# Constitutive modelling and numerical simulation of multivariant phase transformation in superelastic shape-memory alloys

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#### SUMMARY

This work concerns the micromechanical constitutive modelling, algorithmic implementation and numerical simulation of polycrystalline superelastic alloys under multiaxial loading. The model is formulated in finite deformations and incorporates the effect of texture. The numerical implementation is based on the constrained minimization of the Helmholtz free energy with dissipation. Simulations are conducted for thin tubes of Nitinol under tension-torsion, as well as for a simplified model of a biomedical stent. Copyright © 2004 John Wiley & Sons, Ltd.

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# 1. INTRODUCTION

Shape-memory alloys are currently used in a wide array of engineering systems ranging from microactuators to cell phone antennas. These materials exhibit superelastic behaviour, namely they can recover their undeformed state upon hysteretic unloading from moderately large strains at sufficiently high and constant temperature. Superelasticity is microscopically induced by the displacive solid–solid phase transformation of the crystalline material between a highly-ordered austenitic and less-ordered martensitic phases, as well as by the stress-induced self-accommodating reorientation of the martensitic variants, known as twinning. A brief illustrative description of superelasticity, as well as the related shape-memory effect, can be found in References [1, 2].

The constitutive characterization of superelasticity has evolved from early one-dimensional phenomenological models of pure tension [3-5] to fully three-dimensional polycrystalline models that account, in some form, for the material microstructure [2, 6-8]. In parallel, numerical

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implementations of specific constitutive models have been pursued by several researchers using techniques from computational plasticity, see, e.g. References [9-11]. The present work proposes a numerical method for the solution of the constitutive equations resulting from a generalization of the habit plane model by Siredey *et al.* [8]. Habit plane models have a distinct advantage over lattice deformation models, because the habit plane variants are essential elements in the modelling of the twinning process, see Reference [12]. The numerical method is based on the constrained minimization of the Helmholtz free energy (with dissipation) and can handle both forward and reverse transformation. Given that the superelastic plateau in many superelastic alloys can reach strains up to 5-10%, the model is formulated in finite deformations. Also, the model incorporates the effects of texture, which can dramatically affect the overall mechanical response of shape-memory alloys. In this paper, the constitutive modelling and numerical simulations are focused exclusively on Nitinol, a nearly-equiatomic Ni-Ti alloy that is by far the most popular superelastic material. The multiaxial response of Nitinol is analysed in connection with a series of recent tension-torsion experiments on thin-walled tubes, which are the starting material for biomedical stents widely used in angioplasty procedures [13]. In addition, numerical simulations are presented for a simplified model of such a biomedical stent.

The organization of the article is as follows: Section 2 summarizes essential background from continuum mechanics and introduces the main ingredients of a plasticity-based theory of superelasticity. This is followed by the description of the specific model in Section 3 and a brief discussion of texture characterization for thin-walled tubes in Section 4. The numerical implementation of the model and a series of numerical simulations are presented in Sections 5 and 6. Concluding remarks appear in Section 7.

#### 2. BALANCE LAWS, THERMODYNAMICS AND CONSTITUTIVE ASSUMPTIONS

#### 2.1. Balance laws and thermodynamics

Let the motion  $\chi$  of a continuum take a typical point **X** from a fixed reference configuration to  $\mathbf{x} = \chi(\mathbf{X}, t)$  at time *t*. Recall that the velocity and acceleration of **X** at time *t* are defined respectively as  $\mathbf{v} = \partial \chi / \partial t$  and  $\mathbf{a} = \partial^2 \chi / \partial t^2$ , while the (relative) deformation gradient is defined as  $\mathbf{F} = \partial \chi / \partial X$ . In addition, the Lagrangian strain is given by  $\mathbf{E} = \frac{1}{2} (\mathbf{F}^T \mathbf{F} - \mathbf{I})$ , where **I** is the referential second-order identity tensor.

The linear and angular momentum balance equations are written in local referential form as

$$\operatorname{Div}(\mathbf{FS}) + \rho_0 \mathbf{b} = \rho_0 \mathbf{a}$$

$$\mathbf{S} - \mathbf{S}^{\mathrm{T}}$$
(1)

where **S** is the second Piola–Kirchhoff stress tensor,  $\rho_0$  is the mass density per unit referential volume, and **b** is the body force per unit mass. Likewise, the energy equation can be expressed as

$$\rho_0 \dot{\varepsilon} = \rho_0 r - \text{Div}\,\mathbf{q}_0 + \mathbf{S} \cdot \dot{\mathbf{E}} \tag{2}$$

in terms of the internal energy per unit mass  $\varepsilon$ , the heat supply per unit mass r, and the heat flux vector  $\mathbf{q}_0$  resolved over the geometry of the reference configuration.

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In this work, the Clausius–Duhem inequality is assumed to hold and be an expression of the Second Law of Thermodynamics. A local referential statement of this inequality is of the form

$$\rho_0 \dot{\eta} \theta \ge \rho_0 r - \text{Div} \, \mathbf{q}_0 + \frac{\mathbf{q}_0 \cdot \text{Grad} \, \theta}{\theta} \tag{3}$$

where  $\eta$  denotes the entropy per unit mass and  $\theta$  the absolute temperature.

### 2.2. Constitutive assumptions

Although the fundamental physics of martensitic phase transformations in polycrystalline solids is very different from that of plastic deformation, the underlying structure of plasticity theory is sufficiently broad to be applicable to the study of superelasticity. This is because in both plastic and superelastic materials, the macroscopic response during cyclic loading is characterized by the existence of elastic and inelastic ranges with sharply defined transitions from one to the other, as well as by strongly dissimilar stress response between loading and unloading at all inelastic states. For this reason, many models for shape-memory alloys have been developed or can be interpreted within the framework of plasticity theory, see, e.g. References [8, 10, 14].

This section outlines the main assumptions of a general plasticity-like theory that is broadly based on the Lagrangian approach advocated by Green and Naghdi [15], and further specialized to the micromechanical modelling of shape-memory alloys. These are:

(a) The existence of a Lagrangian strain tensor  $\mathbf{E}^{t}$  which quantifies the inelastic part of the deformation during phase transformation. This transformation strain tensor is related to the martensitic volume fraction set

$$\{\xi_{\alpha}\} = \left\{ (\xi_1, \xi_2, \dots, \xi_{nv}) \left| \sum_{\beta=1}^{nv} \xi_\beta \leqslant 1, \ \xi_\beta \geqslant 0 \right\}$$
(4)

according to

$$\mathbf{E}^{\mathsf{t}} = \hat{\mathbf{E}}^{\mathsf{t}}(\{\xi_{\alpha}\}) \tag{5}$$

where nv is the total number of martensitic variants which, depending on the crystalline structure, can be as high as nv = 24. The function  $\hat{\mathbf{E}}^t$  is subject to the homogeneity condition

$$\hat{\mathbf{E}}^{\mathsf{t}}(\{0\}) = \mathbf{0} \tag{6}$$

where {0} denotes the zero element of the set  $\{\xi_{\alpha}\}$ . Unlike classical multi-surface plasticity, the transformation strain itself (as opposed to its rate) is expressed here as an algebraic function of variables  $\{\xi_{\alpha}\}$ .

(b) The admittance of a stress response function  $\hat{\mathbf{S}}$ , such that

$$\mathbf{S} = \hat{\mathbf{S}}(\mathbf{E}, \{\xi_{\alpha}\}, \theta) \tag{7}$$

The function  $\hat{\mathbf{S}}$  is assumed invertible for fixed  $\{\xi_{\alpha}\}$  and  $\theta$ , namely there exists a function  $\hat{\mathbf{E}}$  such that

$$\mathbf{E} = \mathbf{E}(\mathbf{S}, \{\xi_{\alpha}\}, \theta) \tag{8}$$

The invertibility of the stress response permits all constitutive functions to be equivalently expressed in strain- or stress-space for given  $\{\xi_{\alpha}\}$  and  $\theta$ .

(c) The existence of transformation functions  $\hat{Y}^{\rm f}_{\alpha}$  and  $\hat{Y}^{\rm r}_{\alpha}$  of the form

$$Y_{\alpha}^{f} = \hat{Y}_{\alpha}^{f}(\mathbf{E}, \{\xi_{\beta}\}, \theta), \quad Y_{\alpha}^{r} = \hat{Y}_{\alpha}^{r}(\mathbf{E}, \{\xi_{\beta}\}, \theta)$$
(9)

associated with the forward or reverse transformation of variant  $\alpha$ . In a state of forward (respectively reverse) transformation,  $Y_{\alpha}^{f} = 0$  (respectively  $Y_{\alpha}^{r} = 0$ ). These conditions define the sets of forward (respectively reverse) *active* variants at given strain and temperature as  $\mathscr{J}^{f}(\mathbf{E}, \theta) = \{\alpha \mid \hat{Y}_{\alpha}^{f}(\mathbf{E}, \{\xi_{\beta}\}, \theta) = 0, \xi_{\alpha} > 0\}$  and  $\mathscr{J}^{r}(\mathbf{E}, \theta) = \{\alpha \mid \hat{Y}_{\alpha}^{r}(\mathbf{E}, \{\xi_{\beta}\}, \theta) = 0, \xi_{\alpha} > 0\}$ , respectively. In order to guarantee positive dissipation,  $Y_{\alpha}^{f} < Y_{\alpha}^{r}$ , for all  $\alpha$ . Taking into account (8), the transformation functions can be also expressed in stress space as

$$Y_{\alpha}^{f} = \tilde{Y}_{\alpha}^{f}(\mathbf{S}, \{\xi_{\beta}\}, \theta), \quad Y_{\alpha}^{r} = \tilde{Y}_{\alpha}^{r}(\mathbf{S}, \{\xi_{\beta}\}, \theta)$$
(10)

