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A finite-strain thermomechanical behavior model for Iron-based Shape Memory Alloys accounting for coupling between phase transformation and plastic slip

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Abstract

Shape Memory Alloys (SMAs) have the main interesting property to recover an inelastic strain induced by martensitic transformation. The initial shape can be recovered directly after unloading or with the application of an additional heating. Iron-based SMAs (Fe-SMAs) are characterized by a high coupling between phase transformation and plastic slip at low temperatures under small stress levels. Thermomechanical constitutive models describing such coupling developed based on small-strains are not suitable for higher loading levels. This motivates the proposed development of a finite-strain constitutive model for Fe-SMAs considering thermomechanical coupling between phase transformation and plastic slip, and by extending the small-strain model within a finite-strain thermodynamical framework in order to describe large strains mainly induced by plastic hardening in Fe-SMA material point. The model here has two internal variables (volume fraction of martensite and the accumulative plastic strain). It is based on the assumption of the local multiplicative split of the deformation gradient into elastic and inelastic parts with a total Lagrangian formulation. The inelastic deformation gradient splits also into a transformation and a plastic parts. The developed model is implemented into the commercial software Matlab. The results obtained for thermomechanical loadings are discussed and, a good agreement with

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experimental results is also observed.

Keywords: Iron-based SMAs, Finite strain behavior law, Phase transformation, Plastic slip, Multiplication decomposition.

1. Introduction

Conventional materials have long been used for their structural properties. However, continuous technological innovation in advanced fields such as aeronautics, bio-medical, energy production and automotive, as well as the progress made over the few decades in the development of materials with high multiphysical coupling have led to fulfill other functionalities such as sensing, actuation, etc. In this category of so-called functional, adaptive or intelligent materials, the most widely used materials are those having electrical/mechanical (piezoelectric), magnetic/mechanical (magnetostrictive) or thermal/mechanical (shape memory alloys) coupling (e.g. [Kim and Kwon \(2015\)](#); [Ojha and Sehitoglu \(2016\)](#); [Lookman et al. \(2017\)](#); [Xue et al. \(2018\)](#); [Jella et al. \(2019\)](#)).

The evolution of research on Shape Memory Alloys (SMAs) allowed to better understand the physical mechanisms as the phase transformation and plastic slip occurring on the microstructure, leading to innovative industrial applications. The latter have main characteristics known as the shape memory effect and the pseudo-elasticity (super-elasticity). In the past, many studies have been undertaken making it possible to modelize and characterize the behaviors of these alloys both metallurgically and thermomechanically (e.g. [Christ and Reese \(2009\)](#); [Xiao \(2014\)](#); [Cissé et al. \(2016a,b\)](#); [Xu et al. \(2018\)](#)).

Three SMAs families are currently used: Copper-based SMAs (Cu-Al-Be, Cu-Zn-Al, etc.), Nickel-Titanium-based SMAs (Ni-Ti, Ni-Ti- Nb, etc.) and Iron-based SMAs (Fe-Mn-Si, Fe-Ni-Co, etc.). In particular, Iron-based SMAs (Fe-SMAs) are distinguished from other SMAs by their thermomechanical coupling between martensitic transformation and plastic slip. [Koval et al. \(1979\)](#) noticed a shape memory effect on Fe-Ni-Co-Ti steel. The discovery of this new material was better recognized after the research of [Sato et al. \(1982\)](#) on Fe-Mn-Si that reveals the same shape memory effect. Since then these new materials have been recognized by the name Iron-based SMAs. Fe-SMAs drew a lot of attention for their use of various applications due to their low cost and their good mechanical properties. The shape

27 memory effect in the case of the Fe-SMAs comes, on the one hand, from the mechanically
28 induced phase transformation, from the γ -austenite FCC phase to the ε -martensite HCP
29 phase, and, on the other hand, from the reverse transformation activated only by heating.
30 More studies have been carried out on the phase transformation behavior (Kokorin et al.,
31 1993), the plastic slip behavior (Bouraoui et al., 2008; Khalil et al., 2013), the rubber effect
32 (Torra et al., 2015), the pseudo-elasticity (Sawaguchi et al., 2005), the physical properties
33 (Lin and Lin, 1996) and the improvement of the shape memory effect (Mamivand et al., 2014;
34 Wang et al., 2016). The non-Schmid effect, well known for Ni-Ti and Cu-based SMAs (Alkan
35 et al., 2018; Alkan and Sehitoglu, 2017, 2019), is less noticeable at the macroscopic scale for
36 Fe-SMAs. In fact, the difference between tension and compression in phase transformation
37 and the hardening anisotropy are much less pronounced in Fe-SMAs (Cao and Iwamoto,
38 2019; Nishimura et al., 1996, 1997b)

