

Modeling the interaction between instabilities and functional degradation in shape memory alloys[†]

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Abstract

Localization of the stress-induced martensitic phase transformation plays an important role in the fatigue behavior of shape memory alloys (SMAs). The phenomenon of return-point memory that is observed during the subloop deformation of a partially-transformed SMA is a clear manifestation of the interaction between localized phase transformation and degradation of the functional properties. The present study aims to demonstrate this structure–material interaction in the modeling of return-point memory. It seems that this crucial aspect has been overlooked in previous modeling studies. For this purpose, we developed a gradient-enhanced model of pseudoelasticity that incorporates the degradation of functional properties in its constitutive description. The model is employed to reproduce the hierarchical return-point memory in a pseudoelastic NiTi wire under isothermal uniaxial tension with nested subloops. Additionally, a detailed analysis is carried out for a NiTi strip with more complex transformation pattern. Our study highlights the subtle morphological changes of phase transformation under different loading scenarios and the resulting implications for return-point memory.

Keywords: Shape memory alloys; Phase transformation; Functional degradation; Propagating instabilities; Subloop deformation; Modeling

1. Introduction

1 The practical interest in shape memory alloys (SMAs), especially NiTi, stems from their ability
2 to withstand and recover large strains. This ability is exhibited through mechanical loading and
3 unloading at sufficiently high temperatures (pseudoelasticity) or through mechanical loading and
4 unloading followed by heating (shape memory effect). The underlying mechanism is the crystallo-
5 graphically reversible martensitic phase transformation that occurs between the austenitic parent
6 phase (stable at higher temperatures, possessing higher crystal symmetry) and the martensitic prod-
7 uct phase (stable at lower temperatures, possessing lower crystal symmetry) [1]. By leveraging the
8 unique characteristics of SMAs, they have found a broad range of applications across various fields,
9 from micro-scale biomedical devices to macro-scale industrial components [2, 3]. The operational

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10 lifespan of SMAs in most of the applications involves enduring cyclic mechanical/thermal loadings,
11 which highlights the great importance of identifying their fatigue behavior. It is well-recognized
12 that, due to the martensitic phase transformation, fatigue in SMAs is more complex than in common
13 engineering metals and is mainly classified into two aspects: degradation of functional properties
14 (such as recoverable strain, transformation stress, and hysteresis loop area), known as functional
15 fatigue, and the evolution of damage in the material, known as structural fatigue [4]. This complex
16 nature demands special attention and, as a result, has prompted a tremendous number of stud-
17 ies that focus on the fatigue characterization of SMAs from a variety of perspectives and on the
18 underlying micromechanical processes [3–13].

19 Stress-induced martensitic transformation in pseudoelastic NiTi appears (typically, in tension-
20 dominated loadings) as localized instabilities in the form of martensite bands, and subsequently
21 progresses via propagation of the instabilities in the form of patterned interfaces (macroscopic trans-
22 formation fronts) that separate the domains of low-strained austenite and high-strained martensite,
23 e.g., [14–17]. Due to the high strain incompatibilities that exist within the transformation front
24 and the ensuing large local stresses, it can be reasonably inferred that propagating instabilities can
25 vitally influence both the functional fatigue and structural fatigue of the material. Despite the
26 longstanding recognition of this crucial aspect [4, 18–21], its direct validation was provided only a
27 few years ago in the experiments conducted by Zheng et al. [8, 22, 23]. It was demonstrated that
28 in view of the repetitive nucleation and propagation of the localized transformation in NiTi strips
29 under cyclic uniaxial tension, a rapid degradation of pseudoelasticity occurs that accelerates the
30 fatigue crack initiation and fatigue failure.

31 An interesting manifestation of the interaction between propagating instabilities and functional
32 degradation is found in the subloop deformation of a partially-transformed SMA specimen under
33 displacement-control loading. The subloop deformation has been extensively investigated experi-
34 mentally, notably for NiTi [18, 19, 23–26] but also for other SMAs [27, 28]. Fig. 1(a), reproduced
35 from Tobushi et al. [24], depicts the mechanical response of a NiTi wire subjected to subloop paths.
36 For a more intuitive description of the phenomenon, hypothetical schematics of the corresponding
37 transformation front evolution are provided in Fig. 1(b). As the front propagates along the wire,
38 it leaves behind transformation-induced microstructural defects, such as dislocations and stabilized
39 (locked-in) martensite. During the subloop unloading (for instance, the first subloop, which starts
40 at point A), the front travels backward over an already swept zone (from A to B), hence intensify-
41 ing the generated defects. Accordingly, during the subloop reloading, the propagation of the front
42 over the twice-swept zone occurs with a lower stress level compared to the original transformation
43 plateau. Upon entering the pristine zone (at point A), which is virtually free of transformation-
44 induced defects, the front experiences the transformation-onset stress characteristic to the initial
45 material state. This causes the stress to catch up with the original plateau by passing through the
46 subloop unloading point. This trait is known as the return-point memory. The process repeats in
47 the subsequent subloops and culminates in an intriguing hierarchical return-point memory.

48 Motivated by the experimental results, numerous attempts have been made to develop SMA
49 models capable of capturing the phenomenon of return-point memory during the subloop deforma-
50 tion, either through incorporating the permanent strain contribution and degradation of functional
51 properties [29–32] or by merely refining the constitutive equations of (non-cyclic) model of pseudoe-

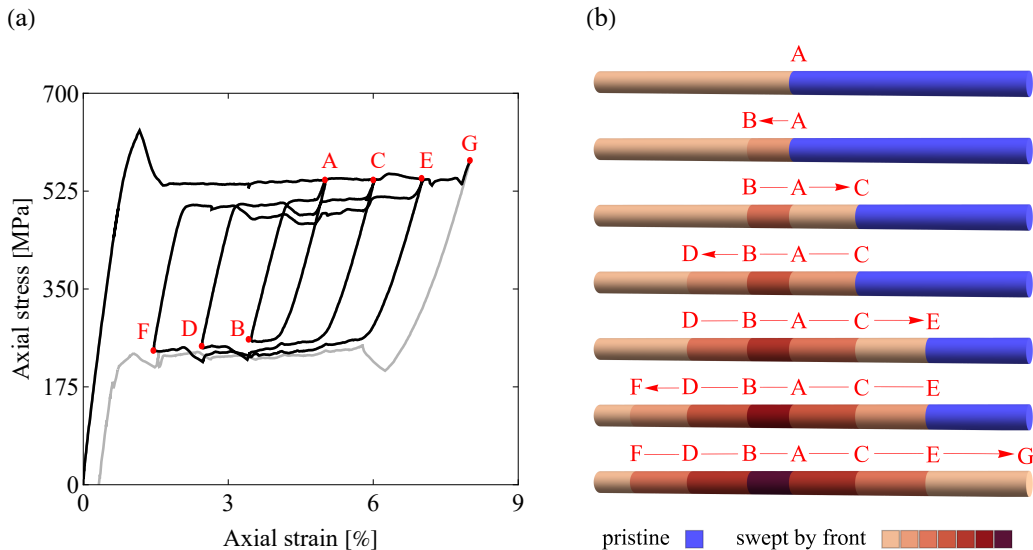


Figure 1: Return-point memory in NiTi wire subjected to uniaxial tension with three nested subloop paths: (a) the structural stress–strain response, and (b) hypothetical schematics of the corresponding transformation front evolution. The stress–strain response in panel (a) is reproduced from Tobushi et al. [24] (courtesy of R. Matsui). The red arrows in panel (b) indicate the trajectory of the front propagation, and the color scales quantify the recurrence of the front’s traversal over the wire’s segments.

52 elasticity [25, 33, 34]. In fact, a physically-relevant approach for modeling the return-point memory
 53 should hinge on the interaction between the propagating instabilities (structural inhomogeneities)
 54 and the functional degradation of the material. Nevertheless, most of the existing models (including
 55 those referenced above) postulate a homogeneous martensitic phase transformation, while address-
 56 ing a problem with a transformation of localized nature. Albeit this simplifies the computations
 57 significantly, it is not a plausible assumption in the present context. To the best of our knowledge,
 58 the only related modeling study that has accounted for this structure–material interaction is the 1D
 59 model of Bartel et al. [32]. In their model, however, instabilities do not originate from a softening-
 60 type intrinsic material response but are rather treated as weak displacement discontinuities that
 61 separate the transformed and untransformed material points (indeed, experiments, e.g., [35, 36],
 62 have confirmed that the true intrinsic response of NiTi is characterized by a significant soften-
 63 ing branch). It should be remarked that recently Xiao and Jiang [37, 38] have acknowledged this
 64 structure–material interaction in their simulations, however, their applications did not specifically
 65 pertain to the subloop deformation and return-point memory.

66 In light of the above premise, this work aims to provide a detailed analysis of the phenomenon
 67 of return-point memory by accounting for the interaction between propagating instabilities and the
 68 degradation of the functional properties of the material. To achieve this, a gradient-enhanced model
 69 of pseudoelasticity with functional degradation is developed in this work. The model is formulated
 70 within the small-strain theory. The basic structure of the model follows the non-gradient model of
 71 pseudoelasticity developed by Stupkiewicz and Petryk [39] and is based on the energy minimization
 72 principle. The gradient-enhancement, micromorphic regularization, and thermomechanical coupling
 73 are adopted from our previously-developed gradient-enhanced model [40, 41]. This previous model
 74 has demonstrated its capability in reproducing the complex patterns of phase transformation in

75 pseudoelastic NiTi specimens under uniaxial tension [41], including the effect of loading rate and
 76 latent heat of transformation on martensite domain formation, and in pseudoelastic NiTi tubes
 77 under combined tension–torsion [42, 43]. The main advancement of the model in the present work
 78 compared to the previous version lies in the incorporation of permanent inelastic strain and the
 79 enrichment of the constitutive equations with functional degradation effects. Consequently, given
 80 its ability to treat localization effects via gradient-enhancement and micromorphic regularization,
 81 the model can be considered a suitable tool for addressing problems where both cyclic loading and
 82 transformation localization are at play.

83 In what follows, we first introduce the model in Section 2. The model is employed to analyze the
 84 problem of subloop deformation in NiTi wire and strip under uniaxial tension. The corresponding
 85 results are presented and discussed in Section 3. In addition, a simplified version of the model is
 86 provided in Appendix A.

2. A small-strain model of pseudoelasticity with functional degradation

87 The present model falls in the category of phenomenological models. Accordingly, the consti-
 88 tutive relations are tailored, in a simple phenomenological manner, to mimic the pseudoelasticity
 89 degradation effects. Since the focus of this study is on the analysis of the return-point memory,
 90 which is relevant at the macroscopic scale, a phenomenological description seems to adequately
 91 fulfill the intended purpose. In Section 2.1, we introduce the constitutive model in an isothermal
 92 format. Subsequently, in Section 2.2, micromorphic regularization, thermomechanical coupling, and
 93 finite-element implementation are briefly discussed.

2.1. Constitutive model

94 We begin the model description by noting that functional fatigue in SMAs is typically attributed
 95 to a number of mechanisms. Among them, generation of dislocation slip [4, 44], formation of
 96 stabilized martensite [21, 45] and non-transforming austenite [45, 46] are the most likely involved
 97 mechanisms. In the present model, a subdivision into the possible mechanisms and their mutual
 98 interaction is not attempted, instead, they are unitedly represented by phenomenological evolution
 99 equations, and are directly linked to the martensitic phase transformation through the accumulated
 100 martensite volume fraction η^{acc} . In line with this notion, the inelastic mechanism responsible for
 101 functional degradation is herein denoted as transformation-induced plasticity (TRIP).

102 The material state at each point is characterized by two quantities, namely the total strain
 103 $\boldsymbol{\varepsilon} = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$, with \mathbf{u} as the displacement vector, and the martensite volume fraction η .
 104 The total strain is additively decomposed into

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^t + \boldsymbol{\varepsilon}^p, \quad (1)$$

105 where $\boldsymbol{\varepsilon}^e$ denotes the elastic contribution, $\boldsymbol{\varepsilon}^t$ denotes the martensitic transformation contribution
 106 and $\boldsymbol{\varepsilon}^p$ is the permanent strain associated with TRIP. At the same time, it is assumed that during
 107 the martensitic transformation a fraction of martensite stabilizes and does not transform back
 108 to austenite. Hence, the martensite volume fraction η is split into the reversible part η^{rev} and

109 irreversible part η^{ir} , viz.,

$$\eta = \eta^{\text{rev}} + \eta^{\text{ir}}, \quad (2)$$

110 and the following inequality constraints hold,

$$0 \leq \eta^{\text{ir}} \leq \eta \leq 1 \quad \implies \quad 0 \leq \eta^{\text{rev}} \leq 1 - \eta^{\text{ir}}. \quad (3)$$

111 The material is in the fully austenitic state when $\eta = \eta^{\text{rev}} = 0$ and is in the fully martensitic state
 112 when $\eta = 1$. Nevertheless, once the material starts transforming to martensite from a pristine
 113 austenitic state, η^{ir} becomes immediately nonzero, as indicated by Eqs. (4)–(6) below, and thereby,
 114 a fully austenitic state will not be recoverable.