(d) The admittance of two sets of transformation conditions signifying the cumulative growth or shrinkage of the martensitic variants. In particular, the transformation conditions from a state of forward transformation  $(\mathscr{J}^{f} \neq \emptyset)$  are stipulated in the form

$$\sum_{\alpha \in \mathscr{J}^{\mathrm{f}}} W_{\alpha}^{\mathrm{f}} \frac{\partial \hat{Y}_{\alpha}^{\mathrm{f}}}{\partial \mathbf{E}} \cdot \dot{\mathbf{E}} \begin{cases} > 0 \Leftrightarrow \text{ forward transformation} \\ = 0 \Leftrightarrow \text{ neutral forward transformation} \\ < 0 \Leftrightarrow \text{ elastic unloading} \end{cases}$$
(11)

where  $W_{\alpha}^{f} = \hat{W}_{\alpha}^{f}(\mathbf{E}, \{\xi_{\beta}\}, \theta)$  are constitutively specified positive functions. Equation (11) illustrates that the transformation conditions from a state of forward transformation depend on a *scalar* variable which quantifies the orientation of the weighted 'normal' vector  $\sum_{\alpha \in \mathscr{J}^{f}} W_{\alpha}^{f} \partial \hat{Y}_{\alpha}^{f} / \partial \mathbf{E}$  relative to the direction  $\dot{\mathbf{E}}$  of loading in strain space. Likewise, the transformation conditions from a state of reverse transformation ( $\mathscr{J}^{f} = \emptyset, \ \mathscr{J}^{r} \neq \emptyset$ ) are taken to be

$$\sum_{\alpha \in \mathscr{J}^{\mathrm{r}}} W_{\alpha}^{\mathrm{r}} \frac{\partial \hat{Y}_{\alpha}^{\mathrm{r}}}{\partial \mathbf{E}} \cdot \dot{\mathbf{E}} \begin{cases} > 0 \Leftrightarrow \text{ elastic reloading} \\ = 0 \Leftrightarrow \text{ neutral reverse transformation} \\ < 0 \Leftrightarrow \text{ reverse transformation} \end{cases}$$
(12)

in terms of the positive constitutive functions  $W_{\alpha}^{r} = \hat{W}_{\alpha}^{r}(\mathbf{E}, \{\xi_{\beta}\}, \theta)$ . Equations (11) and (12) constitute an extension of the loading conditions proposed by Naghdi and Trapp [16] for single-surface plasticity theory in strain space. Note that Equations (11) and (12) differ substantially from those of the multi-surface plasticity treatment in Reference [17, Section 5.1.2], where independent loading/unloading conditions are formulated for each active yield surface. This is because, unlike plasticity, where plastic strain increases monotonically with loading, here forward transformation can (and, in fact, often does) occur by simultaneous growth of certain variants and shrinkage of others. In such a case, all transforming variants are considered active and contribute to the identification of the overall transformation state by means of the proposed transformation conditions. (e) The existence of a representative volume element  $\mathcal{D}$  of volume  $V_{\mathcal{D}}$  at each referen-

tial point X, such that macroscopic second Piola-Kirchhoff stress S, Lagrangian strain E and Lagrangian transformation strains  $E^{t}$  are volumetric averages of corresponding



Figure 1. Schematic representation of a plasticity-like model for shape-memory alloys.

microscopic quantities  $\sigma$ ,  $\varepsilon$ , and  $\varepsilon^{t}$ , namely

$$\mathbf{S} = \frac{1}{V_{\mathscr{D}}} \int_{\mathscr{D}} \boldsymbol{\sigma} \, \mathrm{d}V, \quad \mathbf{E} = \frac{1}{V_{\mathscr{D}}} \int_{\mathscr{D}} \boldsymbol{\varepsilon} \, \mathrm{d}V, \quad \mathbf{E}^{\mathsf{t}} = \frac{1}{V_{\mathscr{D}}} \int_{\mathscr{D}} \boldsymbol{\varepsilon}^{\mathsf{t}} \, \mathrm{d}V \tag{13}$$

The applicability of plasticity-like theory with two sets of yield surfaces is schematically illustrated in Figure 1 for the special case of single variant superelastic transformation at constant temperature  $\theta$  above the austenitic finish value  $A_f$ . During forward transformation (region (a)–(b)), the yield surface  $Y^f = 0$  is active and expands in stress space, while the material traces the forward transformation plateau. Upon further loading, the material moves past the final forward yield surface in stress space and behaves elastically (region (b)–(c)). After elastic unloading back to (d), the material enters the reverse transformation plateau, where the yield surface  $Y^r = 0$  becomes active and contracts in stress space until full recovery of the austenite phase is attained at point (e).

The superelastic material can be viewed as a parametrized thermoelastic material for given  $\{\xi_{\alpha}\}$ , see Reference [18] for an analogous argument in the context of thermoplasticity. Indeed, if  $\Psi = \hat{\Psi}(\mathbf{E}, \{\xi_{\alpha}\}, \theta)$  is the Helmholtz free energy, such that

$$\Psi = \rho_0(\varepsilon - \eta\theta) \tag{14}$$

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then Equations (2) and (3) imply that, during a homothermal superelastic process,

$$\left(\mathbf{S} - \frac{\partial \hat{\Psi}}{\partial \mathbf{E}}\right) \cdot \dot{\mathbf{E}} - \sum_{\alpha=1}^{nv} \frac{\partial \hat{\Psi}}{\partial \xi_{\alpha}} \cdot \dot{\xi}_{\alpha} \ge 0$$
(15)

Given that **E** and  $\xi_{\alpha}$  can be varied independently due to the existence of elastic processes at all states, the standard Coleman and Noll argument can be applied to Equation (15), leading to

$$\mathbf{S} = \frac{\partial \hat{\Psi}}{\partial \mathbf{E}} \tag{16}$$

and

$$\dot{D} = -\sum_{\alpha=1}^{nv} \frac{\partial \hat{\Psi}}{\partial \xi_{\alpha}} \cdot \dot{\xi}_{\alpha} \ge 0$$
<sup>(17)</sup>

Equation (17) shows that the dissipation rate  $\hat{D}$ , defined as the rate of work done by the totality of the thermodynamic forces  $-\partial \hat{\Psi}/\partial \xi_{\alpha}$ , is non-negative.

During persistent forward transformation under constant temperature, Equation (17) implies that

$$\sum_{\alpha \in \mathscr{J}^{\mathrm{f}}} \left( -Y_{\alpha}^{\mathrm{f}} - \frac{\partial \hat{\Psi}}{\partial \xi_{\alpha}} \right) \dot{\xi}_{\alpha} \ge 0$$
(18)

Persistency of forward transformation also necessitates that

$$\dot{Y}_{\alpha}^{f} = \frac{\partial \dot{Y}_{\alpha}^{f}}{\partial \mathbf{E}} \cdot \dot{\mathbf{E}} - \sum_{\beta \in \mathscr{J}^{f}} Q_{\alpha\beta} \dot{\xi}_{\beta} = 0$$
<sup>(19)</sup>

where  $Q^{\rm f}_{\alpha\beta}$  is defined as

$$Q^{\rm f}_{\alpha\beta} = -\frac{\partial \hat{Y}^{\rm f}_{\alpha}}{\partial \xi_{\beta}} \tag{20}$$

and quantifies the coupling between variants in the transformation conditions. It is further stipulated at this stage that the rate of change of each volume fraction can be uniquely determined from (19). This, in turn, implies that the matrix  $[Q^f]$  with components  $Q^f_{\alpha\beta}$  is invertible. As a result, during persistent forward transformation of variant  $\beta$ ,

$$\dot{\xi}_{\beta} = \sum_{\alpha \in \mathscr{J}^{\mathrm{f}}} \mathcal{Q}_{\alpha\beta}^{\mathrm{f}-1} \frac{\partial \hat{Y}_{\alpha}^{\mathrm{f}}}{\partial \mathbf{E}} \cdot \dot{\mathbf{E}}$$
(21)

where  $Q_{\alpha\beta}^{f-1}$  are the components of the matrix  $[Q^f]^{-1}$ . However, note that  $\dot{\xi}_{\beta}$  in (21) is not necessarily positive, as the forward transformation process may require shrinkage of variant  $\beta$ . Taking into account (18) and (21) it is readily concluded that during persistent forward transformation

$$\sum_{\alpha \in \mathscr{J}^{\mathrm{f}}} \sum_{\beta \in \mathscr{J}^{\mathrm{f}}} \mathcal{Q}_{\alpha\beta}^{\mathrm{f}-1} \left( -Y_{\beta}^{\mathrm{f}} - \frac{\partial \hat{\Psi}}{\partial \xi_{\beta}} \right) \frac{\partial \hat{Y}_{\alpha}^{\mathrm{f}}}{\partial \mathbf{E}} \cdot \dot{\mathbf{E}} \ge 0$$
(22)

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By comparing (22) to (11), it is immediately clear that the Clausius–Duhem inequality yields a restricted form of the weighting function  $W_{\alpha}^{f}$  as

$$W_{\alpha}^{f} = \sum_{\beta \in \mathscr{J}^{f}} \mathcal{Q}_{\alpha\beta}^{f-1} \left( -Y_{\beta}^{f} - \frac{\partial \hat{\Psi}}{\partial \xi_{\beta}} \right)$$
(23)

An analogous argument can be made for the case of persistent reverse transformation, leading to counterparts of Equations (18)-(23).