39 Unlike NiTi and Cu-based SMAs, very few constitutive models are available for Fe-SMAs.
40 The modeling of these materials has attracted many researchers leading to relatively large
41 number of studies (Nishimura et al. (1997a); Nishimura and Tanaka (1998); Goliboroda
42 et al. (1999); Nishimura et al. (2003); Jemal et al. (2009); Khalil et al. (2012); Cissé et al.
43 (2017)). Jemal et al. (2009) constructed the first three-dimensional model describing the
44 thermomechanical behavior of Fe-SMAs. This model is based on the description of a macro-
45 scopic behavior of a representative volume element (RVE). They defined the accumulative
46 plastic strain γ with the martensite volume fraction χ as the internal variables and the
47 stress Σ with the temperature T as controlling variables. The expression of the Gibbs free
48 energy is assumed taking into account of the phase transformation, the plastic slip and the
49 interaction energies leading to linear hardening. Khalil et al. (2012) developed a model us-
50 ing a thermodynamic/energetic approach while retaining the same internal variables as the
51 model of Jemal et al. (2009). It rectifies this latter by introducing a loading function for the
52 reverse phase transformation. They Modified the yield force of plasticity by considering the
53 temperature dependence, and improved the description of inter-granular and intra-granular
54 interactions to predict the experimentally observed non linear hardening. More recently,
55 Cissé et al. (2017) introduced a new model for Fe-SMAs based on the Zaki and Mounni
56 (2007) model for NiTi SMAs, and presented an energetic formulation. The Helmholtz free

57 energy Φ is written as a function of that in the austenite, Φ_a , martensite, Φ_m , and an in-
58 teraction energy, Φ_{int} introduced by $\Phi = (1 - \xi)\Phi_a + \xi\Phi_m + \Phi_{int}$, with ξ being the volume
59 fraction of martensite. All these constitutive models were built assuming the small-strain.
60 However, Fe-SMAs can reach large strain levels because of their ductility. Therefore, a
61 small-strain formulation may not be suitable, and it is necessary to account for the evolu-
62 tion of the deformed configuration during loading. This motivates the present authors to
63 develop a finite-strain behavior law for Fe-SMAs.

64 Plastic slip coupled or uncoupled with respect to phase transformation, could lead to
65 large inelastic strains in ductile metals and alloys as TRansformation Induced Plasticity
66 (TRIP) (Wei et al., 2007) and TWinning Induced Plasticity (TWIP) (Kalsar and Suwas,
67 2017) steels and also Fe-SMAs (Wen et al., 2014). This motivated the application of the
68 finite strain formulation for the conventional elasto-plastic material behavior modeling. The
69 basic equations for the mechanics of solids in finite strains can be found in many references.
70 Among these references (Taylor, 1938); (Malvern, 1969); (Lion, 2000); (Sidoroff and Dogui,
71 2001). The finite strain plasticity formulation is a difficult and controversial topic, both
72 conceptually and technically (Sidoroff and Dogui, 2001). The starting point of this formula-
73 tion can be a multiplicative decomposition. The total deformation gradient \mathbf{F} breaks down
74 as $\mathbf{F} = \mathbf{F}_{el}\mathbf{F}_{pl}$, with \mathbf{F}_{el} and \mathbf{F}_{pl} representing the elastic and plastic deformation gradients
75 (Lee, 1969); (Sidoroff and Dogui, 2001); (Vladimirov et al., 2010); (Grilo et al., 2016). Finite
76 strain models are developed either for the classical SMAs or to TRIP and TWIP steels. Be-
77 ginning with the classical SMAs, in literature, a large number of models have been proposed.
78 The work of Christ and Reese (2009) dealt with two typical and important phenomenon of
79 SMA behavior: Pseudo-Elasticity (PE) and Shape Memory Effect (SME). As in classical
80 plasticity, an unconstrained intermediate state decouples the elastic deformation gradient
81 of the deformation gradient that are induced by phase transformation $\mathbf{F}_t = \mathbf{F}_e^{-1}\mathbf{F}$ (Christ
82 and Reese, 2009). Evangelista et al. (2009) proposed a phenomenological model in finite
83 transformations for SMAs describing PE and SME behavior. Its model was based on a local
84 multiplicative formulation of the deformation gradient into an elastic part and a phase trans-
85 formation part $\mathbf{F} = \mathbf{F}_e\mathbf{F}_t$. Constitutive model equations were written with respect to the
86 undeformed configuration (Lagrangian approach). Arghavani et al. (2011) developed a fi-

