations during parts of its load-unload history. Results from an experiment on a NiTi strip are presented, followed by a brief outline of the modeling framework and its calibration to tensile and compressive material responses. The model is then implemented in a finite element model that is used to simulate the strip experiment.

2. EXPERIMENTS AND RESULTS

a. Tensile Test on a NiTi Strip

A tensile test was performed on a polycrystalline NiTi strip in the pseudoelastic temperature regime. The material has an alloy composition of 50.5 at. % Ni with $A_s = -12.8$ °C

and $A_f = 15.5\text{ }^{\circ}\text{C}$ (the same material used in [Shaw and Kyriakides, 1997](#); [Hallai and Kyriakides, 2013](#)). The strip tested had an overall length of 120 mm (4.75 in), width $w = 3.95\text{ mm}$ (0.1555 in) and wall thickness $t = 0.40\text{ mm}$ (0.0157 in). The test was performed at room temperature ($23\text{ }^{\circ}\text{C}$) in a standard screw-type testing machine using custom flat specimen grips and a calibrated 22 kN (5000 lb) capacity load cell. Clamping the specimen in the grips left behind a 48.8 mm (1.92 in) long (L) gage section. To minimize any effects of self-heating/cooling of the specimen caused by the latent heats of transformation, the tension test was performed at a slow displacement rate that resulted in an average strain rate of $0.83 \cdot 10^{-5}\text{ s}^{-1}$. The in-plane deformation history of the gage section was recorded using Digital Image Correlation (DIC—ARAMIS software). To accommodate the DIC measurements, the specimen surface was covered with a fine black speckle pattern painted over a white undercoat. Images of the full gage section were recorded at 30 s intervals with a 4288×2848 pixel resolution.

Figure 1 shows the recorded nominal axial stress (σ) plotted against the average axial strain ($\bar{\epsilon}$) in the gage section (evaluated from the DIC images). Figure 2 shows a set of 18 full field DIC axial strain contours corresponding to the numbered bullets on the response in Fig. 1 (selected from the more than 500 recorded). The response exhibits the distinctive pseudoelastic closed hysteresis of NiTi. It first rises stiffly to a stress of 374 MPa (54.2 ksi) followed by an extended stress plateau. In the process the initial austenitic phase (A) deforms elastically and homogeneously as depicted by the representative image ①. (As observed in previous studies, the small nonlinearity in the response above a stress of about 250 MPa (36.3 ksi) is an indication that some transformation is already taking place.) The first abrupt stress knee is associated with the onset of localized deformation that accompanies transformation to martensite (M). The nucleation stress is typically higher than the stress of steady-state propagation of localized deformation. In the present set up the stress concentrations at the gripped ends are sufficient to suppress the nucleation stress peak. Thus, transformation which nucleates first at the left clamped end, is without the usual initiation stress peak (for more details on initiation see Fig. 7 and related text in [Shaw and Kyriakides, 1997](#)). A single narrow inclined transformation front that separates transformed and untransformed material has appeared in image ②. The band propagates to the right as depicted by images ③ and ④ while the stress remains essentially constant. The strain of the transformed material corresponds to that at the end of the stress plateau while that of the untransformed is at the level of the beginning of the plateau. The band

front is initially rather straight with an inclination (ϕ) of 55-60° and its width is about 5-8 mm (see expanded image ③ in Fig. 3). As observed previously, the steep gradient across such inclined bands causes local kinking of the specimen in the plane of the strip (for NiTi strips see [Shaw and Kyriakides \[1998\]](#), and for strips deformed by Lüders banding see [Lomer \[1952\]](#), [Butler \[1962\]](#), [Kyriakides and Miller \[2000\]](#)). For the present specimen the kink angle, γ , is of the order of 2° (Fig. 3), which results in the build up of a local in-plane moment. In an effort to relieve the moment, transformation along the second characteristic with an inclination of $-\phi$ tends to be activated. In the current experiment, this did not materialize during loading but the second characteristic had the effect of making the front curved, with one side having an inclination of approximately 55° and the other a larger value. (A more complete deformation history can be seen in the video [NiTi_TensionExperiment.mp4](#) included as supplementary material).

At some point during loading, a second front initiated from the clamped end on the right (see image ⑤). It has the same inclination as the first front as this is again a moment relieving mechanism. Subsequently the two fronts propagated simultaneously towards each other meeting in image ⑦, causing the small stress valley just after point ⑦ on the response. The inhomogeneous part of the response has now been completed and the response recovers stiffness associated with the mainly *M*-phase.

Plotted in Fig. 4 is the time history of the axial position of the front (undeformed coordinates). A single front starts propagating at approximately 2000 s into the test. It moves at a velocity, c , that is in accordance with the expression

$$c = \frac{\dot{d}}{nDe_L} \quad (1)$$

where $\dot{d}$ is the applied displacement rate, De_L is the upper plateau strain and n the number of fronts propagating simultaneously in the gage section ([Butler \[1962\]](#); [Shaw and Kyriakides \[1995\]](#)). Thus, when the second front starts to also propagate, at about 5000 s into the test, the velocity drops by a factor of 2 as indicated by the reduction of the slope of the data.

Unloading from point ⑧ initially occurs with homogeneous deformation as depicted by image ⑨. At a stress of 152 MPa the martensitic phase stops being stable and the specimen starts transforming back to austenite. Transformation nucleates with an increase in the load at about the same location that the forward transformation terminated at. It is again in the form of two inclined parallel fronts that propagate away from each other (image ⑩). Transformation returns

the material to the strain level at the end of the lower stress plateau while that remaining in the M -phase is at a strain of about 4.6% at the beginning of the lower plateau. By point ⑫ the right front has reached the clamped end and subsequently the specimen transforms with the propagation of a single front towards the left end (images ⑫ and ⑬). In the neighborhood of point ⑭ the moment associated with the asymmetry of the deformed section can no longer be sustained; transformation nucleates along the second characteristic developing the more symmetric crisscross pattern observed in image ⑭. Soon there after the front reverts back to a single front (image ⑮) but now with the opposite inclination to the ones seen thus far (see expanded view of image ⑮ in Fig. 3). These events are reflected on the corresponding part of the $S - \bar{\epsilon}$ response as stress undulations. Soon after image ⑯, the whole specimen is back to the A -phase. It unloads homogenously along the same stiff response as that of loading (image ⑰).