115 It has been repeatedly observed in the experiments that the degradation of pseudoelasticity in
 116 conventional polycrystalline NiTi are mostly pronounced during the first tens of cycles, gradually
 117 diminishing and eventually reaching saturation as the material passes the so-called shakedown
 118 stage, e.g., [22, 47, 48]. In view of this general consensus, we adopt the assumption that both the
 119 irreversible volume fraction η^{ir} and the permanent strain ϵ^{p} follow exponential-type evolution laws.
 120 Note that this assumption is not unique to the present model and has been exploited in various
 121 SMA models that account for functional degradation, e.g., [37, 49–51]. With this assumption in
 122 place, we first introduce the accumulated volume fraction η^{acc} as

$$\dot{\eta}^{\text{acc}} = |\dot{\eta}^{\text{rev}}| \quad \implies \quad \eta^{\text{acc}} = \int_0^t |\dot{\eta}^{\text{rev}}| d\tau, \quad (4)$$

123 where the overdot denotes the rate of change of the variable and t denotes the time. The evolution
 124 equation for the irreversible volume fraction η^{ir} is then explicitly postulated as

$$\eta^{\text{ir}} = h_{\text{ir}}^{\text{sat}} (1 - \exp(-C_{\text{p}} \eta^{\text{acc}})), \quad (5)$$

125 which results from the time-integration of the following rate equation (with $\eta^{\text{acc}}|_{t=0} = 0$ and
 126 $\eta^{\text{ir}}|_{t=0} = 0$, as for the initial conditions),

$$\dot{\eta}^{\text{ir}} = h_{\text{ir}}^{\text{sat}} C_{\text{p}} \exp(-C_{\text{p}} \eta^{\text{acc}}) \dot{\eta}^{\text{acc}}. \quad (6)$$

127 Analogously, the evolution equation for the permanent strain ϵ^{p} is postulated as

$$\dot{\epsilon}^{\text{p}} = \epsilon_{\text{p}}^{\text{sat}} C_{\text{p}} \exp(-C_{\text{p}} \eta^{\text{acc}}) \dot{\eta}^{\text{acc}} \mathbf{N}_{\text{p}}. \quad (7)$$

128 In Eqs. (5)–(7), $h_{\text{ir}}^{\text{sat}}$ and $\epsilon_{\text{p}}^{\text{sat}}$ represent the respective saturation values for irreversible volume
 129 fraction and permanent strain, C_{p} is the degradation rate, and \mathbf{N}_{p} is the direction tensor which is
 130 defined such that the rate of the permanent strain $\dot{\epsilon}^{\text{p}}$ is aligned with the martensitic transformation
 131 strain ϵ^{t} , i.e.,

$$\mathbf{N}_{\text{p}} = \frac{\epsilon^{\text{t}}}{\|\epsilon^{\text{t}}\|}, \quad \|\epsilon^{\text{t}}\| = \sqrt{\text{tr}(\epsilon^{\text{t}})^2}. \quad (8)$$

132 Note that, in view of the definition of the accumulated volume fraction η^{acc} , the variables η^{ir} and
 133 ϵ^{p} evolve continuously during both the forward and backward transformations.

134 Martensitic transformation in SMAs usually exhibits negligible volumetric change [1]. The
 135 transformation strain $\boldsymbol{\varepsilon}^t$ is therefore assumed to be deviatoric (i.e., $\text{tr } \boldsymbol{\varepsilon}^t = 0$). Moreover, since
 136 the stress-induced transformation renders the martensite variants to be oriented in the direction
 137 of the applied stress, martensite is here considered to appear in a fully-oriented state so that the
 138 transformation strain $\boldsymbol{\varepsilon}^t$ is defined as a function of the reversible volume fraction η^{rev} and the
 139 transformation strain of fully-oriented martensite $\bar{\boldsymbol{\varepsilon}}^t$,

$$\boldsymbol{\varepsilon}^t = \eta^{\text{rev}} \bar{\boldsymbol{\varepsilon}}^t, \quad \bar{\boldsymbol{\varepsilon}}^t \in \bar{\mathcal{P}} = \{ \bar{\boldsymbol{\varepsilon}}^t : g(\bar{\boldsymbol{\varepsilon}}^t) = 0 \}. \quad (9)$$

140 The set $\bar{\mathcal{P}}$ defines the admissible limit transformation strain tensors characterized by the surface
 141 $g(\bar{\boldsymbol{\varepsilon}}^t) = 0$ which is expressed in the following form [52],

$$g(\bar{\boldsymbol{\varepsilon}}^t) = \left[(-I_2)^{3/2} - bI_3 - cI_4^3 \right]^{1/3} - a. \quad (10)$$

142 In Eq. (10), I_2 and I_3 denote the principal invariants of the limit transformation strain tensor $\bar{\boldsymbol{\varepsilon}}^t$
 143 while I_4 denotes a mixed invariant, defined as

$$I_2 = -\frac{1}{2} \text{tr}(\bar{\boldsymbol{\varepsilon}}^t)^2, \quad I_3 = \det \bar{\boldsymbol{\varepsilon}}^t, \quad I_4 = \mathbf{m} \cdot \bar{\boldsymbol{\varepsilon}}^t \mathbf{m}, \quad (11)$$

144 where \mathbf{m} is the axis of the transverse isotropy. The parameters a , b and c characterize the shape
 145 and size of the surface $g(\bar{\boldsymbol{\varepsilon}}^t) = 0$ and are specified as

$$a = \epsilon_{\text{T}} \left[\frac{3\sqrt{3}}{4(1+\alpha^3)} \right]^{1/3}, \quad b = \frac{\sqrt{3}}{6} \frac{9\alpha^3\beta^3 - 7\alpha^3 + 7\beta^3 - 9}{(1+\alpha^3)(1+\beta^3)}, \quad c = \frac{2\sqrt{3}}{3} \frac{\alpha^3 - \beta^3}{(1+\alpha^3)(1+\beta^3)}, \quad (12)$$

146 with ϵ_{T} as the maximum transformation strain in tension, α as the tension–compression asymmetry
 147 ratio in the direction along the axis of transverse isotropy (i.e., parallel to \mathbf{m}), and β as the tension–
 148 compression asymmetry ratio in the direction perpendicular to the axis of transverse isotropy (i.e.,
 149 perpendicular to \mathbf{m}).

150 It is noteworthy that the deviatoric nature of the transformation strain $\boldsymbol{\varepsilon}^t$ dictates, in accordance
 151 with the definition of the direction tensor \mathbf{N}_{p} , see Eq. (8), that the permanent strain $\boldsymbol{\varepsilon}^{\text{p}}$ is also
 152 deviatoric. Models within the present context often postulate that the permanent inelastic strain
 153 evolves in the direction of stress deviator, e.g., [37, 49, 50]. In the present formulation, it can be
 154 easily shown that the stress deviator is perpendicular to the surface $g(\bar{\boldsymbol{\varepsilon}}^t) = 0$, see [39], and thereby,
 155 the transformation strain $\boldsymbol{\varepsilon}^t$ depends on the direction of stress deviator. This, however, does not
 156 imply that the transformation strain $\boldsymbol{\varepsilon}^t$, and accordingly the permanent strain rate $\dot{\boldsymbol{\varepsilon}}^{\text{p}}$, are colinear
 157 with the stress deviator.

158 Another important aspect to highlight is that the accumulation of the irreversible volume frac-
 159 tion η^{ir} and its impact on the reversible volume fraction η^{rev} cause the magnitude of the transfor-
 160 mation strain $\boldsymbol{\varepsilon}^t$, which serves as the actual transformation strain measure in the present model,
 161 to decrease. However, the surface $g(\bar{\boldsymbol{\varepsilon}}^t) = 0$ and so the limit transformation strain $\bar{\boldsymbol{\varepsilon}}^t$ remain in-
 162 tact throughout the cyclic transformation. This represents an underlying modeling assumption in
 163 the present framework regarding the interaction between phase transformation and cyclic degrada-
 164 tion. It reflects the notion that the inherent characteristics of the transformation strain are not

165 affected during the cyclic degradation. Instead, it is the accumulation of TRIP and the decrease in
 166 the amount of transformable (reversible) martensite that lead to the contraction of the maximum
 167 attainable transformation strain.

We now elaborate on the Helmholtz free energy function and the dissipation potential, both customized to incorporate the degradation effects. Assuming an isothermal process, the Helmholtz free energy ϕ is composed of the following contributions: the chemical energy ϕ_{chem} , the elastic strain energy ϕ_{el} , the austenite–martensite interaction energy ϕ_{int} , the energy of the diffuse interface ϕ_{grad} , and the energy contribution ϕ_{deg} related to the pseudoelasticity degradation, i.e.,

$$\begin{aligned} \phi(\boldsymbol{\varepsilon}, \bar{\boldsymbol{\varepsilon}}^t, \boldsymbol{\varepsilon}^p, \eta^{\text{rev}}, \nabla \eta^{\text{rev}}, \eta^{\text{ir}}) = \\ \phi_{\text{chem}}(\eta^{\text{rev}}, \eta^{\text{ir}}) + \phi_{\text{el}}(\boldsymbol{\varepsilon}, \bar{\boldsymbol{\varepsilon}}^t, \boldsymbol{\varepsilon}^p, \eta^{\text{rev}}) + \phi_{\text{int}}(\eta^{\text{rev}}) + \phi_{\text{grad}}(\nabla \eta^{\text{rev}}) + \phi_{\text{deg}}(\eta^{\text{rev}}, \eta^{\text{ir}}). \end{aligned} \quad (13)$$

168 Among the contributions to the Helmholtz free energy ϕ , only ϕ_{deg} is specific to the present model.
 169 The remaining contributions are rather standard and adhere to the non-cyclic model of pseudoelasticity [39–41] and are formulated as

$$\phi_{\text{chem}}(\eta^{\text{rev}}, \eta^{\text{ir}}) = (1 - \eta)\phi_0^a + \eta\phi_0^m = \phi_0^a + \Delta\phi_0\eta, \quad (14)$$

$$\phi_{\text{el}}(\boldsymbol{\varepsilon}, \bar{\boldsymbol{\varepsilon}}^t, \boldsymbol{\varepsilon}^p, \eta^{\text{rev}}) = \mu \text{tr}(\boldsymbol{\varepsilon}_{\text{dev}}^e)^2 + \frac{1}{2}\kappa(\text{tr} \boldsymbol{\varepsilon}^e)^2, \quad \boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon} - \eta^{\text{rev}}\bar{\boldsymbol{\varepsilon}}^t - \boldsymbol{\varepsilon}^p, \quad (15)$$

$$\phi_{\text{int}}(\eta^{\text{rev}}) = \frac{1}{2}H_{\text{int}}(\eta^{\text{rev}})^2, \quad (16)$$

$$\phi_{\text{grad}}(\nabla \eta^{\text{rev}}) = \frac{1}{2}G\nabla \eta^{\text{rev}} \cdot \nabla \eta^{\text{rev}}. \quad (17)$$

174 Here, $\Delta\phi_0 = \phi_0^m - \phi_0^a$ is the phase transformation chemical energy, μ is the elastic shear modulus
 175 and is calculated via applying the Reuss averaging scheme based on the total volume fraction η to
 176 the shear moduli of austenite μ_a and martensite μ_m (i.e., $1/\mu = (1 - \eta)/\mu_a + \eta/\mu_m$), κ is the elastic
 177 bulk modulus (assumed constant), H_{int} is the parameter that characterizes the material response
 178 (softening- or hardening-type) within the transformation regime, and $G > 0$ is the gradient energy
 179 coefficient. Note that the parameter H_{int} can be adapted such that it reflects a loading-dependent
 180 material response (typically, a softening-type response in tension and hardening-type response in
 181 compression), e.g., [42]. However, for simplicity, H_{int} is here considered as a constant parameter.
 182 Given that the simulations in this study involve predominantly tensile loading, see Section 3, this
 183 simplification does not pose a serious limitation. Note also that the interaction energy ϕ_{int} is
 184 a quadratic function of the volume fraction η^{rev} , resulting in a tri-linear intrinsic stress–strain
 185 response, as illustrated in Fig. 2. This choice is also made for simplicity and can be readily adapted
 186 to more complex functions to achieve a more realistic response [43].