87 nite strain three-dimensional Hencky-based kinematic-hardening constitutive model. They
 88 introduced the decomposition of the deformation gradient like that of [Evangelista et al.](#)
 89 [\(2009\)](#). More recently, [Wang et al. \(2017\)](#) constructed a finite strain constitutive model for
 90 SMAs that takes into account of thermomechanical coupling activation and reorientation
 91 of martensite by extending the small-strain model of [Zaki and Mounni \(2007\)](#). To further
 92 explain the thermomechanical coupling, [Wang et al. \(2017\)](#) decomposed the total deforma-
 93 tion gradient \mathbf{F} into, elastic \mathbf{F}_e , inelastic (transformation) \mathbf{F}_{ine} and thermal \mathbf{F}_θ elements
 94 introduced by $\mathbf{F} = \mathbf{F}_e \mathbf{F}_{ine} \mathbf{F}_\theta$, inspired from the previous work of [Levitas \(1998\)](#). The phase
 95 transformation of the austenitic state to the martensitic state takes place in the so-called
 96 austenitic steels ([Hallberg et al., 2007](#)). It treats a finite strain model for the austenitic steel
 97 with phase transformation and it treats the phase transition through an internal variables
 98 (the phase fraction). The local multiplicative decomposition of the total deformation gra-
 99 dient \mathbf{F} has been splitted into elastic \mathbf{F}_e and irreversible \mathbf{F}_{ir} parts, expressed as $\mathbf{F} = \mathbf{F}_e \mathbf{F}_{ir}$.
 100 The related physical phenomena of the TRIP steels are detailed in the review paper ([Fis-
 101 cher et al., 2000](#)). In [Tjahjanto et al. \(2008\)](#), a micromechanics-based model is highlighted
 102 and it is formulated within a finite strain framework. The kinematic description inside a
 103 single-crystal grain of austenite was introduced by the multiplicative decomposition of the
 104 total deformation gradient \mathbf{F} through elastic \mathbf{F}_e , plastic \mathbf{F}_p , and transformation \mathbf{F}_{tr} parts as
 105 $\mathbf{F} = \mathbf{F}_e \mathbf{F}_p \mathbf{F}_{tr}$. [Mahnken et al. \(2012\)](#) presented a finite strain macroscopic material model
 106 which predicts TRIP steel behavior on the hybrid-forming process cases. Another model
 107 was developed by [Mahnken et al. \(2013\)](#) treating the strain-rate and temperature-dependent
 108 asymmetric plastic material behavior accompanied by phase transformation. The total de-
 109 formation gradient splits multiplicatively as $\mathbf{F} = \mathbf{F}_{iso} \mathbf{F}_{vol} = \mathbf{F}_{iso}^e \mathbf{F}_i \mathbf{F}_{vol}$. Here, \mathbf{F}_{iso} , \mathbf{F}_{iso}^e ,
 110 \mathbf{F}_i and \mathbf{F}_{vol} represent, respectively, the deformation gradient of, isochoric, elastic isochoric,
 111 irreversible, and volumetric parts. This model enhances that of [Mahnken et al. \(2012\)](#) as it
 112 is built and specialized in TRIP-steels production processes.