The front spacial-temporal history during unloading is included in the $x-t$ diagram in Fig. 4. Depicted is the initial two-front propagation, followed by propagation in a single front beyond about 13000 s. Once again, the slopes of the data are captured through Eq. (1) by adopting the strain associated with the $M \rightarrow A$ transformation (i.e., De_L of the unloading plateau).

3. ANALYSIS

We adopt the basic constitutive model framework developed in [Jiang et al. \[2016b\]](#) (see also [Jiang and Landis, 2016](#)) tailored to the needs of the tensile problem outlined in Section 2 and use it in a FE model to simulate the reversible unstable behavior observed. For completeness, we start with an outline of the main features of the constitutive framework. Special emphasis is given to the adoption of softening over the unstable branches of the strip response and their calibration to the forward and reverse transformations associated with the upper and lower stress plateaus.

a. Constitutive Model

Let S_{ij} and s_{ij} be the stress tensor components and the deviatoric counterparts. The elastic deformation is enclosed by a transformation surface defined by

$$F = 3(s_{ij} - s_{ij}^B)(s_{ij} - s_{ij}^B)/2 - S_o^2 = 0 \quad (1)$$

where s_{ij}^B represent the back stress and S_o represents the size of the transformation surface.

The strain increment is decomposed into elastic and transformation strain increments, i.e. $\dot{e}_{ij} = \dot{e}_{ij}^e + \dot{e}_{ij}^t$. Elastic deformations are linear and isotropic with constants (E, n) . The stress rate components are given by

$$\dot{S}_{ij} = C_{ijkl}(\dot{e}_{kl} - \dot{e}_{kl}^t) \quad (2)$$

where

$$C_{ijkl} = \frac{E}{(1+n)} \frac{1}{2} (d_{ik}d_{jl} + d_{il}d_{jk}) + \frac{n}{1-2n} d_{ij}d_{kl}.$$

The transformation strain increment is taken to be normal to the transformation surface such that

$$\dot{e}_{ij}^t = L(s_{ij} - s_{ij}^B) \quad (3)$$

where $L > 0$ is the plastic multiplier.

The back stress is related to the transformation strain through a potential as follows

$$S_{ij}^B = \frac{\Psi}{\Psi_{ij}^t}. \quad (4)$$

The tension/compression asymmetry in the stress-strain behavior is introduced through the following representation of this potential

$$\Psi = \chi \Psi_c^t(e_e^t) + (1 - \chi) \Psi_t^t(e_e^t), \quad (5)$$

where Ψ_c^t and Ψ_t^t are potentials that are calibrated to the measured uniaxial compression and tension stress-transformation strain responses, and e_e^t is an equivalent transformation strain that governs the strain asymmetry. The following definition of equivalent transformation strain is adopted

$$e_e^t = J'_2 f(J_r), \quad J_r = J'_3 / J'_2, \quad (6a)$$

with

$$f = \cos\{\cos^{-1}[1 - a(J_r^3 + 1)]/3\}, \quad (6b)$$

where the following definitions of the deviatoric strain invariants hold

$$J'_2 = (2e_{ij}^t e_{ij}^t / 3)^{1/2}, \quad J'_3 = (4e_{ij}^t e_{jk}^t e_{ki}^t / 3)^{1/3}, \quad \text{and} \quad e_{ij}^t = e_{ij}^t - e_{kk}^t d_{ij} / 3. \quad (6c)$$

The function f scales the uniaxial compressive transformation strain to the tensile one.

The weight function χ , chosen to be a function of the ratio of the deviatoric strain invariants, J_r , facilitates the generalization of these results to arbitrary strain states. $J_r = 1$

represents uniaxial extension and $J_r = -1$ represents uniaxial contraction. Thus, $\chi(J_r)$ with $\chi(-1) = 1$ and $\chi(1) = 0$, interpolates between the tensile and compressive responses. In addition, to ensure that the hardening moduli remain finite as $J_r \rightarrow 0$

$$\chi(0) = 0, \chi'(0) = 0, \chi^{iv}(0) = 0 \text{ and } \chi^v(0) = 0. \quad (7)$$

The back stress then becomes

$$S_{ij}^B = \chi \frac{d\mathcal{Y}_c^t}{de_e^t} \frac{\mathbb{I}e_e^t}{\mathbb{I}e_{ij}^t} + (1 - \chi) \frac{d\mathcal{Y}_t^t}{de_e^t} \frac{\mathbb{I}e_e^t}{\mathbb{I}e_{ij}^t} + \chi(J_r)(\mathcal{Y}_c^t - \mathcal{Y}_t^t) \frac{\mathbb{I}J_r}{\mathbb{I}e_{ij}^t}. \quad (8)$$

It can be shown that reduction of (8) to uniaxial stress states (see Appendix A of [Jiang et al. 2016b](#)) results in

$$S_{11c}^B = \frac{d\mathcal{Y}_c^t}{de_e^t} \frac{\mathbb{I}e_e^t}{\mathbb{I}e_{11}^t} \text{ and } S_{11t}^B = \frac{d\mathcal{Y}_t^t}{de_e^t} \frac{\mathbb{I}e_e^t}{\mathbb{I}e_{11}^t} \quad (9)$$

for compression and tension respectively. In view of the kinematic hardening model adopted, and the reductions in Appendix A of [Jiang et al. \[2016b\]](#), Eqs. (9) imply:

$$|S_{11c}| - f(-1) \frac{d\mathcal{Y}_c^t}{de_e^t} = S_o \text{ and } S_{11t} - f(1) \frac{d\mathcal{Y}_t^t}{de_e^t} = S_o \quad (10)$$

for loading, where S_o is the size of the transformation surface.