It is common in the materials science literature of solid-solid phase transformations to describe thermodynamic equilibrium in terms of the Gibbs free energy  $G = \tilde{G}(\mathbf{S}, \{\xi_{\alpha}\}, \theta)$ . The latter is obtained from the Helmholtz free energy by a Legendre transform as

$$G = \Psi - \mathbf{S} \cdot \mathbf{E} = \rho_0(\varepsilon - \eta\theta) - \mathbf{S} \cdot \mathbf{E}$$
(24)

where use is made of (14). The Gibbs energy is preferred when experiments are conducted under constant stress and temperature, as is the case in one-dimensional solid-solid phase transformation. It is debatable whether constant (or even nearly constant) stress conditions apply to multi-dimensional solid-solid transformation experiments. On the other hand, the Helmholtz free energy is the natural choice when formulating constitutive equations of solids for finite element implementation. This is because, in the majority of finite element methods, the solution of the constitutive equations takes place at the integration point level under prescribed total strain history.

## 3. A SIMPLE MULTI-VARIANT MODEL OF PHASE TRANSFORMATION

This section introduces a simple habit plane-based model within the general assumptions presented in Section 2.2. This model is a reformulation and extension of an earlier model by Siredey *et al.* [8]. Here, the macroscopic Lagrangian transformation strain is assumed to depend linearly on the volume fractions of the martensitic variants, namely

$$\mathbf{E}^{\mathsf{t}} = \sum_{\alpha=1}^{nv} \xi_{\alpha} \mathbf{E}_{\alpha}^{\mathsf{t}} \tag{25}$$

where  $\mathbf{E}_{\alpha}^{t}$  are variant transformation strain tensors to be defined. The above constitutive choice is consistent with (5) and well-motivated on micromechanical grounds. Indeed, assume that the microscopic transformation strain  $\boldsymbol{\epsilon}^{t}$  vanishes in the austenitic phase and recall that the microscopic displacement vector of martensitic phase  $\alpha$  is expressed at each referential point **X** as

$$\mathbf{u}_{\alpha}^{n} = g\mathbf{m}_{\alpha}(\mathbf{X} \cdot \mathbf{n}_{\alpha}) \tag{26}$$

where  $\mathbf{m}_{\alpha}$  is the unit vector along the direction of transformation,  $\mathbf{n}_{\alpha}$  is the outward unit normal vector to the habit plane, and g is the transformation displacement, see Figure 2. Equation (25) follows by appealing to (13)<sub>3</sub> and arguing that the variant transformation strain is piecewise constant inside the representative volume element. It is further concluded from (26) that

$$\mathbf{E}_{\alpha}^{t} = \frac{1}{2} g(\mathbf{m}_{\alpha} \otimes \mathbf{n}_{\alpha} + \mathbf{n}_{\alpha} \otimes \mathbf{m}_{\alpha} + g\mathbf{n}_{\alpha} \otimes \mathbf{n}_{\alpha})$$
(27)

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Figure 2. Kinematic variables in martensitic transformation.

Following Siredey *et al.* [8], the Helmholtz free energy  $\Psi$  is decomposed into an elastic part consisting of a quadratic isotropic strain energy in  $\mathbf{E} - \mathbf{E}^{t}$  and a linear chemical energy in  $\theta - \theta_0$ , namely

$$\Psi = \hat{\Psi}(\mathbf{E}, \{\xi_{\alpha}\}, \theta) = \frac{1}{2} \left( \mathbf{E} - \sum_{\alpha=1}^{nv} \xi_{\alpha} \mathbf{E}_{\alpha}^{t} \right) \cdot \mathbb{C} \left( \mathbf{E} - \sum_{\alpha=1}^{nv} \xi_{\alpha} \mathbf{E}_{\alpha}^{t} \right) + B(\theta - \theta_{0}) \sum_{\alpha=1}^{nv} \xi_{\alpha}$$
(28)

where  $\mathbb{C}$  is the fourth-order isotropic elasticity tensor, *B* is a constant chemical energy coefficient, and  $\theta_0$  is the equilibrium temperature. The linear form of the chemical energy is easily justified for small variations of the temperature away from its equilibrium value [19]. The proposed Helmholtz free energy ignores the effect of interactions between the martensitic variants. This simplification is justified by the authors' own experiments in which the interaction energy does not appear to be of significance, see Section 6.1.1. At the same time, the standard quadratic form  $\sum_{\alpha=1}^{nv} \sum_{\beta=1}^{nv} \frac{1}{2} \xi_{\alpha} H_{\alpha\beta} \xi_{\beta}$  of the interaction energy renders the local phase transformation problem ill-defined and requires some form of relaxation to yield a unique solution. The second Piola–Kirchhoff stress can be shown with the aid of (16) and (28) to be

$$\mathbf{S} = \mathbb{C} \left( \mathbf{E} - \sum_{\alpha=1}^{n\nu} \xi_{\alpha} \mathbf{E}_{\alpha}^{\mathsf{t}} \right)$$
(29)

Note that stress response function is invertible for fixed  $\{\xi_{\alpha}\}$  for  $\mathbb{C}$  non-singular, as required by the general theory (see assumption (b) in Section 2.2). Although it is not employed in the ensuing algorithmic development, the Gibbs free energy corresponding to (28) is deduced from (24) with the aid of (29), and recorded here for completeness:

$$G = \tilde{G}(\mathbf{S}, \{\xi_{\gamma}\}, \theta) = -\frac{1}{2} \mathbf{S} \cdot \mathbb{C}^{-1} \mathbf{S} - \mathbf{S} \cdot \left(\sum_{\alpha=1}^{n\nu} \xi_{\alpha} \mathbf{E}_{\alpha}^{\mathsf{t}}\right) + B(\theta - \theta_0) \sum_{\alpha=1}^{n\nu} \xi_{\alpha}$$
(30)

The yield-like condition associated with forward and reverse transformation of a typical variant  $\alpha$  characterises a state in which the thermodynamic force  $-\partial \hat{\Psi}/\partial \xi_{\alpha}$  acting on the variant due to the elastic and chemical energy reaches a critical value, see Reference [20]. Due to symmetry of the variants, this critical value  $\mathscr{F}^{c}$  is independent of the particular variant.

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As is widely done in the literature [7,21], this critical value is also assumed to be the same for both forward and reverse transformation on the basis of equal resistance of the atoms in the lattice to  $A \rightarrow M$  and  $M \rightarrow A$  phase changes. It follows that the forward and reverse transformation functions  $Y^{f}_{\alpha}$  and  $Y^{r}_{\alpha}$  are defined as

$$Y_{\alpha}^{f} = -\frac{\partial \hat{\Psi}}{\partial \xi_{\alpha}} - \mathscr{F}^{c} = -\frac{\partial \tilde{G}}{\partial \xi_{\alpha}} - \mathscr{F}^{c}$$

$$Y_{\alpha}^{r} = -\frac{\partial \hat{\Psi}}{\partial \xi_{\alpha}} + \mathscr{F}^{c} = -\frac{\partial \tilde{G}}{\partial \xi_{\alpha}} + \mathscr{F}^{c}$$
(31)

Using (28), the above functions are expressed as

$$Y_{\alpha}^{f} = \hat{Y}_{\alpha}^{f}(\mathbf{E}, \{\xi_{\beta}\}, \theta) = \mathbb{C}\left(\mathbf{E} - \sum_{\beta=1}^{nv} \xi_{\beta} \mathbf{E}_{\beta}^{t}\right) \cdot \mathbf{E}_{\alpha}^{t} - (B(\theta - \theta_{0}) + \mathscr{F}^{c})$$

$$Y_{\alpha}^{r} = \hat{Y}_{\alpha}^{r}(\mathbf{E}, \{\xi_{\beta}\}, \theta) = \mathbb{C}\left(\mathbf{E} - \sum_{\beta=1}^{nv} \xi_{\beta} \mathbf{E}_{\beta}^{t}\right) \cdot \mathbf{E}_{\alpha}^{t} - (B(\theta - \theta_{0}) - \mathscr{F}^{c})$$
(32)

Taking into account (20) and (32), the coupling matrices  $[Q^{f}]$  and  $[Q^{r}]$  have components

$$Q_{\alpha\beta}^{\rm f} = Q_{\alpha\beta}^{\rm r} = \mathbf{E}_{\alpha}^{\rm t} \cdot \mathbb{C}\mathbf{E}_{\beta}^{\rm t} = Q_{\alpha\beta}$$
(33)

and the transformation conditions (11) and (12) are defined accordingly. It is concluded from (33) that the matrix  $[Q](=[Q^f]=[Q^r])$  is symmetric and of rank at most 6; hence, in general, it is positive semi-definite. This means that the stipulation in Section 2.2 that  $[Q^f_{\alpha\beta}]$  and  $[Q^r_{\alpha\beta}]$  be invertible places a restriction on the cardinality of the active sets  $\mathcal{J}^f$  and  $\mathcal{J}^r$ . This point is further discussed in Section 5.

During persistent forward transformation, Equations (19), (23) and (31)<sub>1</sub> imply that the loading conditions  $(11)_{1,2}$  are equivalent to the condition

$$\sum_{\alpha \in \mathscr{J}^{f}} \dot{\xi}_{\alpha} \ge 0 \tag{34}$$

The latter simply states that during persistent forward loading, the cumulative martensitic volume fraction is increasing. Condition (34), as well as its counterpart for persistent reverse transformation, play an important role in the ensuing algorithmic development. Also during persistent forward transformation, it follows from Equation  $(31)_1$  that

$$\sum_{\alpha \in \mathscr{J}^{\mathrm{f}}} \left( -\frac{\partial \hat{\Psi}}{\partial \xi_{\alpha}} - \mathscr{F}^{\mathrm{c}} \right) \dot{\xi}_{\alpha} = 0$$
(35)

Given that

$$\frac{\partial^2 \hat{\Psi}}{\partial \xi_{\alpha} \partial \xi_{\beta}} = Q_{\alpha\beta} \tag{36}$$

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Equation (35) also implies that, in general, the function  $\Phi^{f} = \Psi + \sum_{\alpha \in \mathscr{J}^{f}} \mathscr{F}^{c} \xi_{\alpha}$  attains a non-unique global minimum at given strain and temperature. Analogous conclusions apply in the case of reverse transformation to the function  $\Phi^{r} = \Psi - \sum_{\alpha \in \mathscr{J}^{r}} \mathscr{F}^{c} \xi_{\alpha}$ .