113 Based on the models discussed in finite strains describing the phenomena of phase trans-
 114 formation and plasticity, a specific finite strain model adapted to Fe-SMAs thermomechan-
 115 ical behavior is detailed in this paper. Determining the behavior laws of Fe-SMAs requires
 116 a good knowledge of kinematics and the evolution laws of martensitic transformation and

117 plasticity. This work is an extension of the [Khalil et al. \(2012\)](#) small-strain behavior law
 118 with some enhancement. The Helmholtz free energy is been used to describe the thermody-
 119 namic framework, and modified the driving and yield forces. An alternative multiplicative
 120 decomposition of the deformation gradient is introduced, in which the total deformation gra-
 121 dient \mathbf{F} was first split into elastic \mathbf{F}_{el} and inelastic \mathbf{F}_{ine} parts. The inelastic part was then
 122 decomposed into contributions for phase transformation \mathbf{F}_{tr} and plastic slip \mathbf{F}_{pl} . The model
 123 constitutive equations are implemented in Matlab software. Obtained results are compared
 124 to the experimental data and numerical results of [Khalil et al. \(2012, 2013\)](#). Results of the
 125 comparison shows the relevance of the proposed model.

126 Section 2, presents an overview of the basic kinematic framework introducing the adopted
 127 local decomposition of the gradient deformation. Section 3 is dedicated to the development
 128 of the constitutive model, beginning with the definition of the Helmholtz free energy and
 129 the inner potential energy to construct the Lagrangian. Then using the second law of
 130 thermodynamics, the loading functions were defined for each behavior. A solution algorithm
 131 is proposed in section 4 to explain the numerical implementation. A comparison with
 132 experimental data is performed in section 5 by adding some finite strain simulations to
 133 predict an Fe-SMA response for higher strain level. The last section 6 gives a conclusion
 134 regarding this work and some prospects.

135 2. Kinematic framework

136 2.1. Deformation gradient

137 The local decomposition of the deformation gradient \mathbf{F} leads to two parts: an elastic part
 138 \mathbf{F}_{el} defined with respect to the intermediate configuration, and an inelastic part, \mathbf{F}_{ine} , de-
 139 fined with respect to the reference configuration. The latter, in the case of Fe-SMAs, is
 140 decomposed into phase transformation induced part \mathbf{F}_{tr} and a plastic induced part \mathbf{F}_{pl} ,
 141 figure 1-(a).

$$\mathbf{F} = \mathbf{F}_{el}\mathbf{F}_{ine} = \mathbf{F}_{el}\mathbf{F}_{tr}\mathbf{F}_{pl} \quad (1)$$

142 The phase transformation-plasticity evolution diagram of yield stresses as a function of
 143 temperature ([Olson and Cohen, 1972](#)); ([Bourauoi et al., 2008](#)), describes the behavior of

144 Fe-SMAs. Two domains are differentiated by the temperature T_0 (labeled Ms^σ in Bouraoui
 145 et al. (2008)) as shown in figure 1-(b). If the temperature of the material is lower than the
 146 temperature T_0 , the phase transformation of the austenite to martensite has priority. Oth-
 147 erwise, the activation of the plasticity in the austenite takes place, preventing the nucleation
 148 of the martensite.

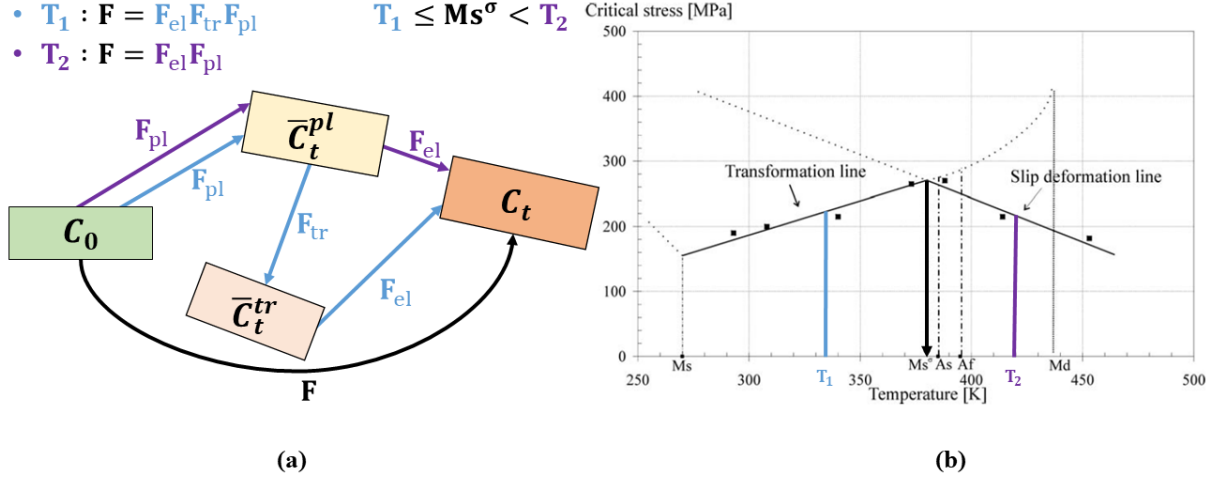


Figure 1: (a) Decomposition of deformation gradients; (b) Stress-Temperature diagram for phase transformation and plasticity (Bouraoui et al., 2008)