The function ξ extends the calibrated model to general strain states and ultimately should be calibrated to experimental results. The following expression has been adopted for the calculations presented here which satisfies the conditions in (7),

$$\chi = \frac{f(J_r) - f(1)}{f(-1) - f(1)}. \quad (11)$$

The constitutive model outlined is implemented into a user-defined material subroutine (UMAT) in ABAQUS. In the UMAT, the constitutive equations are discretized according to a backward Euler routine and are solved by Newton's method.

b. Constitutive Model Calibration

In past works we demonstrated that Lüders-like unstable behavior could be captured by the adoption of a three-regime up-down-up stress-strain response in an appropriate constitutive model. The stress-strain response consists of a stiff hardening branch followed by a mildly

softening one that stretches over the unstable regime of a tensile response and connects to a second hardening response. Such responses introduced in an elastic-plastic constitutive model have been shown to reproduce with significant accuracy the partly unstable behavior exhibited in tensile tests on low-carbon steels (Kyriakides and Miller [2000]; Hallai and Kyriakides [2013]). Similar models were used to reproduce successfully the interaction of Lüders banding with geometric instabilities in more complex structural problems (Corona et al. [2002]; Aguirre et al. [2004]; Kyriakides et al. [2008]; Hallai and Kyriakides [2011a, 2011b]).

Solid-state phase transformations, at least as they materialize in tests under primarily tensile stress states in SMAs in the pseudoelastic temperature regime, exhibit a macroscopically similar material behavior to Lüders banding. Thus in his early work Ericksen [1975] suggested the adoption of an up-down-up stress strain response as a way of modeling the unstable behavior. Abeyaratne and Knowles further developed this concept, at least in the uniaxial setting (see [2006] for a review). In an effort to demonstrate the soundness of such an approach Shaw and Kyriakides [1998] and Shaw [2000] used a J_2 -based elasto-plastic framework to show that the localization and propagation of instabilities exhibited in NiTi strips under tension could be qualitatively reproduced. Of course, among other limitations, such a model does not reproduce the reversibility of pseudoelastic behavior. Other efforts that adopt up-down-up responses in constitutive models to simulate the propagation of fronts include Badnava et al. [2015], Ahmadian et al. [2015], Baldelli et al. [2015], Levitas and Ozsoy [2009], Ozsoy and Babacan [2016], and Zhu et al. [2016].

The phenomenological constitutive framework of Jiang et al. [2016b] was shown to successfully reproduce the buckling and recovery behavior of NiTi tubes in compression. In that problem, the unstable nature of the material exhibited under tension did not play a significant role and was not modeled. In the present problem, the state of stress is tensile throughout the load/unload history and consequently the representation of the unstable tensile uniaxial stress-strain response is of paramount importance. Thus, the aim of the present analysis is to test the capabilities of the model in the tensile setting. We start by describing the calibration of the up-down-up responses that will be adopted to model the measured strip hysteresis. Since compression plays no role in the present solution, the fit of the compressive stress-strain response is included here strictly for completeness of the constitutive model. Furthermore, since the compressive properties of the strip used in the experiments were not available at the writing

of this paper, the response adopted is based on the forward transformation stress and strain of the tube used in [Jiang et al. \[2016b\]](#). In addition, for simplicity, the size of the transformation surface, S_o , is assigned the same value as that of the tensile response. Details of the calibration of the tensile response follow:

- The elastic modulus of A used is similar to the value of the [Hallai and Kyriakides \[2013\]](#) strip experiments. It is somewhat higher than the DIC value of the present strip experiment and this difference is reflected in Fig. 5a. (The DIC parameters were aimed at capturing the inhomogeneous deformation, which lead to some error in the estimation of small deformations associated with the initial modulus.)
- The initial nonlinearity exhibited during the initial homogeneous deformation of A is not fitted and as a result the corresponding model response is somewhat stiffer than that of the measured response.
- The softening modulus of the $A \rightarrow M$ transformation is similar to that extracted from the sandwich experiment on this strip material by [Hallai and Kyriakides \[2013\]](#) (see also [Zhu et al. \[2016\]](#)). Its effect will be studied in the parametric study that follows. Lacking a similar experimental support for the $M \rightarrow A$ transformation, the softening modulus was assumed to be the same as that of the forward transformation.
- The two negative slopes are placed approximately at stress levels that correspond to the corresponding Maxwell stress levels, but the exact positions are determined for best reproduction of the two stress plateaus.
- The size of the transformation surface Φ (S_o in Eq. (1)) corresponds to the stress difference between the measured loading and unloading stress plateaus.
- The initial hardening modulus following the stress valley is fitted to that of the experiment.
- For simplicity, the elastic modulus of M is assumed to be the same as that of A . As a consequence the initial unloading slope of M is higher than that of the experiment. Furthermore, the connection to the lower softening stage is similar to the transition from softening to hardening in the forward transformation.
- The stable and unstable branches are connected by functions that provide algebraic convenience and optimal numerical performance.