# 4. TEXTURE ANALYSIS

Texture, understood here as the (generally non-uniform) distribution of orientation in crystals, has a profound effect on the mechanical response of shape-memory structures, such as polycrystalline Nitinol tubes. Texture depends crucially on the manufacturing process. In thin-walled tubes, such as those used in the authors' experiments and the ensuing simulations, the drawing process induces primarily  $\langle 1 1 1 \rangle \{1 1 0\}$ -type sheet texture that is 'wrapped' around the cylindrical surface, such that the  $\langle 1 1 1 \rangle$  austenite lattice direction is aligned with the longitudinal axis of the tube, see also the work of Gall, Schitoglu *et al.* [12, 22]. To characterize the texture in a cylindrical tube relative to a common fixed right-hand orthonormal basis { $\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3$ }, where  $\mathbf{E}_3$  lies along the longitudinal axis of the cylinder, let

$$\mathbf{p} = \cos \theta \mathbf{E}_1 + \sin \theta \mathbf{E}_2$$

$$\mathbf{q} = -\sin \theta \mathbf{E}_1 + \cos \theta \mathbf{E}_2$$

$$\mathbf{r} = \mathbf{E}_3$$
(37)

form a right-hand orthonormal basis of the austenite lattice vectors, see Figure 3. Equations (37) state that the orthonormal basis { $\mathbf{p}, \mathbf{q}, \mathbf{r}$ } is obtained from { $\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3$ } by a (counterclock-wise) rotation of angle  $\theta$  on the plane of  $\mathbf{E}_1$  and  $\mathbf{E}_2$ . Subsequently, the wrapping of the plane {110} around the cylindrical surface of the tube induces an additional rotation of { $\mathbf{p}, \mathbf{q}, \mathbf{r}$ } by an



Figure 3. Texture distribution over the thin tubular specimen.

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constant angle  $\phi = \pi/4$  on the plane of **p** and **q** to {**p**', **q**', **r**}. These two planar rotations are expressed in terms of the rotation tensor **Q**<sub>1</sub> with components

$$[Q_1] = \begin{bmatrix} \cos(\theta + \phi) & -\sin(\theta + \phi) & 0\\ \sin(\theta + \phi) & \cos(\theta + \phi) & 0\\ 0 & 0 & 1 \end{bmatrix}$$
(38)

relative to  $\{\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3\}$ . Finally, a rotation of  $\{\mathbf{p}', \mathbf{q}', \mathbf{r}'\}$  to  $\{\mathbf{p}'', \mathbf{q}'', \mathbf{r}''\}$  by a constant angle  $\psi = \cos^{-1} 1/\sqrt{3}$  on the plane of  $\mathbf{p}' + \mathbf{q}'$  and  $\mathbf{r}' = \mathbf{r}$  directs the vector  $\langle 1\,1\,1 \rangle$  along the longitudinal axis of the cylinder, and corresponds to rotation tensor  $\mathbf{Q}_2$  with components

$$[Q_2] = \begin{bmatrix} \cos\psi\sin^2\theta + \cos^2\theta & \sin\theta\cos\theta(1 - \cos\psi) & \sin\psi\sin\theta\\ \sin\theta\cos\theta(1 - \cos\psi) & \cos\psi\cos^2\theta + \sin^2\theta & -\sin\psi\cos\theta\\ -\sin\psi\sin\theta & \sin\psi\cos\theta & \cos\psi \end{bmatrix}$$
(39)

relative to  $\{\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3\}$ . Using (38) and (39), the composite rotation can now be expressed by means of the tensor  $\mathbf{Q} = \mathbf{Q}_2 \mathbf{Q}_1$  with components

$$[Q] = \begin{bmatrix} \cos\theta\cos\phi - \sin\theta\sin\phi\cos\psi & -\cos\theta\sin\phi - \sin\theta\cos\phi\cos\psi & \sin\theta\sin\psi\\ \sin\theta\cos\phi + \cos\theta\sin\phi\cos\psi & -\sin\theta\sin\phi + \cos\theta\cos\phi\cos\psi & -\cos\theta\sin\psi\\ \sin\phi\sin\psi & \cos\phi\sin\psi & \cos\psi \end{bmatrix}$$
(40)

relative to the fixed basis  $\{E_1, E_2, E_3\}$ . Hence, the components of the 'textured' transformation strain  $E_{texture}^t$  are related to those of its 'untextured' counterpart by

$$[E_{\text{texture}}^{\text{t}}] = [Q][E^{\text{t}}][Q]^{\text{T}}$$
(41)

Note that materials typically exhibit a variation of the texture ('wobble'), which is ignored in this analysis.

### 5. ALGORITHMIC IMPLEMENTATION

The algorithmic problem at the Gauss point level amounts to the minimization of  $\hat{\Phi}^{t}(\mathbf{E}, \theta, \{\xi_{\alpha}\})$  and  $\hat{\Phi}^{r}(\mathbf{E}, \theta, \{\xi_{\alpha}\})$  at given strain and temperature, as argued in Section 3. This minimization determines the volume fractions  $\{\xi_{\alpha}\}$ , subject to the *nv*-dimensional polytope conditions  $\xi_{\alpha} \ge 0$  and  $\sum_{\alpha=1}^{nv} \xi_{\alpha} \le 1$ , see Figure 4 for nv = 3. Note from (28) that  $\hat{\Phi}^{f}$  and  $\hat{\Phi}^{r}$  are quadratic in  $\xi_{\alpha}$ , which reduces the algorithmic problem to one of quadratic programming, see, e.g. Reference [23].

In typical computational treatments of multi-surface plasticity, a predictor–corrector method is employed to first identify the active yield surface(s) and, subsequently, solve for the stresses and plastic strains subject to enforcing the active yield conditions. Here, a somewhat different approach is advocated. In particular, the elastic loading/unloading and forward transformation processes are handled in a unified manner by imposing the appropriate constraints on the functional  $\Phi^{f}$ . An analogous unified treatment applies to elastic loading/unloading and reverse

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Figure 4. Polytope constraint in martensitic transformation.

transformation associated with the functional  $\Phi^r$ . As explained later, an elastic process is handled in terms of  $\Phi^f$  or  $\Phi^r$  depending on the assigned (forward or reverse) state at the current time.

To elaborate on the proposed algorithmic treatment, first note that the constraint conditions for all states of loading and unloading can be expressed as

$$-\xi_{\alpha} \leqslant 0, \quad \bar{\xi}_{l} - \sum_{\alpha=1}^{nv} \xi_{\alpha} \leqslant 0, \quad \sum_{\alpha=1}^{nv} \xi_{\alpha} - \bar{\xi}_{u} \leqslant 0$$

$$\tag{42}$$

where  $\bar{\xi}_1$  and  $\bar{\xi}_u$  are lower and upper values of the total martensitic volume fraction, such that  $0 \leq \bar{\xi}_1 < \bar{\xi}_u \leq 1$ . In case of elastic loading/unloading or forward transformation from a state with initial total martensitic volume fraction  $\xi_{\text{total}}$ , it is clear that  $\bar{\xi}_1 = \xi_{\text{total}}$  and  $\bar{\xi}_u = 1$ . Likewise, in case of elastic loading/unloading or reverse transformation,  $\xi_1 = 0$  and  $\bar{\xi}_u = \xi_{\text{total}}$ . Figure 5 illustrates the above cases for nv = 3. It is easily seen that, when  $\bar{\xi}_1 = 0$ , the constraint in (42)<sub>2</sub> becomes redundant. This, in conjunction with the assumption on the admissible values of  $\bar{\xi}_1$  and  $\bar{\xi}_u$ , implies that there are at most nv simultaneously active constraints,<sup>‡</sup> and that the constraints in (42)<sub>2,3</sub> cannot be both active.

Minimization of  $\Phi^{f}$  and  $\Phi^{r}$ , subject to the inequality constraints (42) requires that

$$\frac{\partial \hat{\Phi}^{\rm f}}{\partial \xi_{\alpha}} + \lambda_{\alpha} + \lambda_{\rm l} - \lambda_{\rm u} = 0, \quad \frac{\partial \hat{\Phi}^{\rm r}}{\partial \xi_{\alpha}} + \lambda_{\alpha} + \lambda_{\rm l} - \lambda_{\rm u} = 0 \tag{43}$$

Here,  $\lambda_{\alpha}$ ,  $\alpha = 1, 2, ..., nv$ ,  $\lambda_1$  and  $\lambda_u$  are non-negative-valued Lagrange multipliers intended to enforce the constraints in (42), subject to the Kuhn–Tucker condition

$$\sum_{\alpha=1}^{n\nu} \lambda_{\alpha}(-\xi_{\alpha}) + \lambda_{l} \left( \bar{\xi}_{l} - \sum_{\alpha=1}^{n\nu} \xi_{\alpha} \right) + \lambda_{u} \left( \sum_{\alpha=1}^{n\nu} \xi_{\alpha} - \bar{\xi}_{u} \right) = 0$$
(44)

 $^{\ddagger}A$  constraint is termed active if the respective constraint condition in (42) is satisfied as an equality.

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Figure 5. Polytope constraints for forward and reverse transformation.