187 On the other hand, the degradation contribution ϕ_{deg} takes the following form

$$\phi_{\text{deg}}(\eta^{\text{rev}}, \eta^{\text{ir}}) = A_{\text{deg}}\eta^{\text{ir}}\eta^{\text{rev}} + \frac{1}{2}H_{\text{deg}}\eta^{\text{ir}}(\eta^{\text{rev}})^2, \quad (18)$$

188 where A_{deg} and H_{deg} represent the degradation parameters. The contribution ϕ_{deg} is specifically
 189 tailored to address two primary effects of pseudoelasticity degradation: it accounts for the reduction

190 of the transformation-onset stress (described by the term $A_{\text{deg}}\eta^{\text{ir}}\eta^{\text{rev}}$) and the conversion of the
 191 mechanical response towards a hardening-type response (described by the term $\frac{1}{2}H_{\text{deg}}\eta^{\text{ir}}(\eta^{\text{rev}})^2$).
 192 In line with the evolution of η^{ir} , Eq. (5), both effects progress exponentially. Note that the approach
 193 of incorporating the cyclic degradation effects into the free energy function has been also used in
 194 other SMA models in the literature, e.g., [53, 54].

195 Finally, a rate-independent dissipation potential is adopted in the following form

$$D(\dot{\eta}^{\text{rev}}, \eta^{\text{acc}}) = f_c(\eta^{\text{acc}})|\dot{\eta}^{\text{rev}}|, \quad (19)$$

196 where $f_c(\eta^{\text{acc}})$, which is called the critical thermodynamic driving force, controls the width of the
 197 hysteresis loop in the stress-strain response. To capture the decrease in the hysteresis loop area
 198 (i.e., the dissipated energy) during the cyclic transformation, the parameter f_c is defined in relation
 199 to the accumulated volume fraction η^{acc} . Similar to the permanent strain ϵ^{p} and the irreversible
 200 volume fraction η^{ir} , Eqs. (5)–(7), f_c evolves exponentially as follows

$$f_c(\eta^{\text{acc}}) = f_c^{\text{fin}} + (f_c^{\text{ini}} - f_c^{\text{fin}}) \exp(-C_f \eta^{\text{acc}}), \quad (20)$$

201 where f_c^{ini} and f_c^{fin} represent, respectively, the initial and final values of f_c , and C_f denotes the
 202 corresponding evolution rate.

203 To formulate the incremental energy minimization problem, we derive the time-discrete version
 204 of the constitutive equations by employing the backward Euler scheme. Having known the variables
 205 related to the previous time step t_n , the variables related to the current time step $t_{n+1} = t_n + \Delta t$ are
 206 sought. We begin by approximating the incremental evolution equation for the irreversible volume
 207 fraction η^{ir} and the permanent strain ϵ^{p} ,

$$\Delta t \dot{\eta}^{\text{ir}} \approx \Delta \eta^{\text{ir}} = h_{\text{ir}}^{\text{sat}} C_p \exp(-C_p \eta^{\text{acc}}) \Delta \eta^{\text{acc}}, \quad \Delta t \dot{\epsilon}^{\text{p}} \approx \Delta \epsilon^{\text{p}} = \epsilon_p^{\text{sat}} C_p \exp(-C_p \eta^{\text{acc}}) \Delta \eta^{\text{acc}} N_p, \quad (21)$$

208 where

$$\eta^{\text{acc}} = \int_0^{t_{n+1}} \Delta \eta^{\text{acc}} d\tau, \quad \Delta \eta^{\text{acc}} = |\Delta \eta^{\text{rev}}|, \quad \Delta \eta^{\text{rev}} = \eta^{\text{rev}} - \eta_n^{\text{rev}}, \quad (22)$$

209 with η_n^{rev} as the value of the reversible volume fraction from the previous time step t_n . At the same
 210 time, the incremental form of the rate-independent dissipation potential is obtained as

$$\Delta D(\Delta \eta^{\text{rev}}, \eta^{\text{acc}}) = f_c(\eta^{\text{acc}}) |\Delta \eta^{\text{rev}}|. \quad (23)$$

211 The solution of the problem is determined via the incremental energy minimization principle
 212 [39, 41, 55]. A global incremental potential Π is defined by summing up the increment of the
 213 total Helmholtz free energy $\Delta \Phi$ (where $\Phi = \int_B \phi dV$), the global dissipation potential $\Delta \mathcal{D}$ (where
 214 $\Delta \mathcal{D} = \int_B \Delta D dV$) and the potential of the external loads $\Delta \Omega$, and is subsequently minimized with
 215 respect to the unknowns \mathbf{u} , $\bar{\epsilon}^{\text{t}}$ and η^{rev} , i.e.,

$$\Pi = \Delta \Phi + \Delta \Omega + \Delta \mathcal{D} \rightarrow \min_{\mathbf{u}, \bar{\epsilon}^{\text{t}}, \eta^{\text{rev}}} \quad (24)$$

216 which is subject to the inequality constraints on the reversible volume fraction η^{rev} , Eq. (3), and

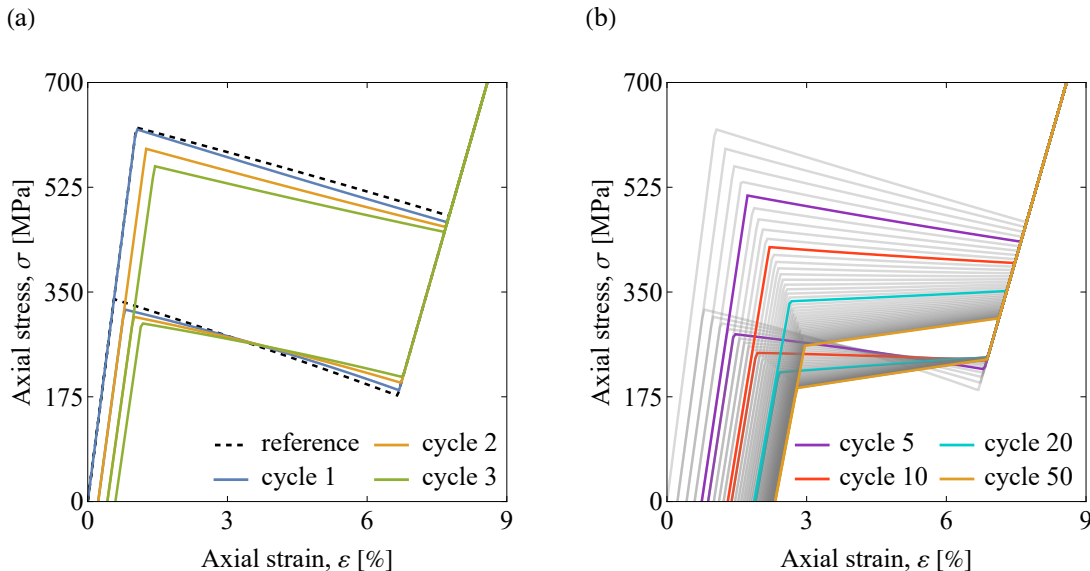


Figure 2: The intrinsic stress–strain response of the model under full-transformation cycles of uniaxial-tension: (a) the first three cycles, and (b) the first 50 cycles. The dashed curve in panel (a), denoted as ‘reference’, represents the pseudoelastic intrinsic response with no degradation effects. The model parameters adopted to produce the intrinsic responses are the same as those in the main simulations, see Section 3.

217 to the constraint related to the limit transformation strain surface, Eq. (9). At the same time,
 218 η^{ir} and ϵ^{p} , which contribute directly to the minimization problem, are explicitly evaluated from
 219 Eq. (21). To provide a clearer idea of the structure of the minimization problem and the underlying
 220 constitutive behavior of the model, a simplified 1D version of the model is elaborated in Appendix
 221 A.

222 Fig. 2 showcases the intrinsic stress–strain response predicted by the model under cyclic tensile
 223 loading. Two cases are highlighted: the pseudoelasticity degradation effects observed within the
 224 first three cycles, relevant to the problem of subloop deformation investigated in this study, and
 225 the degradation effects observed within 50 cycles, which provides a more holistic view of the model
 226 behavior. Note that the material parameters adopted to generate the intrinsic response in Fig. 2
 227 are the same as those adopted in the main simulations in Section 3.

2.2. Further extensions and finite-element implementation

228 The model presented in Section 2.1 is now enriched with micromorphic regularization and is
 229 made thermomechanically coupled. Both extensions have been thoroughly discussed in our previous
 230 works [40, 41]. Hence, we only briefly discuss them here.

231 The purpose of adopting the micromorphic regularization is to facilitate the finite-element imple-
 232 mentation of the gradient-enhanced model by restructuring the minimization problem in a way that
 233 the constitutive complexities are transferred to the local level (for instance, at the Gauss points)
 234 where they can be treated in a more efficient way. To do so, a new degree of freedom $\check{\eta}$ is introduced
 235 and is coupled with the volume fraction η^{rev} through the following penalization term ϕ_{pen} which is
 236 added into the Helmholtz free energy function ϕ , see Eq. (13),

$$\phi_{\text{pen}}(\eta^{\text{rev}}, \check{\eta}) = \frac{1}{2} \chi (\eta^{\text{rev}} - \check{\eta})^2, \quad (25)$$

237 with χ as the penalty parameter. The gradient energy ϕ_{grad} , see Eq. (17), is then redefined in terms
 238 of the gradient of the new variable $\check{\eta}$, i.e.,

$$\phi_{\text{grad}}(\nabla\check{\eta}) = \frac{1}{2}G\nabla\check{\eta} \cdot \nabla\check{\eta}. \quad (26)$$

239 Following this modification, the volume fraction η^{rev} can be considered as a local quantity and the
 240 respective evolution equation can be solved (together with that of $\bar{\epsilon}^{\text{t}}$) at the local level. For further
 241 details regarding the micromorphic regularization, interested readers are referred to [56, 57].

242 To arrive at a thermomechanically-coupled model, two most important couplings are taken
 243 into consideration. First, the chemical energy ϕ_{chem} , Eq. (14), is extended to reflect the effect of
 244 temperature on the mechanical response (the Clausius–Clapeyron relation), i.e.,

$$\phi_0(\eta^{\text{rev}}, \eta^{\text{ir}}, T) = \phi_0^{\text{a}}(T) + \Delta\phi_0(T)\eta, \quad \Delta\phi_0(T) = \Delta s^*(T - T_{\text{t}}), \quad (27)$$

245 where Δs^* represents the transformation entropy change, T is the temperature, and T_{t} is the
 246 transformation equilibrium temperature. Next, the internal heat source \dot{R} is defined to encompass
 247 the latent heat of transformation and the heat release by mechanical dissipation, viz.,

$$\dot{R} = \Delta s^* T \dot{\eta}^{\text{rev}} + f_c(\eta^{\text{acc}})|\dot{\eta}^{\text{rev}}|. \quad (28)$$

248 Eq. (28) is then introduced into the (isotropic) heat conduction equation

$$\varrho_0 c \dot{T} + \nabla \cdot \mathbf{Q} = \dot{R}, \quad \mathbf{Q} = -K \nabla T, \quad (29)$$

249 where \mathbf{Q} is the heat flux, $\varrho_0 c$ is the specific heat, and the scalar K is the heat conduction coefficient.
 250 It follows from Eq. (28) that the internal heat generation is influenced during the cyclic phase
 251 transformation. This influence is manifested by both the latent heat of transformation and the
 252 mechanical dissipation and operates through the reversible volume fraction η^{rev} and the hysteresis
 253 parameter f_c , cf. Eqs. (3) and (20).

254 The full thermomechanically-coupled model comprises three global unknown fields: the displace-
 255 ment \mathbf{u} , the micromorphic variable $\check{\eta}$ and the temperature T ; and two local unknown variables: the
 256 reversible volume fraction η^{rev} and the limit transformation strain $\bar{\epsilon}^{\text{t}}$. Recall that the irreversible
 257 volume fraction η^{ir} and the permanent strain ϵ^{p} are explicitly integrated by using Eq. (21). The
 258 finite-element discretization of the displacement field \mathbf{u} is performed by using 20-noded quadratic
 259 hexahedral (Serendipity) elements with reduced Gauss integration rule ($2 \times 2 \times 2$). On the other
 260 hand, 8-noded linear hexahedral elements with standard Gauss integration rule ($2 \times 2 \times 2$) are
 261 used for $\check{\eta}$ and T . For the 2D axisymmetric wire problem discussed in Section 3.2, the respective
 262 discretizations have been done by 8-noded quadratic elements and 4-noded linear elements. The
 263 resulting global–local problem is structured as a nested iterative-subiterative scheme and is solved
 264 at both the global and local levels by using the Newton method. Notably, a fully-coupled monolithic
 265 scheme is adopted so that the problem is solved simultaneously with respect to all unknowns.