With these assumptions the derivatives of back stress potentials γ_c^t and γ_t^t in Eq. (10) take the following form:

$$\frac{d\gamma^t}{de_e^t} = h_0 e_e^t + (h_1 - h_0) \left[e_e^t - \frac{1}{b} (1 - e^{-be_e^t}) \right] + (h_2 - h_1) \begin{cases} 0 & 0 \leq e^t \leq e_1 \\ (e_2 - e_1)(z^3/4 + z^2/8) & e_1 \leq e^t \leq e_2 \\ 3(e_2 - e_1)/8 + (e_e^t - e_2) & e_2 \leq e^t \end{cases} \quad (12)$$

$z = (e_e^t - e_1)/(e_2 - e_1)$

with the values for the paramaters $b, h_0, h_1, h_2, e_1, e_2$ listed in Table 1. The constant a in the function f (see Eq. (6b)) is assigned the value of 0.9357. The resultant back stresses responses are shown in Fig. 5b.

Table 1 Model parameters for tensile and compressive responses

Model	E GPa	n	S_o MPa	b	h_o GPa	h_1 GPa	h_2 MPa	e_1 (%)	e_2 (%)
Comp.	68.3	0.425	93.8	2500	1575	2.772	157.5	2.7	3.3
Tens.	68.3	0.425	93.8	2500	1434	-9.751	78.55	2.7	3.3

c. Finite Element Model

The constitutive model is implemented as a UMAT in a finite element model of the strip experiment. The model, shown in Fig. 6 has the dimensions of the strip tested $\{L \times W \times t\} = \{48.8 \times 3.95 \times 0.399\}$ mm. To accommodate the expected strain jumps, as in our past works (e.g., Aguirre et al. [2004], Hallai and Kyriakides [2011a, 2011b, 2013]), we adopt ABAQUS's 3-D incompatible elements C3D8I (see Wilson et al. [1973], Ortiz et al. [1987], Nacar et al. [1989], Simo and Armero [1992]). In order to avoid any directional bias, the meshes adopted are uniform with cubical elements. The mesh used to generate the main results presented in the following section has 2 elements through the thickness, 20 across the width and 245 along the length for a total of 9800 elements. In the experiment, the strip was clamped between flat grips. This is a difficult boundary condition to reproduce; so instead, in the model the boundary conditions are idealized by fixing the degrees of freedom of the nodes at both ends except that the axial

displacement of the nodes on the left end is prescribed incrementally. A small geometric imperfection in the form of a small indentation on the top surface of the strip is introduced in the way of initiating the instability. The imperfection is located a distance W from the left end and is generated by reducing the local width by $0.02t$ over two elements (see Fig. 6).

4. NUMERICAL RESULTS

a. Simulation of the NiTi Strip Tensile Test

The calculated load-unload average nominal stress-elongation ($S - d/L$) response is plotted in Fig. 7a together with the experimental one. Figure 8 shows a set of 21 full-field deformed configurations of the strip corresponding to the solution at the location of the numbered bullets on the response. Superimposed on the configurations with color contours is the calculated axial strain. Initially the strip deforms uniformly with the response following the uniaxial stress-strain response. The stress rises to a local maximum of 439 MPa when it drops sharply down to 362 MPa. As discussed in Appendix A, this drop is a "jump" caused by unloading in the rest of the strip. It does not affect the events that follow and thus for simplicity the displacement controlled loading is used in the rest of the study. Localized deformation has initiated from the imperfection in the form of a narrow band of higher strain. The band can be seen in the expanded view of image ① in Fig. 9. It is rather weak, with a width of a couple of elements and an inclination of 53° to the direction of loading, which is very close to that of the Hill [1952] characteristics of 54.7° (see also Bijlaard [1940]). The band can be seen fully developed covering the width of the strip in image ② that corresponds to the bottom of the load drop. It has the same inclination, its width now covers four elements, and the center of the band has reached a strain of about 5.6%, which corresponds to the value at the end of the stress plateau. (A more complete deformation history can be seen in the video [NiTi_TensionAnalysis.mp4](#) included as supplementary material).

As discussed in the experimental section (see also Shaw and Kyriakides [1998], Kyriakides and Miller [2000]), inclined zones of higher strain result in the built up of in-plane moment in these strips. The moment acting on the left edge of the strip, M , will be monitored in Fig. 7b where it is plotted against the applied end displacement (normalized by $M_o = S_{NM}tw^2/6$). It can be observed that the sudden appearance of the band between the stress maximum and point ②, has resulted in a sharp built up of moment. Beyond point ②, the stress

starts to trace a somewhat ragged plateau during which the band of high strain propagates initially toward the right. The shear deformation of the highly deformed zone causes local kinks in the strip and increases the moment. In image ③ in Fig. 9, the kink angle is approximately 1.8° and the moment reaches a local maximum. At this point, a small band along the second characteristic initiates from the upper left corner of the specimen that can be seen in image ④. The new band has a straightening effect and results in a reduction in the moment of about 30% between image ③ and ④. The small zone of material on the left end is soon fully deformed and the ensuing deformation takes place strictly by the propagation of the right front. As this takes place the moment increases again. This is not sustainable and some deformation along the second characteristic is activated which results in the front developing some curvature that can be seen in image ⑤. The additional increase in the moment observed after image ⑤ again cannot be sustained causing the front to flip its inclination along the second characteristic as observed in image ⑥. Associated with the new front is a kink of about 1.9° while its inclination is now about 71° (see Fig. 9). This is because the moment remains large and the second characteristic is active. The front propagates with the new inclination for a short distance but because of the large moment the band initiation starts to alternate between the two characteristics producing the crisscross patterns observed in images ⑦ and ⑧ (see also the expanded view in Fig. 9). These patterns have a straightening effect on the structure and result in the moment fluctuations and the reducing trend observed in Fig. 7b. The alternating initiation of bands leaves behind small islands of undeformed material, each of which is deformed somewhat later. In addition, the multiple initiations and terminations of localized deformation result in the higher amplitude stress undulations that can be observed between points ⑦ and ⑨ in Fig. 7a. By point ⑨ the front has reached the right end. A small island of undeformed material finally deforms but with a small increase of stress to 399 MPa at point ⑩. At the end of the plateau at point ⑨ the average strain is 5.62% a value that closely corresponds to the end of the stress plateau recorded in the experiment.