In particular, taking into account (28), the constraint minimization of  $\Phi^{f}$  and  $\Phi^{r}$  at time  $t = t_{n+1}$  leads to the forward and reverse conditions

$$\mathbb{C}\left(\mathbf{E}_{n+1} - \sum_{\beta=1}^{nv} \xi_{\beta,n+1} \mathbf{E}_{\beta}^{t}\right) \cdot \mathbf{E}_{\alpha}^{t} - (B(\theta - \theta_{0}) + \mathscr{F}^{c}) + \lambda_{\alpha,n+1} + \lambda_{l,n+1} - \lambda_{u,n+1} = 0$$

$$\mathbb{C}\left(\mathbf{E}_{n+1} - \sum_{\beta=1}^{nv} \xi_{\beta,n+1} \mathbf{E}_{\beta}^{t}\right) \cdot \mathbf{E}_{\alpha}^{t} - (B(\theta - \theta_{0}) - \mathscr{F}^{c}) + \lambda_{\alpha,n+1} + \lambda_{l,n+1} - \lambda_{u,n+1} = 0$$

$$(45)$$

subject to

$$\sum_{\alpha=1}^{n\nu} \lambda_{\alpha,n+1}(-\xi_{\alpha,n+1}) + \lambda_{l,n+1} \left( \bar{\xi}_{l,n+1} - \sum_{\alpha=1}^{n\nu} \xi_{\alpha,n+1} \right) + \lambda_{u,n+1} \left( \sum_{\alpha=1}^{n\nu} \xi_{\alpha,n+1} - \bar{\xi}_{u,n+1} \right) = 0 \quad (46)$$

As noted in Section 3, a restriction needs to be placed on the active sets  $\mathcal{J}^{f}$  and  $\mathcal{J}^{r}$  to guarantee the positive-definiteness of [Q], hence the existence of unique global minima of  $\Phi^{f}$  and  $\Phi^{r}$  at specified strain and temperature. Such a restriction is also supported by experimental evidence, where for proportional loading paths only one to three variants appear to be simultaneously active in each grain [22]. The identification of a specific set of potentially active variants depends on the loading path, and is discussed in Sections 6.1 and 6.2, in connection with the two sets of numerical simulations. More general methodologies for selecting and deselecting potentially active variants are discussed in a forthcoming paper by the authors. Upon identifying a suitable set of six potentially active variants, the constraint minimization of  $\Phi^{f}$  and  $\Phi^{r}$  reduces to classical definite quadratic programming. This, in turn, can be dealt

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with by an active set strategy in which a feasible descent direction for each of the functionals  $\Phi^{f}$  and  $\Phi^{r}$  is obtained by gradient projection on the active set of linear constraints rather than on the entire constraint set, see, e.g. Reference [23].

Preliminary to formulating an active set strategy, define the extended set of Lagrange multipliers as an eight-dimensional column vector

$$[\lambda_{n+1}^e] = [\lambda_1 \ \cdots \ \lambda_6 \ \lambda_1 \ \lambda_u]_{n+1}^{\mathrm{T}}$$

$$\tag{47}$$

and, the set of the corresponding martensitic volume fractions as a six-dimensional column vector

$$[\xi_{n+1}] = [\xi_1 \ \cdots \ \xi_6]_{n+1}^{\mathrm{T}} \tag{48}$$

Then, the Kuhn-Tucker condition (46) can be expressed in matrix form as

$$[\lambda_{n+1}^e]^{\mathrm{T}}([A][\xi_{n+1}] - [h_{n+1}]) = [0]$$
(49)

where

$$[A] = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} [a_1]^T \\ [a_2]^T \\ \vdots \\ [a_6]^T \\ [a_7]^T \\ [a_8]^T \end{bmatrix}$$
(50)

and

$$[h_{n+1}] = [0 \ 0 \ \cdots \ 0 \ -\bar{\xi}_{1,n+1} \ \bar{\xi}_{u,n+1}]^{\mathrm{T}}$$
(51)

Also, let  $[\Pi_{n+1}]$  be the  $na \times 8$ -dimensional projection matrix from the eight-dimensional space of all constraints to the *na*-dimensional space of all *active* constraints, where, as argued earlier,  $na \leq 6$ . It follows that  $[\bar{\lambda}_{n+1}] = [\Pi_{n+1}][\lambda_{n+1}^e]$ , where  $[\bar{\lambda}_{n+1}]$  is the *na*-dimensional column vector of the multipliers associated with active constraints. Now, Equations (45) and (46) are written, respectively, in matrix form as

$$[Q][\xi_{n+1}] + ([\Pi_{n+1}][A])^{\mathrm{T}}[\bar{\lambda}_{n+1}] = [c_{n+1}] [\Pi_{n+1}][A][\xi_{n+1}] = [\Pi_{n+1}][h_{n+1}]$$
(52)

where the six-dimensional column vector  $[c_{n+1}]$  has components

$$c_{\alpha,n+1} = \begin{cases} \mathbf{E}_{\alpha}^{t} \cdot \mathbb{C}\mathbf{E}_{n+1} - (B(\theta - \theta_{0}) + F^{c}) & \text{(forward)} \\ \mathbf{E}_{\alpha}^{t} \cdot \mathbb{C}\mathbf{E}_{n+1} - (B(\theta - \theta_{0}) - F^{c}) & \text{(reverse)} \end{cases}$$
(53)

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Since [Q] is positive-definite and  $[\Pi_{n+1}][A]$  is a  $na \times 6$ -dimensional matrix of rank na, the system (52) can be solved uniquely for  $[\xi_{n+1}]$  and  $[\overline{\lambda}_{n+1}]$  in the form

$$[\xi_{n+1}] = [\Xi_{n+1}][c_{n+1}] + [\Delta_{n+1}]^{1} [\Pi_{n+1}][h_{n+1}]$$

$$[\bar{\lambda}_{n+1}] = [\Delta_{n+1}][c_{n+1}] - \left[ [\Pi_{n+1}][A][Q]^{-1} ([\Pi_{n+1}][A])^{\mathrm{T}} \right]^{-1} [\Pi_{n+1}][h_{n+1}]$$
(54)

where

$$[\Xi_{n+1}] = [Q]^{-1} - [Q]^{-1} ([\Pi_{n+1}][A])^{\mathrm{T}} \left[ [\Pi_{n+1}][A][Q]^{-1} ([\Pi_{n+1}][A])^{\mathrm{T}} \right]^{-1} [\Pi_{n+1}][A][Q]^{-1}$$
(55)

and

$$[\Delta_{n+1}] = \left[ [\Pi_{n+1}][A][Q]^{-1} ([\Pi_{n+1}][A])^{\mathrm{T}} \right]^{-1} [\Pi_{n+1}][A][Q]^{-1}$$
(56)

The active constraints are determined iteratively using a standard active set strategy, see, e.g. Reference [23, Chapter 14]. Once the active constraints are specified at an iteration k (hence, the matrix  $[\Pi_{n+1}^{(k)}]$  is known), they are enforced in equality form as in (52)<sub>2</sub>. To reduce the cost of identifying the active constraints, the initial guess for the active set at any given time is taken to coincide with the active set determined at the previous solution time.

Discrete counterparts of (11) and (12) are employed to distinguish between the various transformation conditions starting from a state of forward or reverse transformation. Specifically, recalling that the constraint  $(42)_2$  is enforced, the conditions

$$\Delta \xi_n^{\rm f} = \sum_{\alpha=1}^6 \left( \xi_{\alpha,n+1}^{\rm f} - \xi_{\alpha,n} \right) \begin{cases} > 0 & \Leftrightarrow \text{ forward transformation} \\ = 0 \text{ and } \lambda_1 = 0 & \Leftrightarrow \text{ neutral forward transformation} \\ = 0 \text{ and } \lambda_1 > 0 & \Leftrightarrow \text{ elastic unloading} \end{cases}$$
(57)

are employed to distinguish between the various states of loading starting from a state of forward transformation at time  $t_n$ , where  $\xi_{\alpha,n+1}^{f}$  are computed by minimization of  $\Phi^{f}$ . Taking into account (34), it is clear that (57)<sub>1</sub> corresponds exactly to (11)<sub>1</sub>. However, (57)<sub>2,3</sub> are modified in order to account for the explicit enforcement of (42)<sub>2</sub>. In this case, the distinction between neutral forward transformation and elastic unloading is made by means of the Lagrange multiplier corresponding to the constraint (42)<sub>2</sub>. Likewise, starting from a state of reverse transformation at time  $t_n$ , the conditions

$$\Delta \xi_n^{\rm r} = \sum_{\alpha=1}^6 \left( \xi_{\alpha,n+1}^{\rm r} - \xi_{\alpha,n} \right) \begin{cases} = 0 \text{ and } \lambda_{\rm u} > 0 \quad \Leftrightarrow \quad \text{elastic reloading} \\ = 0 \text{ and } \lambda_{\rm u} = 0 \quad \Leftrightarrow \quad \text{neutral reverse transformation} \\ < 0 \qquad \qquad \Leftrightarrow \quad \text{reverse transformation} \end{cases}$$
(58)

describe the three possible states, where  $\xi_{\alpha,n+1}^{r}$  are computed by minimization of  $\Phi^{r}$ . In analogy to the loading case, (58)<sub>3</sub> corresponds exactly to (12)<sub>3</sub>, while the distinction between (58)<sub>1,2</sub> is made with the aid of the Lagrange multiplier that enforces the constraint condition (42)<sub>3</sub>.

Since the proposed algorithm is based on a unified treatment of elastic and transformation states, the elastic processes need also be determined by extremization of  $\Phi^{f}$  or  $\Phi^{r}$ . In order to guarantee that the algorithm is well-defined at all states, it is essential that both sets of discrete loading conditions (57) and (58) be checked at each solution step. To this end, a flag is introduced to keep track of the state at  $t_n$  and resolve any possible indeterminacies resulting from checking both sets of loading conditions. This flag is initially set to 'forward' and is switched to 'reverse' upon satisfaction of (57)<sub>1</sub> and (58)<sub>1</sub> and (57)<sub>1</sub>, etc. The following table summarises the characterization of the state at  $t_{n+1}$  for all combinations of forward and reverse loading conditions.

| $\Delta \xi_n^f$ | +         | 0         |
|------------------|-----------|-----------|
| _                | !flag     | 'reverse' |
| 0                | 'forward' | flag      |

The notation '!flag' in the table denotes switching of the flag. Figure 4 schematically depicts the feasible volume fraction regions of forward and reverse transformation cases for nv = 3.