266 It is worth noting that the local minimization problem of η^{rev} is non-smooth, in view of the
 267 rate-independent dissipation potential, see Eqs. (19) and (23). To address this issue, the aug-

268 mented Lagrangian method is utilized, which handles adeptly both the non-smoothness of the
 269 rate-independent dissipation potential and the inequality constraints on the reversible volume frac-
 270 tion η^{rev} , i.e., $0 \leq \eta^{\text{rev}} \leq 1 - \eta^{\text{ir}}$, see Eq. (3). The local problem has an additional constraint to be
 271 satisfied, namely the equality constraint of the limit transformation strain surface, $g(\bar{\epsilon}^t) = 0$, see
 272 Eq. (9). The latter is addressed by using a standard Lagrange multiplier method. For brevity, the
 273 related technical details are not discussed here, see [39].

274 The model is transformed into a finite-element code using the automatic differentiation tool
 275 AceGen [58, 59], thanks to which the residual vector and the tangent matrix are derived automat-
 276 ically, and thereby, the quadratic convergence of the Newton method is ensured. The simulations
 277 are carried out in the finite-element environment AceFEM.

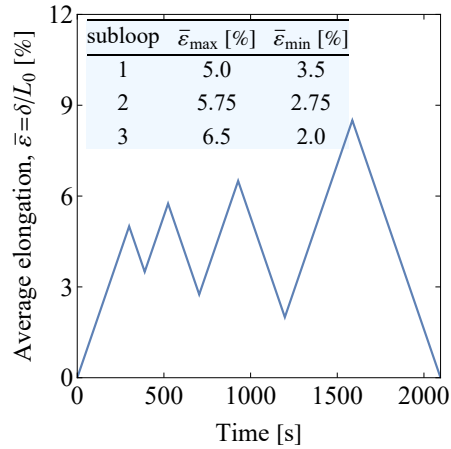
3. Simulations

278 This section is devoted to the analysis of the simulation results. Section 3.1 begins with a
 279 presentation of the simulation setup and calibration of the model parameters, and concludes with
 280 a brief discussion on the results for NiTi wire under full loading–unloading cycles. Our main
 281 modeling study concerns a NiTi specimen subjected to uniaxial tension with subloop loading paths.
 282 Two scenarios are explored. First, in line with the experimental study of Tobushi et al. [24], the
 283 subloop deformation behavior of a NiTi wire is analyzed, see Section 3.2. The loading program in
 284 this scenario encompasses three nested subloops with increasing strain amplitudes, as depicted in
 285 Fig. 3(a). As shown later, this setup enables us to reproduce neatly the hierarchical return-point
 286 memory. Section 3.2 concludes with a supplementary analysis of the TRIP evolution under a large
 287 number of subloops. Next, in Section 3.3, we extend our analysis to a NiTi strip, where we elucidate
 288 how the subloop behavior is influenced by the complexity of the pattern of propagating instabilities.
 289 This scenario is then examined under two additional loading programs, see Fig. 3(b,c).

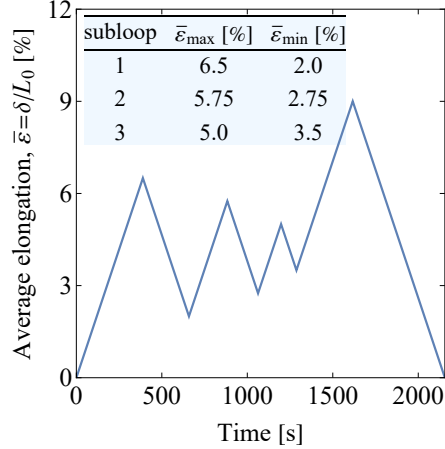
3.1. Preliminaries

290 In all simulations, the loading is exerted in a displacement-control mode at a (constant) low
 291 strain rate of $1.67 \times 10^{-4} \text{ s}^{-1}$. The NiTi wire has a diameter of 0.75 mm and a total length of
 292 $L_0 = 20$ mm. To facilitate this analysis, the wire is justifiably reduced to a 2D axisymmetric
 293 geometry. The corresponding 2D problem is then discretized by a uniform finite-element mesh
 294 consisting of equiaxed elements with an edge size of 0.01 mm. This resulted in 76 000 elements
 295 and approximately 620 000 degrees of freedom. Meanwhile, the NiTi strip is treated as a full 3D
 296 problem. The strip has a thickness of 0.4 mm, a width of 10 mm and a total length of $L_0 = 100$ mm.
 297 It is discretized by a uniform mesh consisting of elements with an in-plane edge size of 0.2 mm and
 298 a through-thickness size of 0.4 mm (i.e., only one element is used through the thickness). This
 299 mesh led to 25 000 elements and nearly 640 000 degrees of freedom. In both problems, the following
 300 boundary conditions are imposed. The displacements at the bottom edge of the specimen are fully
 301 constrained. At the top edge, the axial displacement δ is prescribed and the lateral displacements
 302 are constrained. At the same time, the temperature at both top and bottom edges is set equal to the
 303 ambient temperature, i.e., $T = T_0 = 353$ K, which is the actual ambient temperature maintained
 304 during the experiment [24]. Finally, the heat convection effect is neglected.

(a) Loading program 1



(b) Loading program 2



(c) Loading program 3

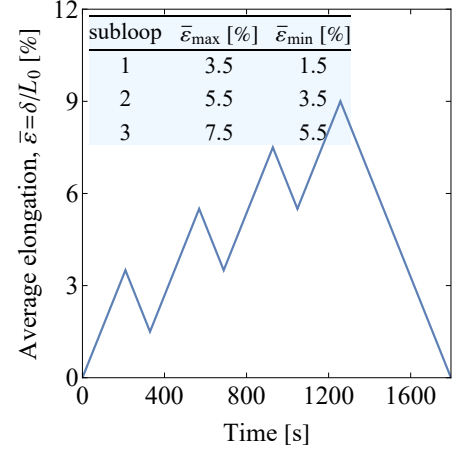


Figure 3: The loading programs used in the simulations. All loading programs represent displacement-control uniaxial tension (with a low strain rate of $1.67 \times 10^{-4} \text{ s}^{-1}$) and incorporate three subloops. Loading program 1 consists of three nested subloops with increasing strain amplitudes. Loading program 2 employs subloops in a reverse order compared to loading program 1. Loading program 3 consists of three equally-spaced subloops with a constant strain amplitude.

305 The model parameters adopted in the simulations are summarized in Tab. 1. Except for the
 306 gradient energy parameter G , all the model parameters are identical in the wire and strip problems.
 307 The parameter G sets the length-scale associated with the phase transformation front and can be
 308 linked to the geometry and micromechanical characteristics [60, 61]. Thus, G takes different values
 309 in each problem. To calibrate G , first, an assumption ought to be made regarding the theoretical
 310 thickness of the macroscopic interface, λ . Subsequently, G is determined through the analytical
 311 relation $G = -H_{\text{int}}\lambda^2/\pi^2$, which is derived from the solution of the 1D small-strain model of
 312 pseudoelasticity [40]. The identification procedure for the remaining model parameters which are
 313 unrelated to TRIP has been thoroughly discussed in our recent study [43], see Section 2.3 and
 314 Appendix E therein, and is not repeated here.

315 Identification of some TRIP-related parameters is guided by the indications obtained from the
 316 structural stress–strain response from the experiment, see Fig. 1(a). These include the significant
 317 decrease in the level of the upper stress plateau during the hierarchical subloop deformation and
 318 the value of the residual strain at the end of the experiment. Accordingly, the parameters $A_{\text{deg}} =$
 319 -45 MPa , $\epsilon_{\text{r}}^{\text{sat}} = 0.4\epsilon_{\text{T}} = 2.4\%$ (recall that ϵ_{T} denotes the maximum transformation strain, Eq. (12))
 320 and $C_{\text{p}} = 0.05$ have been calibrated to produce similar effects. We, however, acknowledge that there
 321 exists a degree of uncertainty in the identification of the remaining parameters, for which we lack
 322 definitive experimental evidence. With this in mind, the parameters $H_{\text{deg}} = 40 \text{ MPa}$, $f_{\text{c}}^{\text{fin}} = 2 \text{ MPa}$,
 323 $C_{\text{f}} = C_{\text{p}} = 0.05$ and $h_{\text{ir}}^{\text{sat}} = 0.4$ are selected such that the changes in the stress–strain response
 324 under a large number of loading cycles (in particular, as it concerns the transition to a hardening-
 325 type response, decrease in the hysteresis loop area and decrease in the extent of the transformation
 326 strain) align with the trends observed in the experiments, e.g., [47, 62–64], see also the discussion
 327 below. The intrinsic response of the model resulting from the adopted parameters is illustrated in
 328 Fig. 2.

Table 1: Model parameters adopted in the simulations.

Category	Parameter	Value	
Elasticity	κ	Bulk modulus	130 GPa
	μ_a	Shear modulus for austenite	21 GPa
	μ_m	Shear modulus for martensite	9 GPa
Martensitic phase transformation	Δs^*	Specific entropy difference	0.24 MPa/K
	T_t	Transformation equilibrium temperature	222 K
	f_c^{ini}	Hysteresis loop parameter (initial)	10 MPa
	H_{int}	Austenite–martensite interaction parameter	-10.5 MPa
	ϵ_T	Maximum tensile transformation strain	6%
	α	Tension–compression asymmetry ratio	1.4
	β	Transverse isotropy parameter	1.0
Macroscopic transformation front	G	Gradient energy parameter (wire problem)	0.04 MPa mm ²
	G	Gradient energy parameter (strip problem)	0.4 MPa mm ²
	χ	Micromorphic regularization parameter	100 MPa
Heat transfer	$\rho_0 c$	Specific heat	2.86 MJ/(m ³ K)
	K	Heat conductivity	18 W/(m K)
TRIP	A_{deg}	Pseudoelasticity degradation parameter	-45 MPa
	H_{deg}	Pseudoelasticity degradation parameter	40 MPa
	ϵ_p^{sat}	Saturated permanent strain	0.4 $\epsilon_T = 2.4\%$
	$h_{\text{ir}}^{\text{sat}}$	Saturated irreversible volume fraction	0.4
	f_c^{fin}	Hysteresis loop parameter (final)	2 MPa
	C_p	Degradation rate	0.05
	C_f	Hysteresis loop degradation rate	0.05

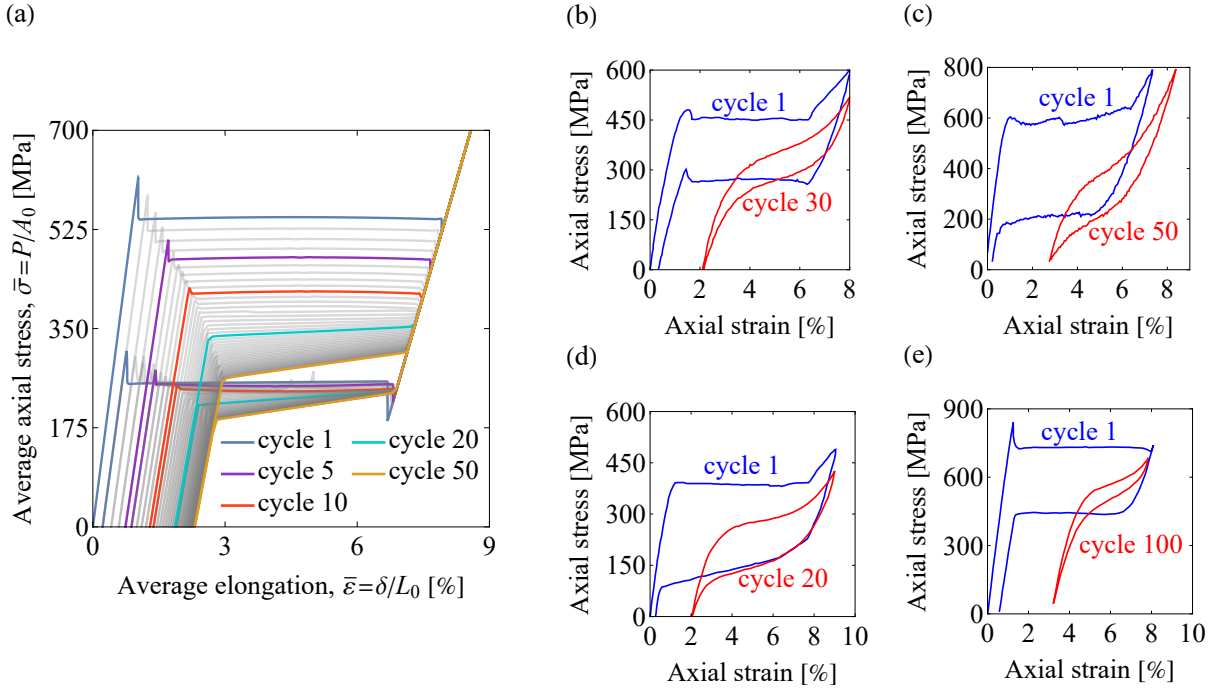


Figure 4: (a) NiTi wire subjected to 50 loading–unloading cycles of uniaxial tension: structural stress–elongation ($\bar{\sigma}$ – $\bar{\epsilon}$) response. The average axial stress $\bar{\sigma}$ and the average elongation $\bar{\epsilon}$ are calculated, respectively, as the reaction force P divided by the initial cross-section area A_0 , and the axial displacement δ divided by the initial length L_0 . The intrinsic responses associated with these structural responses are illustrated in Fig. 2. (b)–(e) Typical cyclic responses of NiTi specimens observed in the experiments, taken from (b) Wang et al. [47], (c) Morin et al. [62], (d) Kan et al. [63], and (e) Sittner et al. [64].