149 2.2. Strain tensors and their time derivatives

150 The deformation gradient \mathbf{F} is not a suitable strain measure. Therefore, a Green-Lagrange
 151 strain \mathbf{E} tensor was adopted to quantify the local strain in a given material point. It is
 152 defined as follows:

$$\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I}) \quad (2)$$

153 where $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ denotes the right Cauchy-Green tensor, and \mathbf{I} the second order identity
 154 tensor. Similarly, the elastic Cauchy-Green tensor is defined as:

$$\mathbf{C}_{el} = \mathbf{F}_{el}^T\mathbf{F}_{el} = \mathbf{F}_{ine}^{-T}\mathbf{C}\mathbf{F}_{ine}^{-1} \quad (3)$$

155 Moreover, the velocity gradient $\mathbf{L} = \frac{\partial \dot{\mathbf{u}}}{\partial \mathbf{x}}$ is decomposed into a, symmetric part \mathbf{D} and anti-
 156 symmetric part \mathbf{W} defined as follow:

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1} = \mathbf{D} + \mathbf{W}; \quad \begin{cases} \mathbf{D} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^T) \\ \mathbf{W} = \frac{1}{2}(\mathbf{L} - \mathbf{L}^T) \end{cases} \quad (4)$$

157 According to (2), the time derivative of the Green-Lagrange strain tensor (Green-Lagrange
158 strain rate) can be calculated as.

$$\dot{\mathbf{E}} = \frac{1}{2}\dot{\mathbf{C}} = \frac{1}{2}(\dot{\mathbf{F}}^T\mathbf{F} + \mathbf{F}^T\dot{\mathbf{F}}) \quad (5)$$

159 Using (4), the Green-Lagrange strain rate can be rewritten as:

$$\dot{\mathbf{E}} = \frac{1}{2}\mathbf{F}^T(\mathbf{L} + \mathbf{L}^T)\mathbf{F} = \mathbf{F}^T\mathbf{D}\mathbf{F} \quad (6)$$

160 For further use, the time derivative of the elastic right Cauchy–Green tensor has been defined
161 as follows:

$$\dot{\mathbf{C}}_{el} = -\mathbf{L}_{ine}^T\mathbf{C}_{el} + \mathbf{F}_{ine}^{-T}\dot{\mathbf{C}}\mathbf{F}_{ine}^{-1} - \mathbf{C}_{el}\mathbf{L}_{ine} \quad (7)$$

162 with $\mathbf{L}_{ine} = \mathbf{L} - \mathbf{L}_{el}$ being the inelastic velocity gradient.

163 3. Fe-SMA thermomechanical constitutive model in finite strains

164 3.1. Free energy function

165 To satisfy the principle of material objectivity, it is assumed that the Helmholtz free energy
166 Ψ depends on the elastic right Cauchy-Green strain tensor \mathbf{C}_{el} , the martensite volume
167 fraction χ , the plastic slip γ , and the temperature T . The Helmholtz free energy of a
168 Fe-SMA is the sum of hyper-elastic and inelastic energies as:

$$\Psi = \Psi(\mathbf{C}_{el}) + \Psi(\chi, \gamma, T) \quad (8)$$

169 The hyper-elastic energy can be defined as (Wang et al., 2017):

$$\Psi(\mathbf{C}_{el}) = \frac{\mu}{2}(I_{\mathbf{C}_{el}} - 3) - \mu \ln J + \frac{\lambda}{2}(\ln J)^2 \quad (9)$$

170 where μ and λ are equivalent Lamé constants by assuming an isotropic elastic behavior
171 with the same properties at the martensitic and austenitic states. $I_{\mathbf{C}_{el}}$ is the first cauchy
172 invariant of \mathbf{C}_{el} and $J = \det(\mathbf{F})$ is the deformation Jacobian (third invariant of \mathbf{F}).