The strip unloads from ⑩ tracing a similar nonlinear path to that of the experiment. In images ⑪ and ⑫ the deformation remains essentially homogeneous and the bending moment is reduced to essentially zero. Inhomogeneous deformation initiates from the right end soon after point ⑫. It is in the form of a crisscross pattern that appears similar to those developed during loading (images ⑬-⑮), while the stress traces a plateau that corresponds to that of the

experiment. The crisscross pattern of the propagating front maintains the moment at a low level but causes fluctuations in the moment as well as in the recorded axial stress. In the neighborhood of point ⑩, one of the characteristics wins and a single front develops with an inclination that is opposite to that developed during the early parts of loading. The asymmetry associated with a single front results in a significant increase in the moment between points ⑩ and ⑪. In the neighborhood of point ⑪, a second front with the same inclination initiates from the left. In images ⑪-⑬ the two fronts propagate towards each other and in the process the bending moment gradually reduces. In the expanded view in Fig. 9, the inclinations of the fronts in image ⑬ have returned back to 53° and 57° . The last remaining sliver of high strain material in image ⑬ has an inclination of 54° . Beyond this point the deformation is homogeneous as the strip unloads along the stiff path followed during loading.

Comparison between the numerical and experimental results leads to the following observations:

- In the experiment transformation initiates from one of the clamped ends due to the inherent stress concentration. In the simulation localized deformation is initiated from an imperfection introduced artificially. The location and type of imperfection used influences the initial patterns of localized deformation and its subsequent propagation.
- The calculated stress-displacement response closely follows the experimental one. The small difference in the initial modulus is caused by differences between the modulus of the response used in the calibration and that recorded by the DIC system used in the experiment (see Section 3b).
- In the calculated response, the initial stress peak is governed by the slope of the negative branch and its connection to the initial stable branch, which determines the initial stress maximum of the stress-strain response. It is also influenced to some degree by the type and amplitude of the imperfection used.
- The stress valley in the "reverse transformation" is partly masked by the residual untransformed material at the two ends.
- In the experiment, the transformation propagated mainly through a single band during loading. Reverse transformation propagated also via an inclined front but a crisscross pattern developed towards the end of the transformation. In the simulation, deformation also propagated initially via an inclined band but switched to a crisscross pattern in the second

half of the test. During unloading, the front propagation followed the reverse order to that of loading. Band and kink angles produced in the model matched those of the experiment. The differences in the propagating fronts between experiment and simulation are influenced by the idealized boundary conditions adopted in the model and by the strength of the instability implied by the stress peaks/valleys and the negative slopes assumed. Support for this will be given in the parametric studies that follow.

- The model is an idealization of the experiment, with simpler/cleaner boundary conditions. The islands at the two ends left untransformed in image ⑩ are a consequence of this idealized boundary conditions adopted in the model. They require a higher stress to be transformed.

b. Parametric Study

(i) Mesh Sensitivity of the Solution

The softening branches introduced in the stress-strain response imply some degree of mesh sensitivity of the solution. As in our treatment of Lüders banding in structures, our approach has been to choose a uniform mesh that is fine enough to reproduce the finer features of the localized deformation observed in the experiments. Once this is decided, the addition of mild rate dependence to the constitutive model regularizes the solution removing the sensitivity to the mesh (Needleman [1988]). The alternative approach is to introduce higher order gradients in the formulation with an intrinsic length scale. To date, this length parameter is chosen for best performance of the model—e.g., see He and Sun [2010], Duval et al. [2011] for SMA applications, Maziere et al. [2016] for Lüders banding. The SMA phenomenological constitutive model outlined in Section 3 is rate independent. Consequently, the mesh sensitivity of the strip tension solution presented in the previous section must be examined. To this end, two additional mesh densities were used to simulate the tension test in which the number of cube-shaped elements through the thickness (N_t) was increased to 3 and 4. This respectively increases the number of elements across the width to 30 and 40 and to 33,300 and 78,400 total elements.

The solutions from the two finer meshes are very similar to the one depicted in Figs. 7 and 8 and will be simply outlined here. The mesh refinement had next to no visible effects on the calculated stress-elongation response or on the front initiation and propagation patterns. The main effect of mesh refinement is in the width of the front transition zone. Figure 10a shows

expanded views of the banded localized deformation produced by the three mesh densities. They correspond to point ③ on the calculated response shown in Fig. 7a. The inclinations of the two band fronts, the kink angles, and the secondary band that has initiated at the upper corner of the left end of the strip are essentially the same in the three solutions. However, the front transition zones occupy approximately two elements in each mesh. Consequently, the front is getting narrower as N_t increases. Another illustration of the effect of the mesh on the width of the band is shown in Fig. 10b, where the axial strain along the centerline of the strip in the neighborhood of the right hand front is plotted for the three meshes. All three cases show the strain ahead of the front to be 0.77% and behind it 5.6%. They are connected with transition zones the widths of which decrease as N_t increases.

In summary, in the present problem the width of this transition zone does not affect the solution if the mesh is fine enough to capture the finer features of localized deformation. This is to be contrasted with other problems where localization bands result in failure and must be modeled more accurately

(ii) *Effect of Strain Rate*

The present constitutive model does not incorporate material rate dependence. Here we will demonstrate the effect of rate on the solution using J_2 plasticity with a mild power-law rate dependence calibrated to the same up-down-up stress-strain response as that used in the present model (Fig. 5a). The comparison is limited to loading only. The strip is discretized with the same elements using the three uniform meshes used in the previous section (i.e., $N_t = 2, 3$ and 4) Each case is analyzed first with rate independent plasticity, second using the powerlaw rate model, and then the solutions are compared. Summarized below are the main observations from these comparisons.