329 It is worth noting that in all the simulations, as a way to trigger the phase transformation
 330 instability, a geometric imperfection in the form of a slight indent is applied to the specimen. The
 331 indent is located at a distance equal to the diameter/width of the wire/strip from its lower end.

332 Before entering into the main analysis of subloop deformation, a simulation is performed for
 333 the NiTi wire subjected to 50 loading–unloading cycles of uniaxial tension. Fig. 4 illustrates the
 334 structural response of the wire. Here, as well as in the figures in the following subsections, the
 335 structural response is represented in terms of the average axial stress $\bar{\sigma} = P/A_0$ versus average
 336 elongation (engineering strain) $\bar{\epsilon} = \delta/L_0$, where P denotes the reaction force and A_0 denotes the
 337 initial cross-section area. Recall that δ and L_0 are the axial displacement and the initial length,
 338 respectively. As it is evident in the structural response, the wire undergoes a complete phase
 339 transformation within each cycle. Initially, the wire exhibits a localized phase transformation,
 340 characterized by a stress drop at the transformation onset and a subsequent stress plateau. The
 341 localized transformation persists for about 15 cycles. Thereafter, the transformation proceeds in a
 342 more homogeneous manner, and the structural response displays a mild hardening. As the number
 343 of cycles increases, the slope of the hardening branch also increases. The cyclic behavior captured
 344 in the simulation is in a qualitative agreement with the typical cyclic behavior of NiTi specimens
 345 observed in experiments [47, 62–64], which underscores the reliability of the simulation results.

3.2. NiTi wire subjected to subloop deformation

346 The results pertaining to the subloop behavior of the NiTi wire are presented in Figs. 5 and 6.
347 The phase transformation evolution in Fig. 5(a) and TRIP evolution in Fig. 5(b) are displayed via,
348 respectively, the distribution of the reversible volume fraction η^{rev} and irreversible volume fraction
349 η^{ir} . Note that, for a more natural visualization, the results of the 2D axisymmetric wire are post-
350 processed and presented in a 3D configuration. As anticipated, the transformation initiates at the
351 position of the geometric imperfection. Throughout the entire loading stage of the global cycle
352 (hereinafter, to avoid confusion with the subloops, we use the term ‘global’), the transformation
353 maintains a single propagating front. Interestingly, while the front appears to be a flat (and visibly
354 diffuse) interface in the 3D-wire configuration, e.g., [65], it takes on a spherical-shaped appearance
355 (or ‘cone-shaped’ as described in [60, 66]), as can be conceived from the corresponding pattern in the
356 axisymmetric planes (not shown here). During the global unloading, the backward transformation
357 commences from the wire’s central part. As shown in Fig. 5(b) and discussed below, the highest
358 amount of irreversible volume fraction η^{ir} , thus the highest TRIP, is accumulated within the central
359 part, making it a favorable site for the nucleation of the austenitic band. At the same time, due to
360 a slight asymmetry in the distribution of η^{ir} with respect to the wire’s midpoint, the two evolved
361 fronts do not propagate concurrently. More specifically, the top front reaches the boundary first
362 and annihilates, which manifests as an abrupt stress rise in the structural stress-elongation ($\bar{\sigma}$ - $\bar{\varepsilon}$)
363 response, occurring at an average elongation of about $\bar{\varepsilon} = 4\%$ (see Fig. 6). Subsequently, the bottom
364 front follows suit.

365 Within each subloop path, the front retreats downward during unloading and advances upward
366 during reloading. This cyclic movement prompts the material points inside the front’s sweeping
367 zone to undergo backward-then-forward transformation, and thereby, gives rise to the accumulation
368 of TRIP within the sweeping zone, while the material points beyond it remain unaffected. Note that
369 the loading program adheres to a fixed nominal mean strain (set at $\bar{\varepsilon} = 4.5\%$, which corresponds
370 to the front’s proximity to the wire’s midpoint) but an increasing strain amplitude, see Fig. 3(a).
371 Thus, the sweeping zone expands successively from subloop 1 to subloop 3, and at the same time,
372 the sweeping zone of each subloop encompasses that of the previous one. This therefore results in
373 the highest concentration of TRIP within the central part of the wire and its step-wise decreasing
374 trend as it moves away from it, as can be clearly seen in Fig. 5(b).

375 The hierarchical return-point memory, which is an outcome of the cyclic traversal of the front
376 across the boundaries of the sweeping zones, is correctly reproduced in the structural stress-
377 elongation response in Fig. 6. The reproduced feature is in a reasonable agreement with the
378 experimental result of Tobushi et al. [24], see Fig. 1 and the accompanying discussion. In view
379 of the exponential nature of the pseudoelasticity degradation effects, the reduction in the level of
380 the upper stress plateau is at the highest within the first level of hierarchy (of about $\Delta\bar{\sigma} = 21$
381 MPa) and diminishes to its lowest within the last level of hierarchy (of about $\Delta\bar{\sigma} = 17$ MPa). It is
382 worth noting that in this scenario, where the strain rate corresponds to nearly isothermal conditions
383 (i.e., the temperature variation lies within the range of -2 K to 2 K), the stress, upon reaching
384 the return-point, appears to catch up closely with the corresponding stress plateau before applying
385 the subloop. As shown in Section 3.3 and also observed in the experiments [25, 26], such a close
386 catching up does not occur when thermal effects are at play.

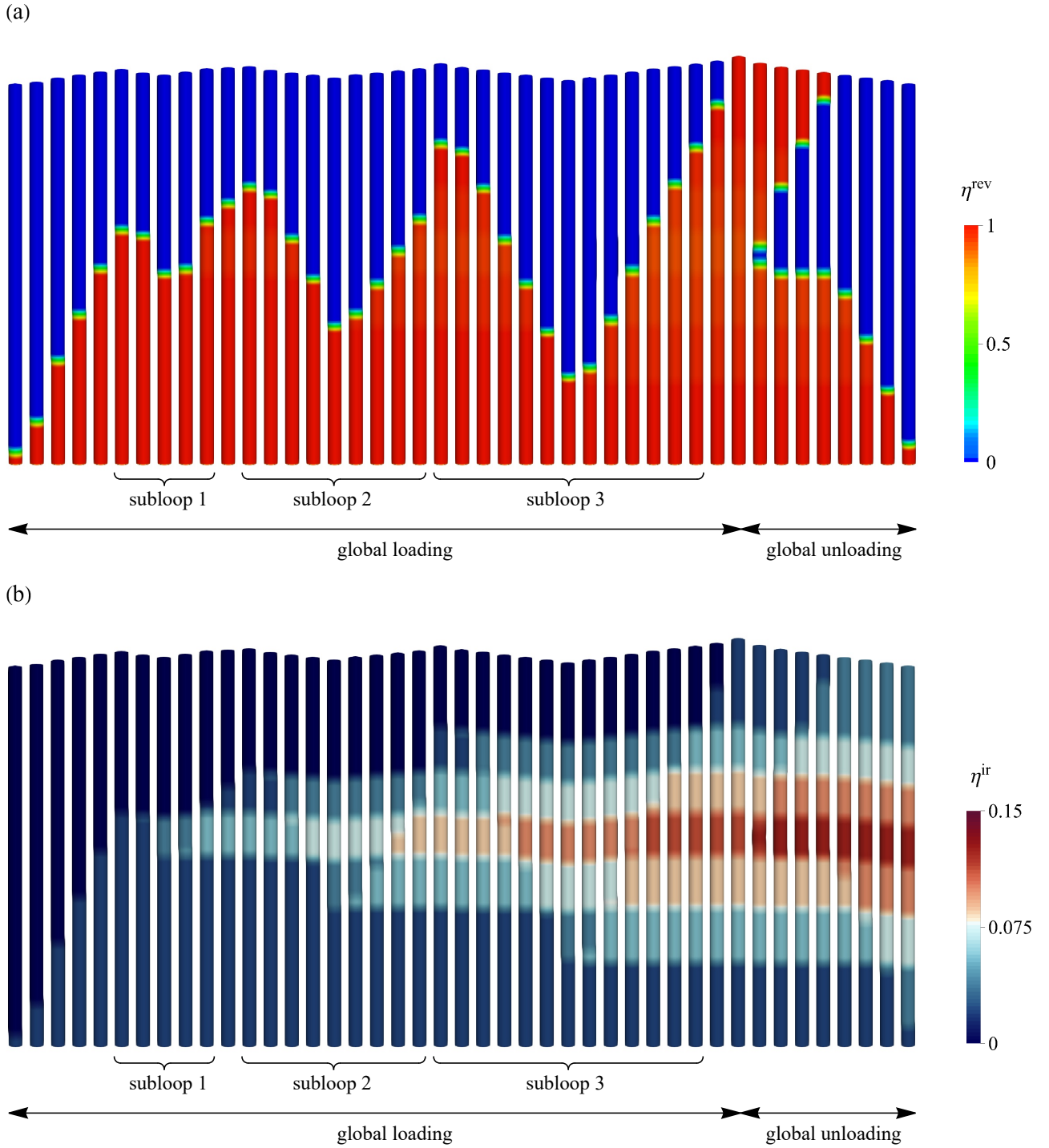


Figure 5: NiTi wire subjected to loading program 1: (a) snapshots of reversible volume fraction η^{rev} illustrating the phase transformation evolution, and (b) snapshots of irreversible volume fraction η^{ir} illustrating the TRIP evolution. For a natural visualization, the axisymmetric wire is presented in full 3D configuration.

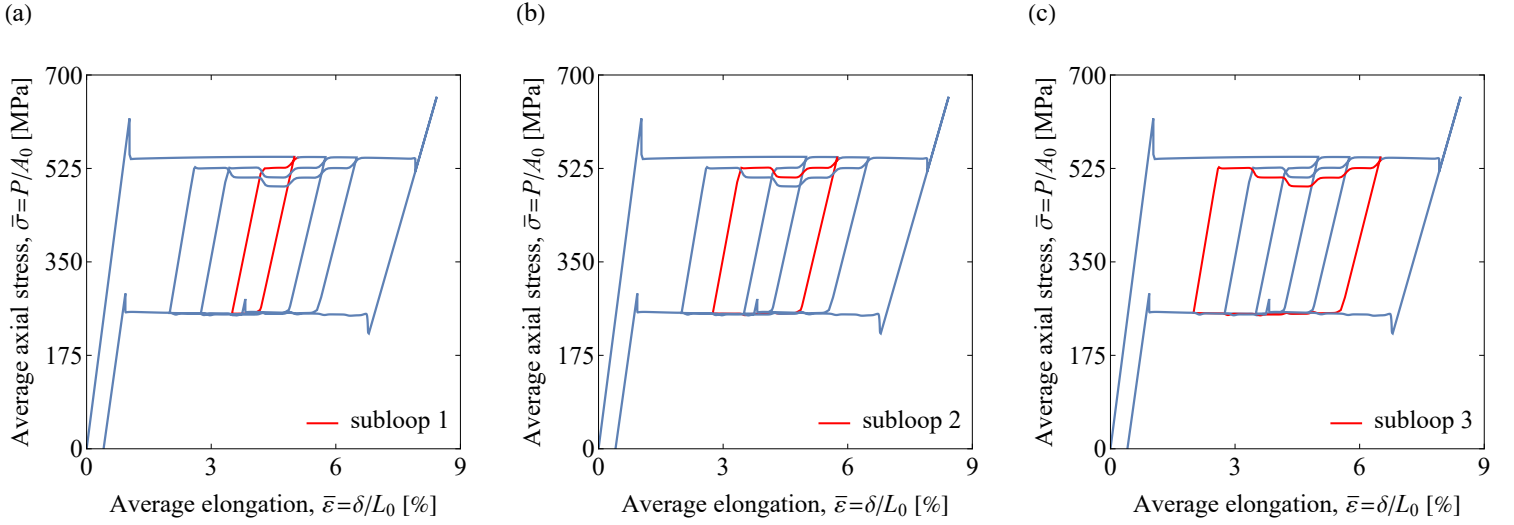


Figure 6: NiTi wire subjected to loading program 1: structural stress–elongation ($\bar{\sigma}$ – $\bar{\epsilon}$) response.