173 The inelastic behavior of Fe-SMAs is induced by phase transformation and plastic slip for
174 a given poly-crystalline RVE (figure 2).

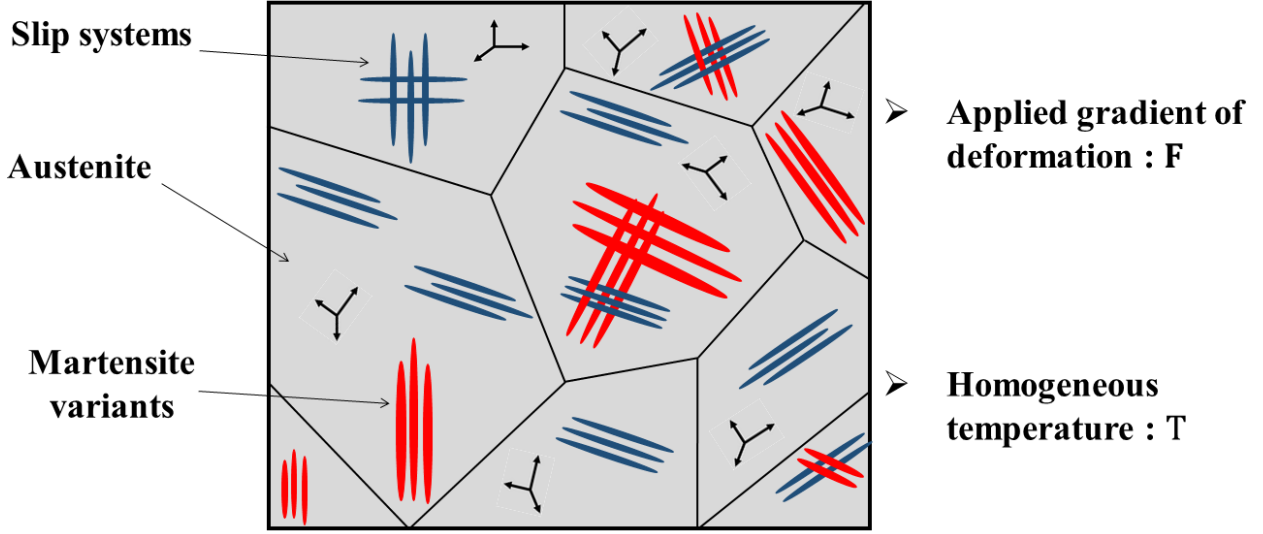


Figure 2: Representative Volume Element of an Fe-SMA

By considering the macroscopic induced effective behavior of this RVE, starting from local micro-mechanical description, a corresponding inelastic free energy is derived. All these steps leading to the adopted constitutive model are detailed in [Khalil et al. \(2012\)](#) for small strain case:

$$\Psi(\chi, \gamma, T) = c_v \left[(T - T_0) - T \ln \left(\frac{T}{T_0} \right) \right] + B (T - T_0) \chi + G_g(\mathbf{E}_{ine}) + [G_v(\chi) + (1 - \chi) G_s(\gamma) + G_{sv}(\gamma, \chi)] \quad (10)$$

175 where T is the current temperature, c_v , B , and T_0 are the material parameters, $G_g(\mathbf{E}_{ine})$
 176 is the intergranular interaction energy and G_v , G_s , G_{sv} are, respectively, the interaction
 177 functions between martensite variants, between plastic slip system, and between martensite
 178 variants and plastic slip systems. They are defined as follows:

$$G_g(\mathbf{E}_{ine}) = \frac{H_g}{(n_g + 1)} (\mathbf{E}_{ine} : \mathbf{E}_{ine})^{n_g + 1} \quad (11)$$

179

$$G_v(\chi) = \frac{H_v}{n_v + 1} \chi^{n_v + 1} \quad (12)$$

180

$$G_s(\gamma) = \frac{H_s}{n_s + 1} \gamma^{n_s + 1} \quad (13)$$

181

$$G_{sv}(\gamma, \chi) = \frac{H_{sv}}{n_{sv} + 1} (\gamma\chi)^{n_{sv} + 1} \quad (14)$$

182 with H_g being a material parameter characterizing intergranular interactions and n_g is a
 183 coefficient characterizing the interaction non linearity evolution. The coefficients n_v , n_s
 184 and n_{sv} reflect the nonlinearities of these interactions. The terms H_v , H_s and H_{sv} are,
 185 respectively, the interaction scalar coefficients between the martensite variants, the slip
 186 systems, and the martensite variants and the slip systems. In order to consider an equivalent
 187 macroscopic approach, the micromechanical formulation is simplified as given in [Peultier](#)
 188 [et al. \(2006\)](#) leading to scalar parameters for interactions. Therefore, only one scalar variable
 189 defines in a global way for each interaction.