- The *loading response* and the evolution of fronts produced using J_2 plasticity models are very similar to those of the constitutive model in Section 3.
- For each mesh density, the rate independent and rate dependent solutions produced front evolutions that are very similar (e.g., see comparison of rate independent and rate dependent configurations in Fig. 11).
- The mesh was not found to affect the evolution of fronts for the rate independent plasticity and, of course, the same was true for the rate dependent case.

- As pointed out in part (i), in the hysteretic model the main effect of the mesh is in the width of the transition zone. The solutions using the rate independent plasticity model exhibit a similar narrowing of the transition zone as the mesh is refined. The addition of rate eliminates this difference

(iii) Effect of Softening Modulus

The softening slope adopted in the model used to simulate the strip experiment was based on the one measured in the sandwich tensile test performed by Hallai and Kyriakides [2013] on the same strip as that used in the present experiment. In order to assess the effect of the strength of softening on the solution to the strip problem, here we will vary the slope of the negative branches, while keeping other characteristics of the up-down-up responses similar. The stress-strain responses considered are shown in Fig. 12a. The response used thus far is designated as 0 and two cases with stronger softening are designated as +1 and +2 and those with weaker softening as -1 and -2.

Figure 12b shows the calculated stress-displacement responses using the mesh of the base case (Fig. 6). The corresponding sets of deformed configurations of the strips are included as Supplementary Material and are designated as [Confs+1](#), [Confs-1](#), etc (the images correspond to approximately the same displacement as that of the bullets on response 0 included in Fig. 12b). All responses exhibit a local stress maximum that of course is higher for the two stronger cases and lower for the two weaker ones. The stress maxima are followed by the usual stress plateaus and stress undulations. The same is repeated for the unloading plateaus.

- All cases develop localized deformation that propagates as the stress plateaus are traced.
- The strength of softening does influence the patterns and the events as follows: During loading, as the softening becomes stronger, the single front propagation persists further into the displacement history, while the crisscross front propagation is less prominent. As the softening gets weaker, the single front propagation terminates earlier and the crisscross pattern becomes dominant.
- During unloading, for +2 and -2 the front propagates from left to right, in other words it does not follow the reverse order to that of loading. For +1, 0 and -1 the front propagated from right to left. For +2 the propagation was dominated by a single front whereas for +1, 0 and -1, the crisscross pattern covered nearly half of the unloading history and in the rest a single

front dominated. In the case of -2, the front propagated with both characteristics active, resulting in the butterfly shaped of the front observed in Confs-2.

5. SUMMARY AND CONCLUSIONS

The phenomenological constitutive model of NiTi pseudoelastic behavior of [Jiang et al. \[2016b\]](#) (see also [Jiang and Landis \[2016\]](#)) has been used in a finite element model to simulate a tensile experiment on a NiTi strip. The strip exhibits the usual pseudoelastic response tracing a closed hysteresis consisting of an upper and a lower stress plateau as the $A \rightarrow M$ and the $M \rightarrow A$ transformations takes place. The transformations lead to inhomogeneous deformation with transformed and untransformed material (relatively large/small deformation) co-existing. The transformed and untransformed materials are usually separated by an inclined front that propagates at a well-defined speed dictated by the rate at which the end of the strip is displaced and the extent of the transformation strain. The major aspects of the experimental results have been observed in the past in similar tests on NiTi strips and on low-carbon steel that exhibit the macroscopically similar phenomenon of Lüders banding. With the benefit of DIC in the present experiment the evolution of inhomogeneous deformation is captured with more detail.

The constitutive model is capable of addressing the tension/compression asymmetry so it is calibrated to both the tensile and compressive responses of the material. Softening moduli are introduced over the extents of the plateaus of the tensile response at approximately the Maxwell stress levels. Guidance on the value of the softening slope for the $A \rightarrow M$ transformation came from the experimental results of [Hallai and Kyriakides \[2013\]](#). Lacking similar experimental support for the reverse transformation, the lower softening slope was assigned the same value as the upper one. The functions used to connect them to the stable branches are chosen mainly for algebraic convenience.

The present form of the constitutive model is rate independent so the usual regularization by the addition of rate was not possible. Instead, a uniform mesh consisting of cubical 3-D solid incompatible elements was chosen fine enough for good reproduction of the finer features of the fronts observed in the experiment. A parametric study demonstrated that the main effect of the mesh is on the width of the transition zones separating the relatively deformed and undeformed zones.

The numerical simulation of the strip tension test reproduced the closed hysteresis with the correct stress plateau levels and extents. The numerical solution exhibits the usual initiation stress peak the level of which depends on the strength of the softening assumed, the manner it is connected to the initial hardening branch, and the amplitude of imperfection used. By contrast in the experiment, the initiation peak was suppressed by the stress concentrations at the clamped ends. Localized deformation is initiated from a small geometric imperfection introduced to the side of the strip model. It takes the form of a single narrow band of higher strain inclined to the axis of the strip at the expected Hill angle ($\sim 55^\circ$). As in the experiment, as the end of the strip is pulled, the high strain zone propagated initially with an inclined front with the stress remaining nearly constant. The shear in the inclined deformed zones causes in-plane local kinking of the strip similar to that observed in the experiment. Kinking causes a built up of in-plane moment, which is relieved by the front first flipping to the alternate characteristic, and subsequently propagating in a crisscross pattern.

The lower stress plateau starts without the usual stress valley recorded in the experiment as localization initiated at one of the ends from a small island of material that was left undeformed during loading. In the experiment the front propagated mostly with a single inclination, developing a crisscross pattern and switching to the alternate characteristic close to the end. In the model, the band propagates with the crisscross front for half the length and then switches to a single inclined front.