387 A notable observation from the experimental curve in Fig. 1(a) is the absence of the return-point
 388 memory during the unloading stages of the subloops. Instead, the lower stress plateau seems to
 389 shift slightly downward from one subloop to the next. Anyway, no attempt was made to adjust the
 390 material parameters to replicate the observed behavior, which is, however, present in the results of
 391 NiTi strip reported in Section 3.3.

392 In concluding the discussion in this section, we present the results of a supplementary analysis
 393 on the NiTi wire subjected to 12 subloops. The aim of this analysis is to illustrate the evolution
 394 of TRIP and subloop deformation behavior over a large number of subloops. The results, as
 395 depicted in Fig. 7, follow an expected trend. However, two specific observations deserve further
 396 comment. Firstly, the stress plateau in a number of subloops exhibits irregularities, specifically a
 397 second stress drop appears ahead of the return-point memory. This is because in these subloops
 398 the transformation during subloop reloading does not proceed by the propagation of the existing
 399 front. Instead, a second front emerges at the opposite end of the sweeping zone and eventually
 400 merges with the original front, thereby, leading to the observed effects. Secondly, as shown in
 401 Fig. 7(b), the sweeping zone continuously expands from one subloop to the next. This is explained
 402 by the accumulation of TRIP within the sweeping zone, which reduces the amount of transformable
 403 martensite. Consequently, since the applied strain amplitude of the subloops is held fixed, the front
 404 gradually moves towards the untransformed segments of the wire to compensate for the reduced
 405 transformation.

3.3. NiTi strip subjected to subloop deformation

406 We begin this section by analyzing the NiTi strip under loading program 1. The primary aim is
 407 to examine the subloop behavior in a notably more involved scenario than the NiTi wire discussed
 408 earlier, arising mainly from a more complex transformation pattern and heightened thermal effects.
 409 The simulation results are presented in Figs. 8 and 9. A quick look at Fig. 9 immediately indicates
 410 that the return-point memory is only observable in the trajectories that lead to the global stress
 411 plateau, while the hierarchical return-point memory is lost. This is undoubtedly an outcome of

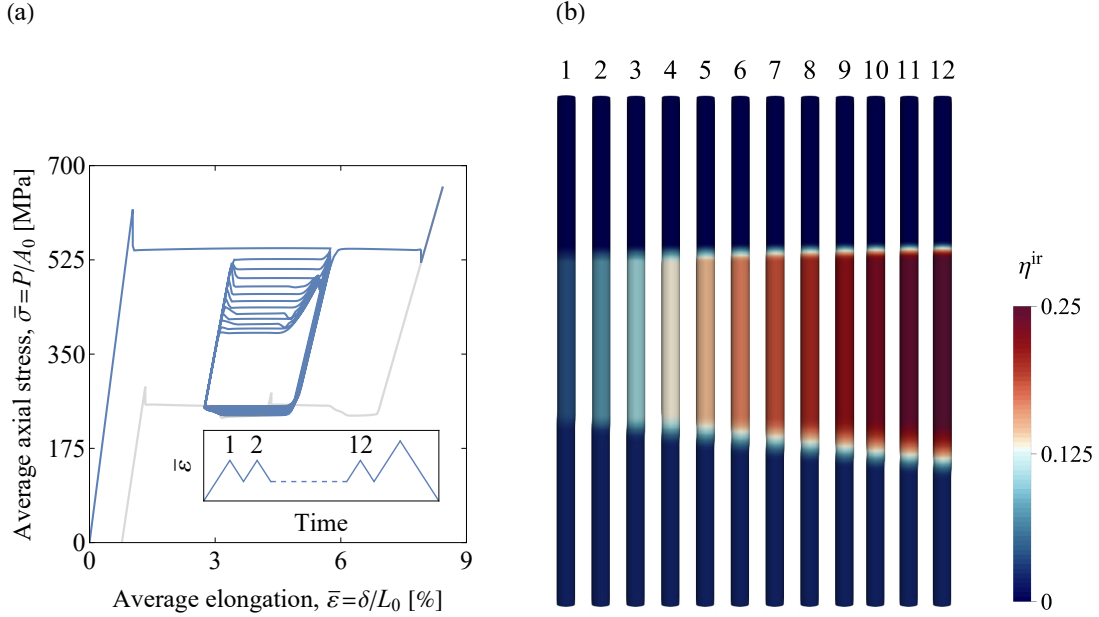


Figure 7: NiTi wire subjected to uniaxial tension with 12 subloop paths: (a) structural stress–elongation ($\bar{\sigma}$ – $\bar{\epsilon}$) response, and (b) snapshots of irreversible volume fraction η^{ir} illustrating the TRIP evolution at the end of each subloop. The inset in panel (a) represents the loading program used for this simulation. The applied subloops have the same mean strain and the same strain amplitude, i.e., $\bar{\epsilon}_{\max} = 5.75\%$ and $\bar{\epsilon}_{\min} = 2.75\%$.

412 the nontrivial pattern of phase transformation and resulting TRIP distribution within the strip.
 413 In contrast to the NiTi wire, where a single phase transformation front remained active during
 414 all subloops, the strip features multiple transformation fronts, each presenting a less predictable
 415 pattern of activation. Below, we provide a more detailed account of the unfolding events.

416 The phase transformation initiates with the nucleation of a single martensite band at the location
 417 of the geometric imperfection. The band is oriented at approximately 54° with respect to the
 418 longitudinal axis, in agreement with the experimental observations [14] and theoretical analysis
 419 [67], and somewhat changes as loading progresses. At an average elongation of about $\bar{\epsilon} = 3\%$,
 420 another martensite band emerges at the opposite end, and henceforth, the two transformation
 421 fronts propagate towards each other. This non-synchronous double nucleation has been commonly
 422 observed in the experiment of NiTi specimens at relatively low strain rates, e.g., [14, 68, 69].
 423 Within subloop 1, the two fronts exhibit a short back-and-forth movement, manifesting a clear
 424 return-point memory in the structural stress–elongation response in Fig. 9(a). During subloop
 425 2, not only the hitherto active fronts but also the fronts near the boundaries become engaged in
 426 the transformation evolution. As a consequence, TRIP is induced via all fronts. This behavior is
 427 reflected in the structural response which takes on an irregular appearance characterized by few
 428 sudden stress changes, thus spoiling the return-point memory in the inner part (Fig. 9(b)). A
 429 similar process recurs within subloop 3, albeit with a more complex phase transformation evolution
 430 during the reloading stage and also more distinct stress events in the structural response. During the
 431 global unloading, the backward transformation proceeds predominantly in a criss-cross mode, which
 432 persists until an average elongation of about $\bar{\epsilon} = 3\%$. Subsequently, the fronts reconfigure into sharp
 433 inclined interfaces that move towards each other until the complete annihilation of the (reversible)

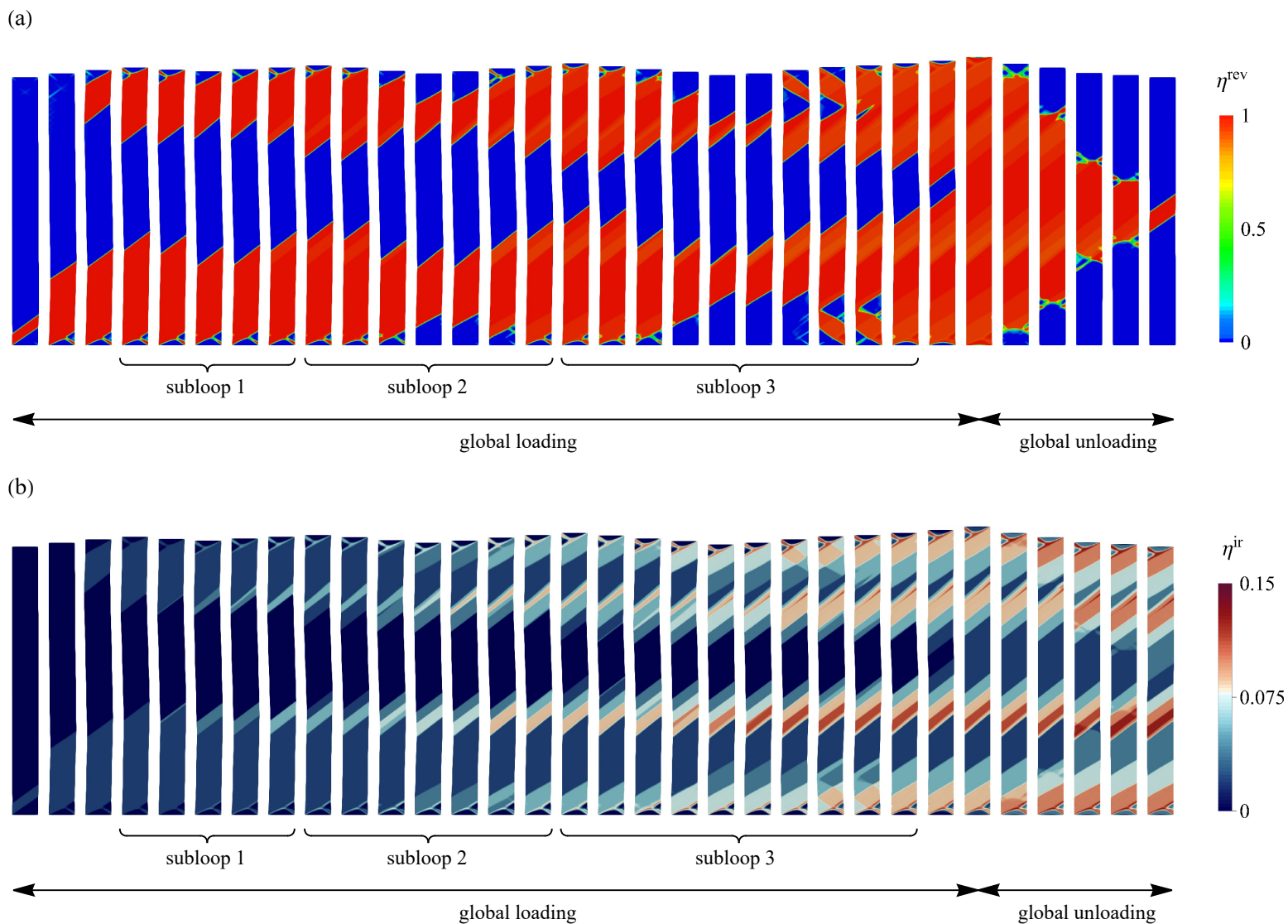


Figure 8: NiTi strip subjected to loading program 1: (a) snapshots of reversible volume fraction η^{rev} illustrating the phase transformation evolution, and (b) snapshots of irreversible volume fraction η^{ir} illustrating the TRIP evolution.

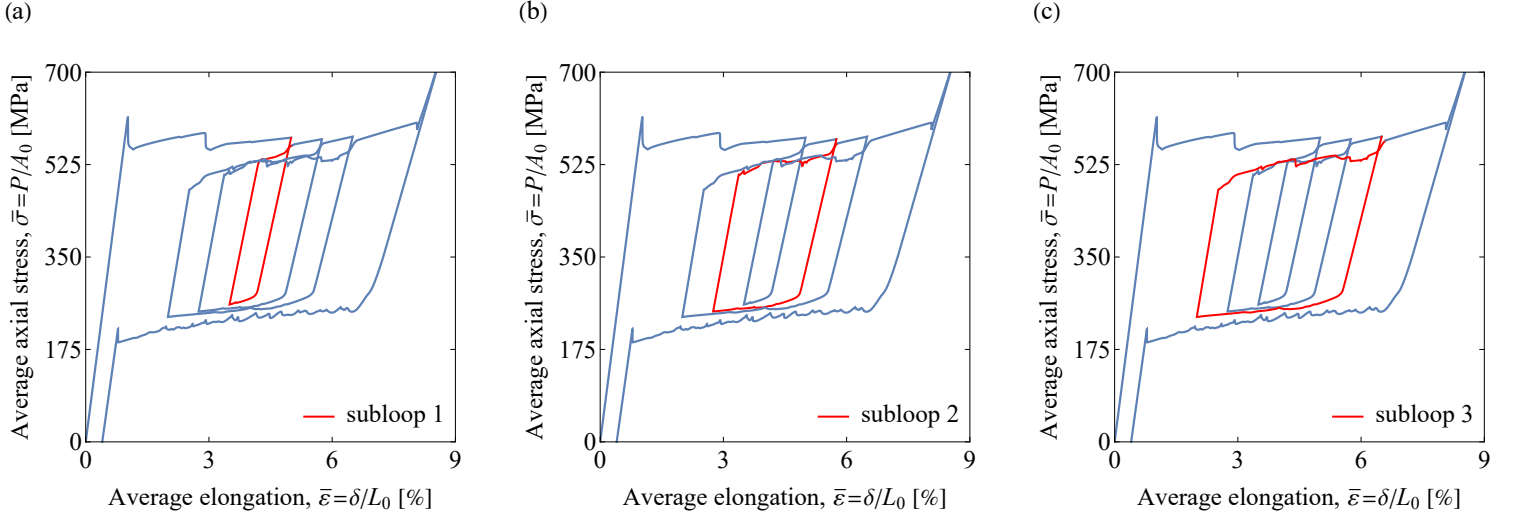


Figure 9: NiTi strip subjected to loading program 1: structural stress–elongation ($\bar{\sigma}$ – $\bar{\epsilon}$) response.