A closed-form expression of the algorithmic tangent modulus  $\partial_{\mathbf{E}_{n+1}} \mathbf{S}_{n+1}$  consistent with the constrained minimization method is easily determined as follows: first, use (29) to conclude that

$$\partial_{\mathbf{E}_{n+1}} \mathbf{S}_{n+1} = \mathbb{C} - \sum_{\alpha=1}^{6} \mathbb{C} \mathbf{E}_{\alpha}^{\mathsf{t}} \partial_{\mathbf{E}_{n+1}} \xi_{\alpha,n+1}$$
(59)

Then, appealing to (53) and (54) leads to

$$\partial_{\mathbf{E}_{n+1}}\xi_{\alpha,n+1} = \sum_{\beta=1}^{6} \Xi_{\alpha\beta,n+1} \mathbb{C}\mathbf{E}_{\beta}^{\mathsf{t}}$$
(60)

hence

$$\partial_{\mathbf{E}_{n+1}} \mathbf{S}_{n+1} = \mathbb{C} - \sum_{\alpha=1}^{6} \sum_{\beta=1}^{6} \Xi_{\alpha\beta, n+1}(\mathbb{C}\mathbf{E}_{\alpha}^{\mathsf{t}}) \otimes (\mathbb{C}\mathbf{E}_{\beta}^{\mathsf{t}})$$
(61)

The local algorithmic procedure is summarised in Appendix A.

# 6. NUMERICAL SIMULATIONS

The constitutive model described in Sections 3 and 4 has been implemented in the finite element code FEAP (see References [24, 25]) using the algorithm of Section 5. Selected numerical simulations have been conducted using 8- and 27-node isoparametric brick elements with the standard displacement formulation. Material properties were chosen from a particular polycrystalline Ni-Ti alloy (Ti 44.5 wt%, Ni 55.5 wt%) that was used by the authors to conduct biaxial loading experiments on thin-walled tubes [13].

| No. |                       | n                     |                       |          | m        |                       | No. |                       | n        |                       |            | m        |          |
|-----|-----------------------|-----------------------|-----------------------|----------|----------|-----------------------|-----|-----------------------|----------|-----------------------|------------|----------|----------|
| 1   | <i>n</i> <sub>1</sub> | $-n_{3}$              | <i>n</i> <sub>2</sub> | $m_1$    | $-m_{3}$ | <i>m</i> <sub>2</sub> | 13  | $-n_{2}$              | $-n_1$   | $-n_{3}$              | $-m_{2}$   | $-m_1$   | $-m_{3}$ |
| 2   | $-n_3$                | $n_1$                 | $-n_{2}$              | $-m_3$   | $m_1$    | $-m_{2}$              | 14  | $-n_{2}$              | $n_1$    | $n_3$                 | $-m_{2}$   | $m_1$    | $m_3$    |
| 3   | $-n_1$                | <i>n</i> <sub>3</sub> | $n_2$                 | $-m_1$   | $m_3$    | $m_2$                 | 15  | $n_2$                 | $n_3$    | $n_1$                 | $m_2$      | $m_3$    | $m_1$    |
| 4   | <i>n</i> <sub>3</sub> | $-n_1$                | $-n_{2}$              | $m_3$    | $-m_1$   | $-m_{2}$              | 16  | $n_2$                 | $-n_{3}$ | $-n_{1}$              | $m_2$      | $-m_{2}$ | $m_3$    |
| 5   | $n_1$                 | $n_3$                 | $-n_{2}$              | $m_1$    | $m_3$    | $-m_{2}$              | 17  | $-n_1$                | $-n_{2}$ | $n_3$                 | $-m_1$     | $-m_{2}$ | $m_3$    |
| 6   | <i>n</i> <sub>3</sub> | $n_1$                 | $n_2$                 | $m_3$    | $m_1$    | $m_2$                 | 18  | $n_1$                 | $-n_{2}$ | $-n_{3}$              | $m_1$      | $-m_{2}$ | $-m_{3}$ |
| 7   | $-n_1$                | $-n_{3}$              | $-n_{2}$              | $-m_1$   | $-m_{3}$ | $-m_{2}$              | 19  | <i>n</i> <sub>3</sub> | $n_2$    | $-n_{1}$              | <i>m</i> 3 | $m_2$    | $-m_1$   |
| 8   | $-n_3$                | $-n_1$                | $n_2$                 | $-m_3$   | $-m_1$   | $m_2$                 | 20  | $-n_3$                | $n_2$    | $n_1$                 | $-m_3$     | $m_2$    | $m_1$    |
| 9   | $n_2$                 | $-n_1$                | $n_3$                 | $m_2$    | $-m_1$   | $m_3$                 | 21  | $-n_1$                | $n_2$    | $-n_{3}$              | $-m_1$     | $m_2$    | $-m_{3}$ |
| 10  | $n_2$                 | $n_1$                 | $-n_{3}$              | $m_2$    | $m_1$    | $-m_{3}$              | 22  | $n_1$                 | $n_2$    | <i>n</i> <sub>3</sub> | $m_1$      | $m_2$    | $m_3$    |
| 11  | $-n_{2}$              | $-n_3$                | $n_1$                 | $-m_{2}$ | $-m_3$   | $m_1$                 | 23  | $-n_3$                | $-n_{2}$ | $-n_{1}$              | $-m_3$     | $-m_{2}$ | $-m_1$   |
| 12  | $-n_2$                | <i>n</i> <sub>3</sub> | $-n_1$                | $-m_{2}$ | $-m_{3}$ | $m_1$                 | 24  | <i>n</i> <sub>3</sub> | $-n_2$   | $n_1$                 | $m_3$      | $-m_{2}$ | $m_1$    |

Table I. Components of the twenty-four habit plane vector pairs  $(\mathbf{n}_{\alpha}, \mathbf{m}_{\alpha})$  for Nitinol.

The elasticity tensor  $\mathbb{C}$  is assumed isotropic with material parameters E = 38.0 GPa and v = 0.3 estimated in the experiments and corresponding to (initial) polycrystal Young's modulus and the Poisson ratio. In the case of Nitinol single crystals, the components of the base crystallographic vectors **n** and **m** are written in component form as

$$[n] = [-0.88888, 0.21523, 0.40443]^{\mathrm{T}}, \quad [m] = [0.43448, 0.75743, 0.48737]^{\mathrm{T}}$$
(62)

relative to the austenite lattice, while g = 0.13078, as in Reference [26]. All twenty-four vector pairs ( $\mathbf{n}_{\alpha}$ ,  $\mathbf{m}_{\alpha}$ ) are generated from the vectors in (62) by appropriate rotations and reflections, see Table I. In addition, the components of the Lagrangian transformation strain after texture distribution are listed for the twenty-four variants in Table II using the cylindrical polar coordinates of Figure 6. In this table, the variants are paired together based on common values of the components  $E_{rr}^{t}$ ,  $E_{\theta\theta}^{t}$ ,  $E_{zz}^{t}$ , and  $E_{\theta z}^{t}$ , which implies that the two variants in a pair are related to each other by a rotation with respect to the  $\mathbf{E}_{r}$ -axis of Figure 6. The remaining relevant material parameters are chosen to be  $B = 0.607 \,\mathrm{MPa}/^{\circ}\mathrm{C}$ ,  $\mathcal{F}^{c} = 7.5 \,\mathrm{MPa}$ , and  $\theta - \theta_{0} = 22.3^{\circ}\mathrm{C}$ .

All simulations assume quasi-static loading conditions. After the constitutive equations are solved locally (i.e. by constrained minimization of  $\Phi^{f}$  or  $\Phi^{r}$  at each Gauss point), the equilibrium equations are enforced globally using Newton's method.

#### 6.1. Uniaxial and biaxial loading of thin-walled tubes

The simulations are supported by direct experimental measurements conducted by the authors' group [13]. Here, thin-walled tubes of 37.8mm length and 4.65mm outer diameter were initially ground down in the 25 mm long centre test section to an outer diameter of 4.3 mm in order to obtain an hourglass shape and minimise end-effects. Thus, the wall thickness in the test section was reduced to 0.2mm, resulting in a thickness-to-radius ratio of 1:10.5. The following loading/unloading programs (referred to respectively as Types A and B) were experimentally traced:

- (A) Load and unload in tension.
- (B) Load and unload simultaneously in tension and torsion.