Overall, the simulation captured the main features of the response and the associated deformation patterns. Differences with the experimental patterns and their evolution are caused by differences in the idealized boundary conditions used in the model, the manner in which the localization is initiated from a local imperfection and by its location, and by the strengths of the two softening branches adopted.

Appendix A: Effect of Loading Scheme on Initial Load Drop

In the numerical simulation of the strip tension tests presented, localized deformation initiates as a narrow inclined band of higher deformation. It causes a drop in load that leads to some unloading in the rest of the strip. For the particular length of strip analyzed, the unloading is large enough that it cannot be handled by the displacement controlled loading scheme adopted. A more rigorous arc length incrementation scheme based on Riks' method shows the response to unload along a path that is to the left of the vertical as depicted in Fig. A1. Thus the vertical part of the solution in Fig. 7a constitutes a "jump." This particular aspect of the response is not of interest in the rest of the study and thus for simplicity the solutions shown are based on a displacement controlled loading.

Fig. A1 Initial parts of the stress-deformation response calculated using "displacement controlled" loading and the Riks arc length incrementation method

Acknowledgments

The authors acknowledge with thanks the financial support received for this work from the National Science Foundation under grant no. CMMI-12000465.

References

- Abeyaratne, R., Knowles, J.K. (2006). *Evolution of Phase Transitions*. Cambridge University Press, New York.
- Aguirre, F., Kyriakides, S., Yun, H.D. (2004). Bending of steel tubes with Lüders bands. *Int. J. Plast.* **20**, 1199-1225.
- Ahmadian, H., Ardakani, S.H., Mohammadi, S. (2015). Strain-rate sensitivity of unstable localized phase transformation phenomenon in shape memory alloys using a non-local model. *Int'l J. Solids Struct.* **63**, 167-183.
- Badnava, H., Kadkhodaei M., Mashayekhi, M. (2015). Modeling of unstable behaviors of shape memory alloys during localization and propagation of phase transformation using a gradient-enhanced model. *J. Intel. Mat. Syst. Str.* **26**, 2531-2546.
- Bechle, N.J., Kyriakides, S. (2014). Localization in NiTi tubes under bending. *Int'l J. Solids Struct.* **51**, 967-980.
- Bechle, N.J., Kyriakides, S. (2016). Evolution of localization in pseudoelastic NiTi tubes under biaxial stress states. *Int'l J. Plasticity* **82**, 1-31.
- Bijlaard, P.P. (1940). Theory of local plastic deformation. Publication of the International Association of Bridge and Structural Engineers **6**, 27-44.
- Butler, J.F. (1962). Lüders front propagation in low-carbon steels. *J. Mech. Physics of Solid* **10**, 313-334.
- Corona, E., Shaw, J.A., Iadicola, M.A. (2002). Buckling of steel bars with Lüders bands. *Int'l J. Solids Struct.* **39**, 3313-3336.
- Duval, A., Haboussi, M., Ben Zineb, T. (2011). Modelling of localization and propagation of phase transformation in superelastic SMA by a gradient nonlocal approach. *Int'l J. Solids Struct.* **48**, 1879-1893.
- Ericksen, J.L. (1975). Equilibrium of bars. *J. Elasticity* **5**, 191-201.
- Gall, K., Sehitoglu, H., Chumlyakov, Y.I. and Kireeva, I.V. (1999). Tension-compression asymmetry of the stress-strain response in aged single crystals and polycrystalline NiTi. *Acta Mater.* **47**, 1203-1217.

- Gall, K., Sehitoglu, H. (1999). The role of texture in tension-compression asymmetry in polycrystalline NiTi. *Int'l J. Plasticity* **15**, 69-92.
- Hallai, J.F., Kyriakides, S. (2011a). On the effect of Lüders bands on the bending of steel tubes. Part I: Experiments. *Int'l J. Solids & Structures* **48**, 3275-3284.
- Hallai, J.F., Kyriakides, S. (2011b). On the effect of Lüders bands on the bending of steel tubes. Part II: Analysis. *Int'l J. Solids & Structures* **48**, 3285-3298.
- Hallai, J.F., Kyriakides, S. (2013). Underlying material response for Lüders-like instabilities. *Int'l J. Plasticity* **47**, 1-12.
- He, Y.J., Sun, Q.P. (2010). Macroscopic equilibrium domain structure and geometric compatibility in elastic phase transition of thin plates. *Int'l J. Mech. Sci.* **52**, 198-211.
- Hill, R. (1952). On discontinuous plastic states, with special reference to localized necking in thin sheets. *J. Mech. Phys. Solids* **1**, 19-30.
- Jacobus, K., Sehitoglu, H. and Balzer, M. (1996). Effect of stress state on the stress-induced martensitic transformation of polycrystalline Ni-Ti Alloy. *Metallu. Mater. Trans. A* **27**, 3066-3073.
- Jiang, D., Bechle, N.J., Landis, C.M., Kyriakides, S. (2016a). Buckling and recovery of NiTi tubes under axial compression. *Int'l J. Solids & Structures* **80**, 52-63.
- Jiang, D., Landis, C.M., Kyriakides, S. (2016b). Effects of tension/compression asymmetry on the buckling and recovery of NiTi tubes under axial compression. *Int'l J. Solids & Structures* **100-101**, 41-53, 2016.
- Jiang, D., Landis, C.M. (2016). A constitutive model for isothermal pseudoelasticity coupled with plasticity. *Shape Memory and Superelasticity* **2**, 360-370.
- Li, Z.Q., Sun, Q.P. (2002). The initiation and growth of macroscopic martensite band in nano-grained NiTi microtube under tension. *Int'l J. Plasticity* **18**, 1481-1498.
- Kyriakides, S. and Miller, J.E. (2000). On the propagation of Lüders bands in steel strips. *ASME J. Appl. Mech.* **67**, 645-654.
- Kyriakides, S., Ok, A. and Corona, E. (2008). Localization and propagation of curvature under pure bending in steel tubes with Lüders bands. *Int'l J. Solids Struct.* **45**, 3074-3087.
- Leon Baldelli, A.A., Maurini, C., Pham, K. (2015). A gradient approach for the macroscopic modeling of superelasticity in softening shape memory alloys. *Int'l J. Solids Struct.* **52**, 45-55.
- Levitas, V.I., Ozsoy, I.B. (2009). Micromechanical modeling of stress-induced phase transformations. Part 2. Computational algorithms and examples. *Int'l J. Plasticity* **25**, 546-583.