434 martensite domain. The reconfiguration of the fronts between criss-cross mode and sharp interfaces
 435 has been also observed in experimental and previous modeling studies, e.g., [36, 70, 71]. It is worth
 436 remarking that the distribution of the irreversible volume fraction η^{ir} within the entire strip at the
 437 end of the global unloading remains consistent with that at the end of the global loading, while its
 438 magnitude increases uniformly.

439 Upon inspecting the return-point memory in Fig. 9, a slight difference can be noticed concerning
 440 the level of the global stress plateau before and after a subloop path. This difference stems from the
 441 thermal effects. Specifically, compared to the NiTi wire, a more pronounced temperature variation
 442 is produced across the specimen during the forward transformation (for instance, of about 10 K
 443 immediately before subloop 1), resulting in a more visible thermal hardening that sustains a higher
 444 stress for the propagation of the front. Within the subloop path, the transformation latent heat is
 445 initially absorbed during the backward transformation (self-cooling) and is subsequently released
 446 when the forward transformation resumes (self-heating). Accordingly, as the front reaches the pris-
 447 tine material, the temperature variation across the specimen is reduced compared to the state before
 448 the subloop (for instance, of about 5 K immediately after subloop 1). Thereby, thermal hardening
 449 diminishes, necessitating a lower stress for interface propagation. Note also that as a result of the
 450 cyclic transformation of the material points, and thus the accumulation of irreversible martensite,
 451 a smaller martensite volume fraction is transformed during the subloop reloading compared to the
 452 state before the subloop, and this contributes to the reduction of the latent heat generation [20],
 453 see Eq. (28).

454 We now proceed with the analysis of the NiTi strip under two additional loading programs, one
 455 consisting of nested subloops with decreasing strain amplitudes, i.e., subloops are applied in a reverse
 456 order compared to loading program 1, and the other consisting of three equally-spaced distinct
 457 subloops with a constant strain amplitude, see Fig. 3(b,c). The corresponding results are shown in
 458 Figs. 10, 11 and 12. The comparison of the snapshots of the reversible volume fraction η^{rev} in the two
 459 additional cases to those of loading program 1 reveals noticeable morphological differences, which are

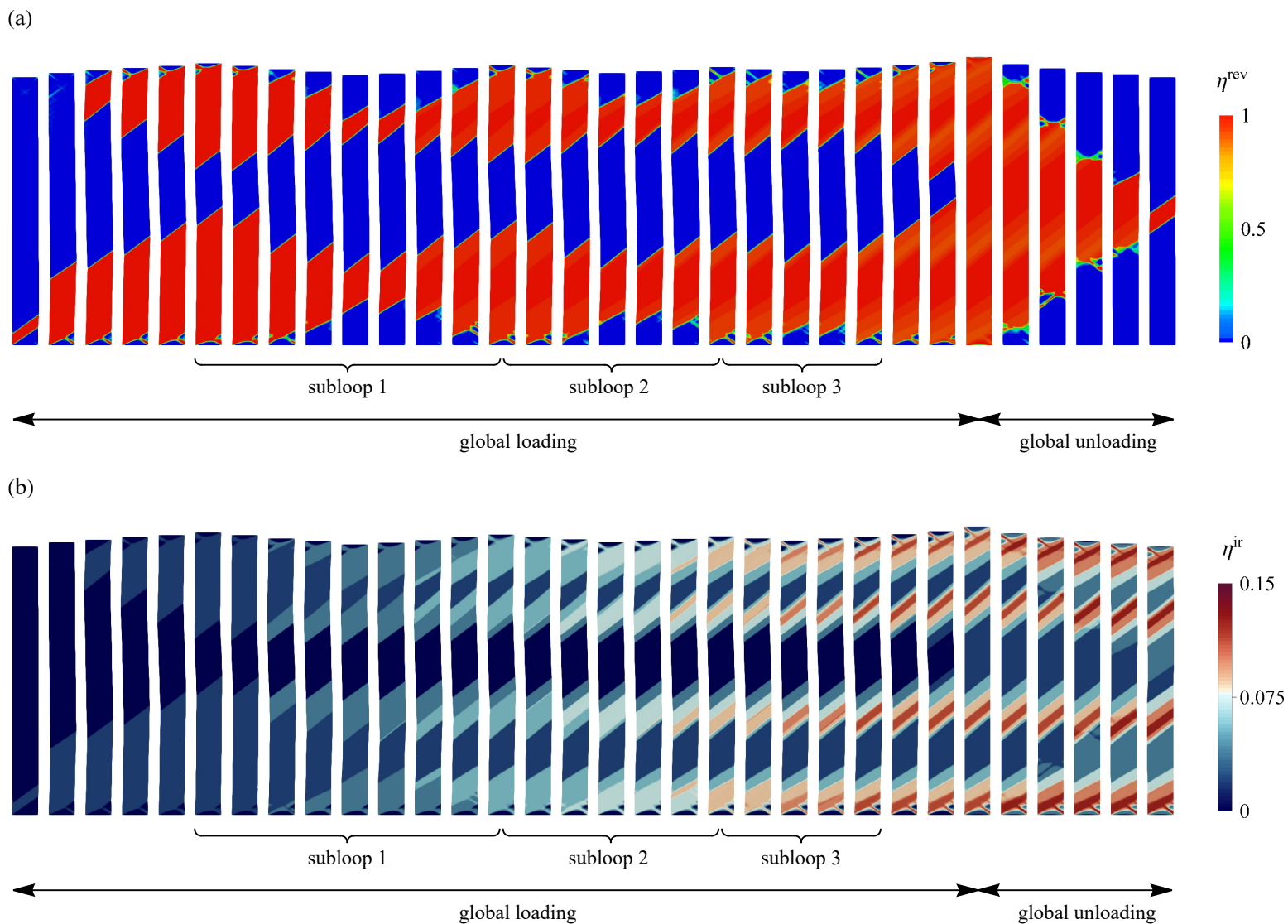


Figure 10: NiTi strip subjected to loading program 2: (a) snapshots of reversible volume fraction η^{rev} illustrating the phase transformation evolution, and (b) snapshots of irreversible volume fraction η^{ir} illustrating the TRIP evolution.

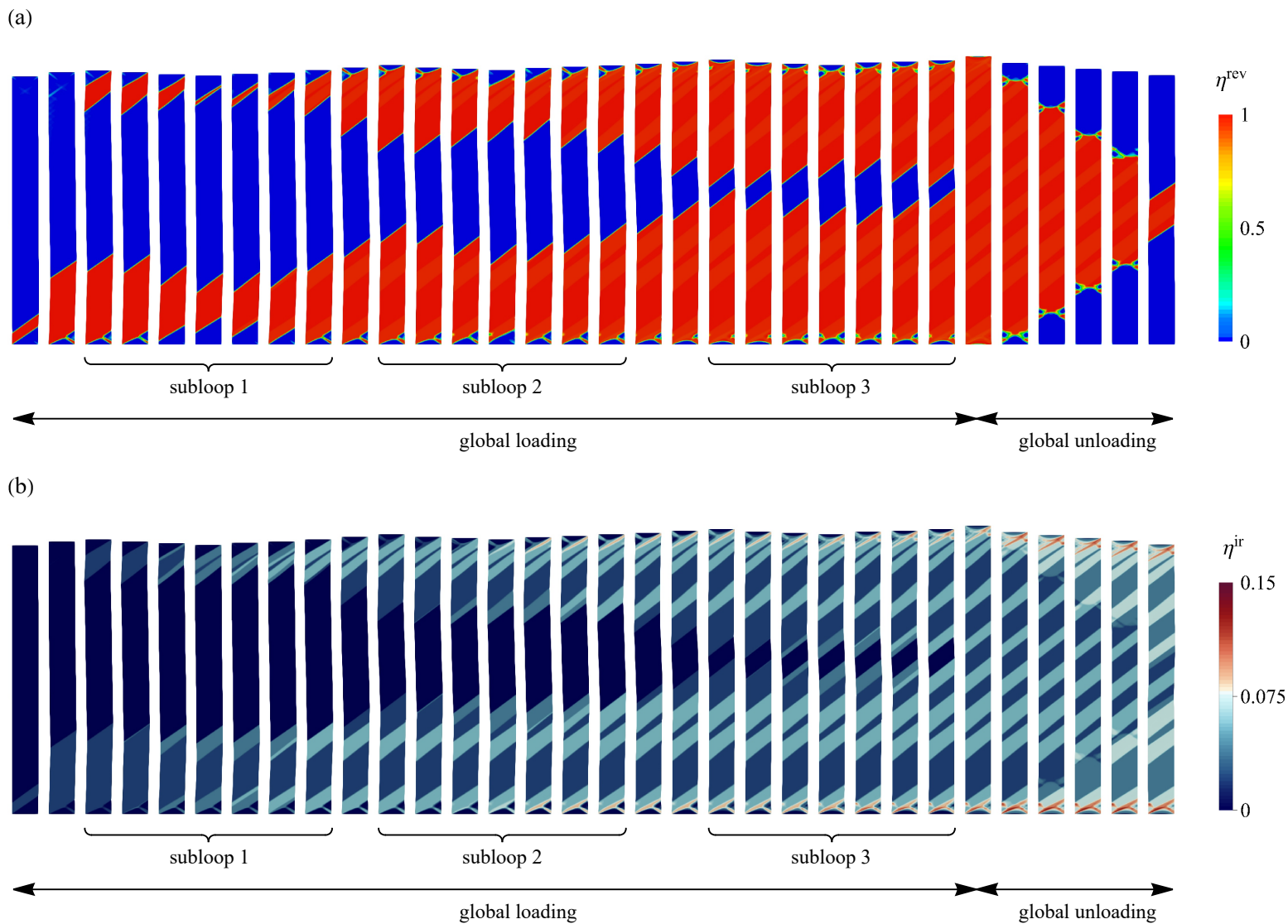


Figure 11: NiTi strip subjected to loading program 3: (a) snapshots of reversible volume fraction η^{rev} illustrating the phase transformation evolution, and (b) snapshots of irreversible volume fraction η^{ir} illustrating the TRIP evolution.

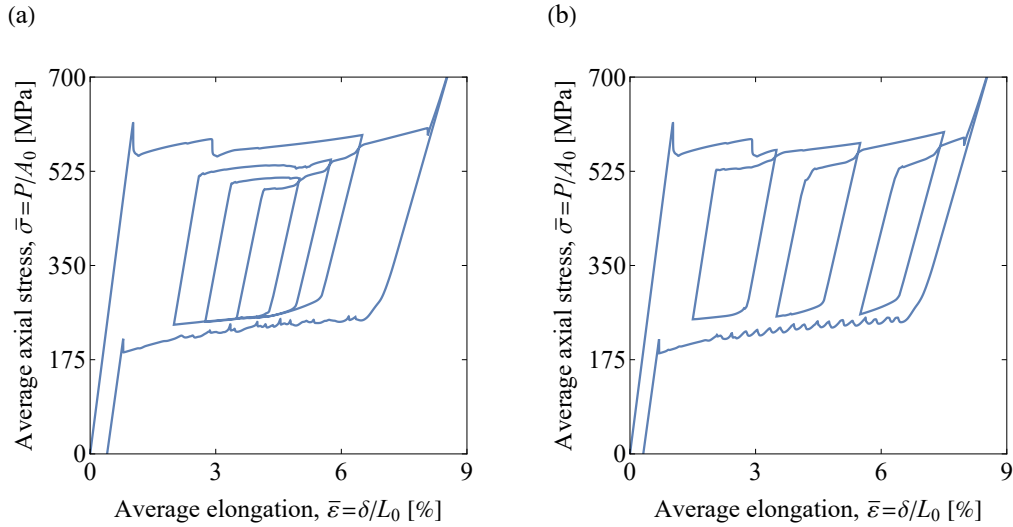


Figure 12: Structural stress–elongation ($\bar{\sigma}$ – $\bar{\varepsilon}$) response of NiTi strip subjected to (a) loading program 2 and (b) loading program 3.