| No | $E_{ m rr}^{ m t}$ | $E^{\mathbf{t}}_{	heta	heta}$ | $E_{zz}^{\mathbf{t}}$ | $2E_{\mathbf{r}	heta}$ | $2E_{	heta z}^{\mathbf{t}}$ | $2E_{zr}^{t}$ |
|----|--------------------|-------------------------------|-----------------------|------------------------|-----------------------------|---------------|
| 1  | -0.2820E-01        | 0.6314E-01                    | -0.2980E-01           | -0.2720E-01            | 0.2216E-01                  | -0.6764E-01   |
| 4  | -0.2820E-01        | 0.6314E-01                    | -0.2980E-01           | 0.2720E-01             | 0.2216E-01                  | 0.6764E-01    |
| 2  | -0.2820E-01        | -0.2643E-01                   | 0.5978E-01            | 0.5470E-01             | -0.4118E-01                 | 0.4819E-01    |
| 3  | -0.2820E-01        | -0.2643E-01                   | 0.5978E-01            | -0.5470E-01            | -0.4118E-01                 | -0.4819E-01   |
| 5  | 0.1162E-01         | -0.2863E-02                   | -0.3620E-02           | -0.1185E+00            | -0.5268E-01                 | -0.3059E-02   |
| 8  | 0.1162E-01         | -0.2863E-02                   | -0.3620E-02           | 0.1185E+00             | -0.5268E-01                 | 0.3059E-02    |
| 6  | 0.1162E-01         | 0.1302E-01                    | -0.1950E-01           | -0.3662E-01            | -0.4145E-01                 | 0.1128E+00    |
| 7  | 0.1162E-01         | 0.1302E-01                    | -0.1950E-01           | 0.3662E-01             | -0.4145E-01                 | -0.1128E+00   |
| 9  | -0.5056E-01        | -0.4070E-02                   | 0.5978E-01            | 0.2888E-01             | -0.2114E-01                 | 0.5976E-01    |
| 18 | -0.5056E-01        | -0.4070E-02                   | 0.5978E-01            | -0.2888E-01            | -0.2114E-01                 | -0.5976E-01   |
| 10 | 0.2853E-01         | 0.6411E-02                    | -0.2980E-01           | 0.9270E-01             | -0.6965E-01                 | 0.1463E-01    |
| 17 | 0.2853E-01         | 0.6411E-02                    | -0.2980E-01           | -0.9270E-01            | -0.6965E-01                 | -0.1463E-01   |
| 11 | -0.3188E-02        | -0.5145E-01                   | 0.5978E-01            | -0.2582E-01            | 0.6232E-01                  | 0.1157E-01    |
| 19 | -0.3188E-02        | -0.5145E-01                   | 0.5978E-01            | 0.2582E-01             | 0.6232E-01                  | -0.1157E-01   |
| 12 | 0.5208E-01         | -0.1714E-01                   | -0.2980E-01           | 0.6550E-01             | 0.4750E-01                  | -0.5301E-01   |
| 20 | 0.5208E-01         | -0.1714E-01                   | -0.2980E-01           | -0.6550E-01            | 0.4750E-01                  | 0.5301E-01    |
| 13 | 0.2853E-01         | -0.3885E-02                   | -0.1950E-01           | -0.1710E-01            | -0.7693E-01                 | 0.9227E-01    |
| 22 | 0.2853E-01         | -0.3885E-02                   | -0.1950E-01           | 0.1710E-01             | -0.7693E-01                 | -0.9227E-01   |
| 14 | -0.5056E-01        | 0.5932E-01                    | -0.3620E-02           | 0.4671E-01             | 0.2369E-01                  | 0.4715E-01    |
| 21 | -0.5056E-01        | 0.5932E-01                    | -0.3620E-02           | -0.4671E-01            | 0.2369E-01                  | -0.4715E-01   |
| 15 | -0.3188E-02        | 0.2783E-01                    | -0.1950E-01           | 0.1952E-01             | 0.1184E+00                  | -0.2049E-01   |
| 23 | -0.3188E-02        | 0.2783E-01                    | -0.1950E-01           | -0.1952E-01            | 0.1184E+00                  | 0.2049E-01    |
| 16 | 0.5208E-01         | -0.4332E-01                   | -0.3620E-02           | -0.7181E-01            | 0.2899E-01                  | 0.4409E-01    |
| 24 | 0.5208E-01         | -0.4332E-01                   | -0.3620E-02           | 0.7181E-01             | 0.2899E-01                  | -0.4409E-01   |

Table II. Pairs of Nitinol variant in thin-walled tube with sheet texture.

Due to the geometry of the specimens and the gripping conditions, all loading paths yield non-uniform stress and strain distributions. To compare the simulations to the experiments, all the results are presented in terms of average equivalent Cauchy stress  $T_{eq}$  versus average equivalent Lagrangian strain  $E_{eq}$ , where

$$T_{\rm eq} = \sqrt{\bar{T}_{\rm t}^2 + 3\bar{T}_{\rm s}^2}, \quad E_{\rm eq} = \sqrt{\bar{E}_{\rm t}^2 + \frac{4}{3}\bar{E}_{\rm s}^2}$$
 (63)

In (63),  $\overline{T}_t$  and  $\overline{T}_s$  denote the average tensile and shearing Cauchy stress, while  $\overline{E}_t$  and  $\overline{E}_s$  the average tensile and shearing Lagrangian strain, respectively. The average tensile and shearing Cauchy stress components in the test section are obtained by dividing the measured forces at



Figure 6. Schematic diagram of the undeformed and deformed thin tube.



Figure 7. Finite element mesh of the thin tubular specimen.

the grips by the current test section area. Appendix B outlines the formulae for the Lagrangian strains and the average equivalent Lagrangian strain in the thin-walled tube.

The finite element mesh used in simulating the loading of the specimen consists of 8-node isoparametric bricks and is shown in Figure 7. Since the texture is uniformly distributed and the austenite lattice vector is aligned with the longitudinal axis of the tube, the centre cross-section is a symmetry plane.

Each element in this mesh is assumed to correspond to a crystal grain with the proper texture, as discussed in Section 4. A set of nv = 6 potentially active variants is identified at the outset as follows: for each of the two loading paths, a series of simulations was run assuming only a single pair of potentially active variants exhibiting rotational symmetry with



Figure 8. Comparison of equivalent stress-strain data from experiments and simulation for Type A loading in thin-walled Nitinol tubes.

respect to the radial direction, see Table II. Given the nearly homogeneous nature of the deformation, these simulations can be run using a coarser mesh or even a single element. With reference to Equation  $(32)_1$ , each of the preliminary runs yields a value for the thermodynamic force at the onset of forward transformation. The set of potentially active variants is chosen to include those with the lowest values of this thermodynamic force. In particular, and taking into account the existing texture, it is deduced here by the preliminary simulations that variant pairs (2, 3) and (11, 19) exhibit the lowest thermodynamic forces in pure tension, while variant pairs (15, 23) and (11, 19) exhibit the lowest thermodynamic forces in pure torsion. Therefore, the potentially active set for all tension and torsion simulations was taken to be comprised of variants (2, 3), (11, 19), and (15, 23).

6.1.1. Pure tension (Type A). The results of this numerical test are plotted in Figure 8 against the experimental results in Reference [13]. Notice that three curves are plotted for the experimental results corresponding to three separate tension experiments. Also, the lack of hardening effect clearly suggests that the interaction energy from the interface between variants does not contribute significantly to the transformation process. The numerical simulation matches well with the experiments during both forward and reverse transformation. The small reduction in stiffness evident in the experimental results during elastic loading is due to the presence of R-phase which is not modelled here. Also, the slight deviation of the numerical results from the experimental measurements during elastic unloading is likely due to the difference in elastic material response between austenite and martensite. Figure 9 illustrates the volume fractions computed for each variant as a function of equivalent strain, as extracted from an element just below the centre cross-section. The distribution of  $T_t$  and the four active variants is depicted in Figures 10 and 11 at 6% equivalent strain. As expected variants 3 and 19 have volume fraction distributions that are mirror images to those of variants 2 and 11, respectively, relative to the centre cross-section.

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Figure 9. Volume fraction vs equivalent strain for Type A loading of thin-walled Nitinol tubes.



Figure 10. Distribution of  $\overline{T}_t$  for Type A loading at 6% equivalent strain.

Figure 12 depicts two partial loading, unloading and reloading paths in pure tension up to 4.6% strain. The first, denoted as Path 1 in the figure, illustrates elastic unloading from a state of forward transformation followed by the elastic reloading back to the forward transformation plateau. The second, denoted as Path 2 in the figure, illustrates elastic reloading from a state of



Figure 11. Distribution of variants 2, 3, 11 and 19 for Type A loading at 6% equivalent strain.

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Figure 12. Equivalent stress–strain response for partial loading, unloading and reloading path for pure tension at up to 4.6%.



Figure 13. Comparison of equivalent stress-strain data from experiments and simulation for Type B loading in thin-walled Nitinol tubes.

reverse transformation, followed by elastic unloading back to the reverse transformation plateau. This simulation confirms the correctness of the proposed loading/unloading criteria, as well as the robustness of the algorithm in selecting and enforcing the appropriate constraints in (42).

6.1.2. Simultaneous tension-torsion (Type B). Figure 13 shows the equivalent stress-strain response under simultaneous tension up to 6.0% and torsion up to 2.0%. The volume fractions

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Figure 14. Volume fraction vs equivalent strain for Type B loading of thin-walled Nitinol tubes.

in Figure 14 are again taken from an element just below the centre cross-section and indicate a reversal in variant dominance from (2, 3) in pure tension to (11, 19) with the presence of torsion. Notice that the pair (15, 23) is still inactive due to the dominance of tension loading over torsion. Contrary to the case of pure tension, Figure 14 illustrates that the activation of variants does not occur simultaneously. In particular, the primary variants (11, 19) are activated at approximately 0.8% equivalent strain, while the secondary variants are essentially activated only at slightly above 2.0% equivalent strain. The overall increase in the stress–strain slope during forward transformation compared to the pure tension case can be attributed to the increased presence of torsion-dominant variants. The distribution of  $T_t$  and the four active variants is depicted in Figures 15 and 16 at maximum loading.