- Lomer, w.M. (1952). The yield phenomenon in polychrystalline mild steel. *J. Mech. Phys. Solids* **1**, 64-73.
- Mao, S.C, Luo, J.F., Zhang, Z., Wu, M.H., Liu, Y., Han, X.D. (2010). EBSD studies of the stress-induced B2-B19' martensitic transformation in NiTi tubes under uniaxial tension and compression. *Acta Materialia* **58**, 3357-3366.
- Maziere, M., Luis, C., Marais, A., Forest, S., Gasperini, M. (2016). Experimental and numerical analysis of the Lüders phenomenon in simple shear. *Int'l J. Solids & Structures* (in press 2016). <http://dx.doi.org/10.1016/j.ijsolstr.2016.07.026>
- Needleman, A. (1988). Material rate dependence and mesh sensitivity in localization problems. *Comp. Methods Appl. Mech. Eng.* **67**, 69-85.
- Nacar, A., Needleman, A. and Ortiz, M. (1989). A finite element method for analyzing localization in rate dependent solids at finite strains. *Comp. Methods Appl. Mech. Eng.* **73**, 235–258.
- Ortiz, M., Leroy, Y. and Needleman, A. (1987). A finite element method for localized failure analysis. *Comp. Methods Appl. Mech. Eng.* **61**, 189–214.
- Ozsoy, I.B., Babacan, N. (2016). Finite element simulations of microstructure evolution in stress-induced martensitic transformations. *Int'l J. Solids Struct.* **81**, 361-372.
- Reedlunn, B., Churchill, C.B., Nelson, E.E., Shaw, J.A., Daly, S.H. (2014). Tension, compression and bending of superelastic shape memory tubes. *J. Mech. Physics Solids* **63**, 506-537.
- Shaw, J.A. and Kyriakides, S. (1995). Thermomechanical aspects of NiTi. *J. Mechanics and Physics of Solids* **43**, 1243-1281.
- Shaw, J.A. and Kyriakides, S. (1997). On the nucleation and propagation of phase transformation fronts in a NiTi alloy. *Acta Materialia* **45**, 683-700.
- Shaw, J.A. and Kyriakides, S. (1998). Initiation and propagation of localized deformation in elasto-plastic strips under uniaxial tension. *Int'l J. Plast.* **13**, 837–871.
- Shaw, J. A. (2000). Simulations of localized thermo–mechanical behavior in a NiTi shape memory alloy. *Int'l J. Plasticity* **16**, 541–562.
- Simo, J.C. and Armero, F. (1992). Geometrically non-linear enhanced strain mixed methods and the method of incompatible modes. *Int'l J. Num. Methods Eng.* **33**, 1413–1449.
- Wilson, E.L., Taylor, R.L., Doherty, W.P. and Ghaboussi, J. (1973). Incompatible displacement models. In: Fenves, S.J. et al. (Eds.), *Numerical and Computer Models in Structural Mechanics*. Academic Press, New York.

Zhu, P., Ping Feng, P., Sun, Q.-P., Wang, J., Dai, H.-H. (2016). Determining the up-down-up response through tension tests of a pre-twisted shape memory alloy tube. *Int'l J. Plasticity* **85**, 52-76.

Figure Legends

Fig. 1 Pseudoelastic tensile stress-elongation response of NiTi strip.

Fig. 2 Set of deformed configuration with DIC axial strain contours superimposed; images correspond to numbered bullets on the response in Fig. 1.

Fig. 3 (a) Geometric variables of inclined bands. (b) Expanded views of inclined transformation bands from configurations ③ (loading) and ⑮ (unloading).

Fig. 4 $x-t$ diagram of the front history in the NiTi strip experiment.

Fig. 5 (a) The assumed softening tensile stress-strain response (red) together with the measured structural response of the strip. (b) The back stress-transformation strain responses for tension and compression used in the model.

Fig. 6 Geometry of the model strip and the finite element mesh used.

Fig. 7 (a) Comparison of calculated and measured stress-elongation responses for the NiTi strip. (b) Moment induced by the inhomogeneous deformation to the end of the strip vs. the applied end-displacement.

Fig. 8 Sequence of calculated strip deformed configuration with axial strain contours superimposed corresponding to numbered bullets on the response in Fig. 7.

Fig. 9 Expanded views of the transformation bands from six configurations in Fig. 8.

Fig. 10 (a) Comparison of the expanded views of the banded deformation in image 3 calculated with FE meshes with $N_t = 2, 3$ and 4. (b) The axial strain profiles of the right front from the three meshes.

Fig. 11 Comparison of the model strip loading deformed configurations produced by rate independent (left) and rate dependent (right) plasticity models ($N_t = 2$).

Fig. 12 (a) A set of assumed stress-strain responses with variable softening slopes ("0" corresponds to that in Fig. 5a. (b) The corresponding strip stress-displacement responses (corresponding sets of deformed configurations uploaded as supplementary material).

Fig. A1 Initial parts of the stress-deformation response calculated using "displacement controlled" loading and the Riks arc length incrementation method.

F1

(a)

(b)

F3

(a)

(b)

F6

(a)

(b)

F8

1

2

3

6

7

18

(a)

(b)

F11

(a)

(b)