460 beyond the differences arising solely from the loading-dependent transformation evolution pathways.
 461 The differences mainly concern the varying number of martensite domains formed during the global
 462 loading stage and the activation pattern of the fronts within the subloops. More specifically, unlike
 463 loading program 1, loading programs 2 and 3 exhibit only two martensite domains during the global
 464 loading. In loading program 2, all four fronts remain consistently active within all subloops, resulting
 465 in a clear demonstration of the hierarchical return-point memory in the stress–elongation response,
 466 as shown in Fig. 12(a). In loading program 3, however, while the involvement of the fronts near the
 467 boundaries is eye-catching within subloop 1, overall, the interior fronts are prominently active. In
 468 this case, the front sweeping zones in the subloops do not interact with each other (as can be also
 469 recognized from the snapshots of η^{ir} in Fig. 11), and the resulting subloops are independent, see
 470 Fig. 12(b). During the global unloading, all cases show a similar transformation evolution pattern
 471 characterized by two active fronts retracting in a criss-cross manner..

472 We conclude this discussion by addressing TRIP accumulation within the strip in relation to
 473 the loading program. Similar to the martensitic transformation, TRIP exhibits characteristics that
 474 are specific to the applied loading program. Given that loading programs 1 and 2 have a reverse
 475 arrangement of the subloops but are otherwise identical, one would intuitively expect that the
 476 resulting TRIP accumulations, in terms of both the pattern and the intensity, would be the same
 477 after applying all the three subloops. A comparison of the snapshots of the irreversible volume
 478 fraction η^{ir} (Figs. 8 and 10) indeed confirms that TRIP hotspots in these two cases are located in
 479 nearly the same regions, with two hotspots near the boundaries and two within the interior of the
 480 strip, corresponding to the regions with the highest activity of the fronts. Yet, minor discrepancies
 481 can be observed, particularly concerning the intensity of TRIP within the hotspot regions. On the
 482 other hand, loading program 3 demonstrates a rather distinct TRIP accumulation characterized by
 483 several regions with mild intensity within the interior and localized hotspots near the boundaries.
 484 As previously noted, this particular TRIP distribution results from the lack of interaction among
 485 the fronts sweeping zones of the independent subloops. As a summary of this discussion, Fig 13

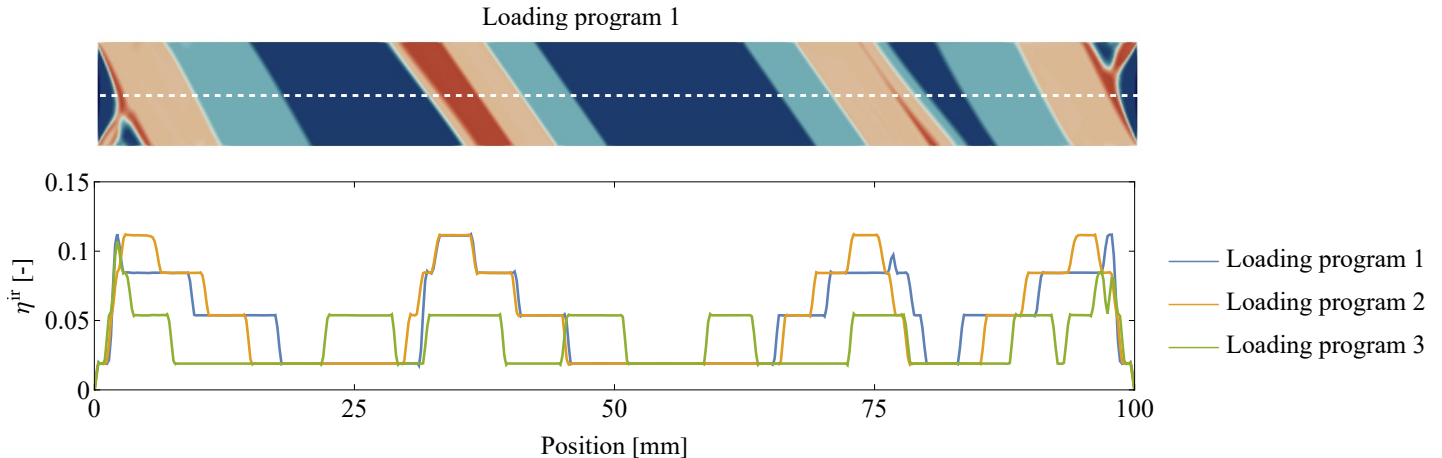


Figure 13: Distribution of the irreversible volume fraction η^{ir} along the entire length of the strip (taken in the reference configuration) at the end of the global loading stage. The graphs correspond to the midsection of the strip, as indicated by the white dashed curve overlaid on the snapshot.

486 compares the distribution of η^{ir} along the entire length of the strip for various loading programs.

4. Conclusions

487 The phenomenon of return-point memory that appears during the subloop deformation of pseudoelastic SMA is an outcome of the interaction between the structural instabilities of phase transformation and the degradation of functional properties. It seems that this crucial aspect has been
 488 generally overlooked in existing modeling approaches. The goal of our study is to demonstrate this
 489 structure–material interaction by modeling the phenomenon of return-point memory. To achieve
 490 this, we have developed a gradient-enhanced model of pseudoelasticity. The developed model represents an advancement over previous versions [39–41], extending the constitutive description to
 491 incorporate pseudoelasticity degradation. The capabilities of the model in reproducing the essential aspects of pseudoelasticity degradation have been shown for NiTi under cyclic uniaxial tension.
 492

493 We examine an illustrative example of a NiTi wire subjected to nearly isothermal uniaxial tension with nested subloops. The obtained results clearly correlate with the experimental observations of
 494 Tobushi et al. [24], especially regarding the hierarchical return-point memory. The accumulation
 495 of TRIP and its distribution during subloop deformation underline the intertwined evolution of
 496 inhomogeneous phase transformation and cyclic degradation.
 497

501 The study is then extended to a more involved scenario of a NiTi strip, where a detailed analysis is performed by examining three different loading programs. The impact of the loading program on
 502 the evolution of phase transformation and TRIP has been highlighted through the activation pattern of phase transformation fronts within the subloops, and its implications on the phenomenon
 503 of return-point memory have been pointed out. In addition, the results hint at the visible contribution of the thermomechanical coupling effects within the subloops, stemming from the self-cooling/heating process of the transforming material.
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Appendix A. A simplified 1D demonstration of the model

519 In this appendix, we derive the governing equation of the transformation stress for a simplified
 520 isothermal 1D model. In 1D setting, the model features four variables, namely the total strain
 521 $\varepsilon = \nabla u$, the reversible volume fraction η^{rev} , the irreversible volume fraction η^{ir} and the permanent
 522 strain ε^{P} . The Helmholtz free energy is thus expressed as follows

$$\phi(\varepsilon, \varepsilon^{\text{P}}, \eta^{\text{rev}}, \eta^{\text{ir}}) = \phi_{\text{chem}}(\eta^{\text{rev}}, \eta^{\text{ir}}) + \phi_{\text{el}}(\varepsilon, \varepsilon^{\text{P}}, \eta^{\text{rev}}) + \phi_{\text{int}}(\eta^{\text{rev}}) + \phi_{\text{deg}}(\eta^{\text{rev}}, \eta^{\text{ir}}) + I(\eta^{\text{rev}}), \quad (\text{A.1})$$

523 where the indicator function I pertains to the inequality constraints on the reversible volume fraction
 524 η^{rev} ($I = 0$ if $0 \leq \eta^{\text{rev}} \leq 1 - \eta^{\text{ir}}$ and $I = \infty$ otherwise). Note that the gradient energy associated
 525 with the austenite–martensite diffuse interface, ϕ_{grad} , is disregarded here.

526 The elastic strain energy ϕ_{el} is formulated as

$$\phi_{\text{el}}(\varepsilon, \varepsilon^{\text{P}}, \eta^{\text{rev}}) = \frac{1}{2} E (\varepsilon - \varepsilon^{\text{t}} - \varepsilon^{\text{P}})^2, \quad \varepsilon^{\text{t}} = \eta^{\text{rev}} \varepsilon_{\text{T}}, \quad (\text{A.2})$$

527 where E is the Young's modulus (for simplicity, E is assumed constant and independent of η) and
 528 the constant ε_{T} is the maximum transformation strain. The remaining components of the free
 529 energy, as well as the dissipation potential, are identical to those of the general 3D model, see
 530 Eqs. (14), (16), (18) and Eq. (23). Moreover, the evolution equations for the permanent strain ε^{P}
 531 and the irreversible volume fraction η^{ir} are postulated as (cf. Eqs. (5)–(7))

$$\dot{\eta}^{\text{ir}} = h_{\text{ir}}^{\text{sat}} (1 - \exp(-C_{\text{p}} \eta^{\text{acc}})), \quad \dot{\varepsilon}^{\text{P}} = \varepsilon_{\text{p}}^{\text{sat}} (1 - \exp(-C_{\text{p}} \eta^{\text{acc}})). \quad (\text{A.3})$$

532 For a given total strain ε , the volume fraction η^{rev} can be determined by minimizing the local
 533 potential $\pi = \Delta\phi + \Delta D$, cf. Eq. (24). It is immediate to see that the local potential π is non-smooth,
 534 due to the presence of the rate-independent dissipation ΔD and the indicator function I . In line
 535 with [40], the minimization of π with respect to η^{rev} is written as a differential inclusion, given by

$$f_{\eta^{\text{rev}}} \in \partial_{\eta^{\text{rev}}} \bar{D}(\eta^{\text{rev}}, \eta^{\text{acc}}) \quad (\text{A.4})$$

536 where $\bar{D} = \Delta D + I$ encompasses the non-smooth components of π and $f_{\eta^{\text{rev}}}$ is the thermodynamic

537 driving force associated with η^{rev} and is expressed as

$$f_{\eta^{\text{rev}}} = - \left(\frac{\partial \phi}{\partial \eta^{\text{rev}}} + \frac{\partial \phi}{\partial \varepsilon^{\text{P}}} \frac{\partial \varepsilon^{\text{P}}}{\partial \eta^{\text{rev}}} + \frac{\partial \phi}{\partial \eta^{\text{ir}}} \frac{\partial \eta^{\text{ir}}}{\partial \eta^{\text{rev}}} \right). \quad (\text{A.5})$$

538 During the forward/backward transformation, i.e., when the bound constraints are inactive, the
539 inclusion (A.4) yields

$$f_{\eta^{\text{rev}}} = \pm f_c, \quad (\text{A.6})$$

540 and gives the following equation for the transformation stress σ_{\pm}^{t} (σ_+^{t} for the forward transformation
541 and σ_-^{t} for the backward transformation),

$$\sigma_{\pm}^{\text{t}} = \frac{\Delta \phi_0 k_1 \pm f_c + H_{\text{int}} \eta^{\text{rev}} + A_{\text{deg}} k_2 + H_{\text{deg}} \eta^{\text{rev}} k_3}{k_4}, \quad (\text{A.7})$$

542 where f_c is defined in Eq. (20) and k_i are expressed as

$$k_1 = 1 + \frac{\partial \eta^{\text{ir}}}{\partial \eta^{\text{rev}}}, \quad k_2 = \eta^{\text{ir}} + \eta^{\text{rev}} \frac{\partial \eta^{\text{ir}}}{\partial \eta^{\text{rev}}}, \quad k_3 = \eta^{\text{ir}} + \frac{1}{2} \eta^{\text{rev}} \frac{\partial \eta^{\text{ir}}}{\partial \eta^{\text{rev}}}, \quad k_4 = \epsilon_{\text{T}} + \frac{\partial \varepsilon^{\text{P}}}{\partial \eta^{\text{rev}}}. \quad (\text{A.8})$$

543 It is important to highlight that the necessary condition for the minimum of π with respect
544 to η^{rev} , which leads to the transformation criteria (A.7), is not computed in a standard manner.
545 This stems from the state-dependence of the dissipation potential D , i.e., the dependence of f_c on
546 the accumulated volume fraction η^{acc} , see Eq. (20). Having the minimization problem formulated
547 in rates (not shown here), it becomes apparent that f_c is treated as a constant when evaluating
548 the necessary condition for the rate $\dot{\eta}^{\text{rev}}$. In the incremental setting, to maintain consistency with
549 the rate-problem, the increment of the martensite volume fraction, $\Delta \eta^{\text{rev}}$, present in the current
550 unknown $\eta^{\text{rev}} = \Delta \eta^{\text{rev}} + \eta_n^{\text{rev}}$ is distinguished from the increment upon which the evolution equation
551 for f_c rely. Despite the two increments coincide, the latter is considered as constant when evaluating
552 the necessary condition. Accordingly, the minimization problem does possess the structure of a quasi-
553 optimization problem and not a genuine optimization problem. To avoid the complexity in the model
554 presentation, this issue is not elaborated here. It should be remarked that upon assuming the same
555 increment $\Delta \eta^{\text{rev}}$ for the current unknown η^{rev} and the evolving parameter f_c , extra differentiation
556 terms arise in the transformation criteria (A.7). However, our auxiliary simulations showed that
557 these extra terms only marginally contribute to the results.

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