# 6.2. Radial expansion of a stent

Stents are small wire-mesh tubes used in a variety of medical applications, including, most notably, coronary artery angioplasty. Stents are typically manufactured from thin-walled tubes by precision laser cutting. Nitinol is increasingly used for stents owing to its superelastic property, biocompatibility, and magnetic resonance compatibility [27]. The stent is first expanded axisymmetrically to its designed configuration and then 'annealed' to yield a new stress-free reference configuration. In angioplasty, stents are compressed into a catheter and deployed at the arterial walls. Upon deployment, the stent attempts to extend back to its original reference configuration. However, due to the superelastic property, the stent applies a smaller pressure load on the vessel walls as it traces its unloading path, while retaining its high resistance to crushing along its loading path. In the present simulation, a unit cell of a stent is considered under periodic boundary conditions. The stress-free reference configuration is taken at four times the diameter of the thin-walled tube. Texture is assumed as in the previous examples, since the stent is cut from the same type of tube. Repeating the procedure used in isolating six potentially active variants in Section 6.1, variant pairs (5, 8), (10, 17), and (2, 3) are considered. As shown



Figure 15. Distribution of  $\overline{T}_t$  for Type B loading at 6% tension and 2% torsion.

in Figure 17, a moderately fine mesh of bricks is used to resolve the stress concentration in the upper and lower section of the stent cell. Furthermore, in order to accurately capture the bending of the stent wires, the finite element analysis is conducted using 27-node isoparametric bricks. The outer radius of the tube is  $R_0 = 2.325$  mm, the thickness is 0.375 mm and the height is 7.0 mm. To replicate the manufacturing process, the initial configuration of the stent was obtained by radial expansion from the tube configuration under displacement control on the outer walls, where the deformation was assumed purely elastic. The resulting configuration was set to coincide with a new stress-free reference configuration and was taken to consist completely of austenitic phase. Subsequently, the stent was radially compressed to radius rusing again displacement control on the outer walls. The average external pressure applied on the outer walls of the stent and resolved on the geometry of the initial configuration is plotted in Figure 18 against the relative change of radius  $(4R_0-r)/R_0$ . This figure illustrates the hysteretic loop obtained during a cycle of compression, followed by self-expansion of the stent. Figures 19 and 20 show the distribution of normal Cauchy stress  $T_{\rm t}$  and the total martensitic volume fraction during the compression/tension cycle. As expected, the stress concentration at the wire connections generates significant martensitic transformation, while the rest of the wire remains largely untransformed. The mechanical behaviour of stents is affected by several design parameters, such as height of the stent cell, number of wire-mesh structures in the circumferential direction, thickness in the radial direction, smoothing of the wire connections, etc. Owing to its excellent predictive capacity, the proposed model can be used in the design and analysis of stents.

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Figure 16. Distribution of variants 2, 3, 11 and 19 for Type B loading at 6% tension and 2% torsion.

### 7. CONCLUSIONS

The article presents in a unified manner a sufficiently general theoretical and computational framework for the analysis of the superelastic effect in shape memory alloys. From a continuum standpoint, the proposed formulation is based on a complete theory which allows for the precise definition of loading/unloading, and the identification and measurement of transformation strain. The algorithmic implementation accurately and robustly replicates the non-smooth transitions during loading and unloading, while the numerical simulations show satisfactory match with experimental results.



Figure 17. Finite element model of a stent.



Figure 18. Pressure vs change of radius for a stent in compression/extension cycle.

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Figure 19. Distribution of  $T_t$  for a stent in compression/extension cycle at six configurations corresponding to outer radii  $r = 4R_0, 3R_0, 2R_0, R_0, 2R_0, 3R_0$ .

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Figure 20. Total martensitic volume fraction distribution for a stent in compression/extension cycle at six configurations corresponding to outer radii  $r = 4R_0, 3R_0, 2R_0, R_0, 2R_0, 3R_0$ .

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# APPENDIX A: OUTLINE OF THE CONSTRAINED MINIMIZATION ALGORITHM

The proposed algorithm for the solution of the constitutive equations at the Gauss point level for time  $t_{n+1}$  is outlined in the following steps.

- 1. Set  $[\xi_{n+1}^{f}]^{(0)} = [\xi_{n+1}^{r}]^{(0)} = [\xi_{n}], \quad \mathscr{J}_{n+1}^{f(0)} = \mathscr{J}_{n}^{f}, \quad \mathscr{J}_{n+1}^{r(0)} = \mathscr{J}_{n}^{r}$  and flag to its value at  $t_{n}$  (flag = f for 'forward' or flag = r for 'reverse'). Also, set counter = 0.
- 2. Calculate  $\begin{bmatrix} h_{n+1}^{\text{flag}} \end{bmatrix}$  and  $\begin{bmatrix} c_{n+1}^{\text{flag}} \end{bmatrix}$ .
- 3. Loop over *i*

(3a) Solve

$$[\mathcal{Q}][d_{n+1}]^{(i)} + ([\Pi_{n+1}]^{(i)}[A])^{\mathrm{T}}[\bar{\lambda}_{n+1}]^{(i)} = [g_{n+1}]^{(i)}$$
$$[\Pi_{n+1}]^{(i)}[A][d_{n+1}]^{(i)} = [0]$$

where  $[g_{n+1}]^{(i)} = \left[c_{n+1}^{\text{flag}}\right] - [Q] \left[\zeta_{n+1}^{\text{flag}}\right]^{(i)}$ . If  $||[d]||^{(i)} < \text{tol, then go to (3d).}$ (3b) Calculate

$$\alpha_{n+1}^{(i)} = \min_{k \mid [a_k]^{\mathrm{T}}[d_{n+1}]^{(i)} > 0} \left\{ 1, \frac{h_{n+1,k} - [a_k]^{\mathrm{T}}[\xi_{n+1}^{\mathrm{flag}}]^{(i)}}{[a_k]^{\mathrm{T}}[d_{n+1}^{(i)}]} \right\}$$

and set  $\left[\xi_{n+1}^{\text{flag}}\right]^{(i+1)} = [\xi_{n+1}^{\text{flag}}]^{(i)} + \alpha_{n+1}^{(i)}[d]^{(i)}$ . (3c) If  $\alpha^{(i)} < 1$ , update  $\mathscr{J}_{n+1}^{\text{flag}(i)}$  to  $\mathscr{J}_{n+1}^{\text{flag}(i+1)}$  by adding the index k, set  $i \leftarrow i+1$ , and return to (3a).

(3d) Determine 
$$\bar{\lambda}_{j}^{(i+1)} = \min_{\alpha \in \mathcal{J}_{n+1}^{\operatorname{flag}(i)}} \bar{\lambda}_{\alpha,n+1}^{(i+1)}$$
. If  $\bar{\lambda}_{j}^{(i+1)} \ge 0$ , set counter  $\leftarrow$  counter +1 and

go to 4. Else, drop the index j from  $\mathscr{J}_{n+1}^{\operatorname{flag}(i)}$ , set  $i \leftarrow i+1$  and go to (3a). 4. Set flag =!flag. If counter = 1 go to 2. 5. If flag = f and  $\sum_{\alpha=1}^{6} \xi_{\alpha,n+1}^{r} < \sum_{\alpha=1}^{6} \xi_{\alpha,n} - \operatorname{tol}$ , set flag = r and

$$\bar{\xi}_1 = 0, \quad \bar{\xi}_u = \sum_{\alpha=1}^{nv} \xi_{\alpha,n}$$

Else if flag = r and  $\sum_{\alpha=1}^{6} \xi_{\alpha,n+1}^{f} > \sum_{\alpha=1}^{6} \xi_{\alpha,n} + \text{tol}$ , set flag = f and  $\bar{\xi}_{l} = \sum_{\alpha=1}^{n\nu} \xi_{\alpha,n}, \quad \bar{\xi}_{u} = 1$ 

6. Compute  $\mathbf{E}_{n+1}^{t}$ ,  $\mathbf{S}_{n+1}$  and  $\hat{\partial}_{\mathbf{E}_{n+1}}\mathbf{S}_{n+1}$ .

#### APPENDIX B: DEFORMATION OF THE THIN-WALLED TUBE

With reference to Figure 6, the combined tension and torsion of a homogeneous circular cylinder tube can be expressed componentwise as

$$r = f(R)$$

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$$\theta = \Theta + \alpha \lambda Z \tag{B1}$$
$$z = \lambda Z$$

where  $(R, \Theta, Z)$  and  $(r, \theta, z)$  are the cylindrical polar co-ordinates in the reference and current configuration. Also,  $\lambda$  is the prescribed stretch along the Z-axis,  $\alpha$  is the prescribed angle of twist per unit referential length, and f is an unknown function of R.

Taking into account (B1), the Lagrangian strain tensor takes the form

$$\mathbf{E} = \frac{1}{2} \left[ (f'(R)^2 - 1) \mathbf{E}_R \otimes \mathbf{E}_R + \left(\frac{r^2}{R^2} - 1\right) \mathbf{E}_\Theta \otimes \mathbf{E}_\Theta + \{\lambda^2 (1 + \alpha^2 r^2) - 1\} \mathbf{E}_Z \otimes \mathbf{E}_Z + \frac{\lambda \alpha r^2}{R} (\mathbf{E}_\Theta \otimes \mathbf{E}_Z + \mathbf{E}_Z \otimes \mathbf{E}_\Theta) \right]$$
(B2)

where  $(\mathbf{E}_R, \mathbf{E}_{\Theta}, \mathbf{E}_Z)$  are the basis vectors associated with the cylindrical polar co-ordinate system of the reference configuration. During the thin-walled tube experiments, the Lagrangian strain of the tube is calculated by measuring  $\alpha \lambda L$ , *r* and *z* in the test section. Upon making a standard thin-wall approximation and recalling the homogeneity of the tube, the average Lagrangian tensile strain  $E_t$  along the *Z*-axis and the average shearing strain  $E_s$  become

$$E_{\rm t} = \frac{1}{2}\lambda^2 [(1 + \alpha^2 r_{\rm o}^2) - 1], \quad E_{\rm s} = \frac{1}{2}\frac{\lambda \alpha r_{\rm o}^2}{R_{\rm o}}$$
(B3)

where  $r_0$  and  $R_0$  are the current and referential outer radii, respectively. The strains (B3) are reported for all experiments and also computed in all thin-walled tube simulations.

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