190 The state variables are subjected to the physical condition that the volume fraction of
 191 martensite can not be less than 0 or greater than 1, expressed by the inequality as:

$$0 \leq \chi \leq 1 \quad (15)$$

192 The introduction of Lagrange multipliers ℓ_1 and ℓ_2 allows to take into account for these
 193 physical constraints. They ensure Kuhn and Tucker conditions as given bellow:

$$\begin{cases} \ell_1 \geq 0 \text{ and } \ell_1 \chi = 0 \\ \ell_2 \geq 0 \text{ and } \ell_2 (1 - \chi) = 0 \end{cases} \quad (16)$$

194 A corresponding inner potential Ψ_{IC} is defined as:

$$\psi_{IC} = -\ell_1 \chi - \ell_2 (1 - \chi) \quad (17)$$

A Lagrangian is then built as the sum of Helmholtz's free energy and the potential of inner conditions as:

$$\begin{aligned} \mathfrak{S} = & \frac{\mu}{2} (I_{C_{el}} - 3) - \mu \ln J + \frac{\lambda}{2} (\ln J)^2 + c_v \left[(T - T_0) - T \ln \left(\frac{T}{T_0} \right) \right] + B (T - T_0) \chi \\ & + G_g(\mathbf{E}_{ine}) + [G_v(\chi) + (1 - \chi) G_s(\gamma) + G_{sv}(\gamma, \chi)] - \ell_1 \chi - \ell_2 (1 - \chi) \end{aligned} \quad (18)$$

195 3.2. Inelastic driving and yield forces

196 At this step, the second law of thermodynamics is taken into account. It asserts that the
 197 entropy production rate ξ is always greater than or equal to the heating rate (heat flux

198 vector \mathbf{q} multiplied by the temperature gradient $\mathbf{grad} T$) divided by the temperature T . As
 199 a result, the Clausius-Duhem inequality takes the following form:

$$-\left(\dot{\mathfrak{S}} + \xi \dot{T}\right) + \mathbf{S} : \dot{\mathbf{E}} - \mathbf{q} \frac{\mathbf{grad} T}{T} \geq 0 \quad (19)$$

200 with \mathbf{S} being the second Piola-Kirchhoff tensor. The temperature is assumed homogeneous
 201 on the RVE.

$$\mathbf{grad} T = 0 \quad (20)$$

202 Assuming that the Lagrangian \mathfrak{S} is an isotropic function of \mathbf{C}_{el} , outcomes that \mathbf{C}_{el} is
 203 coaxial with $\frac{\partial \mathfrak{S}}{\partial \mathbf{C}_{el}}$, this latter property achieves the symmetric property for $\frac{\partial \mathfrak{S}}{\partial \mathbf{C}_{el}}$ which can
 204 be expressed mathematically as follows:

$$\mathbf{C}_{el} \frac{\partial \mathfrak{S}}{\partial \mathbf{C}_{el}} = \frac{\partial \mathfrak{S}}{\partial \mathbf{C}_{el}} \mathbf{C}_{el} \quad (21)$$

205 Additive decomposition of strain rate for different finite strains inelastic processes was in-
 206 troduced in (Levitas, 1996). For a Fe-SMA, the symmetric inelastic strain rate is the sum
 207 of phase transformation and plastic slip strain rates (Feng and Levitas, 2017):

$$\mathbf{D}_{ine} = \mathbf{D}_{tr} + \mathbf{D}_{pl} \quad (22)$$

208

$$\mathbf{D}_{tr} = \dot{\chi} \bar{\epsilon}_{\max}^{tr} \mathbf{N}^{tr} \quad (23)$$

209

$$\mathbf{D}_{pl} = (1 - \chi) \dot{\gamma} \mathbf{N}^{pl} \quad (24)$$

This last relation involves the term $(1 - \chi)$ which translates the assumption of plasticity development only in the austenite phase due to the very high yield stress for the activation of plasticity in martensite variants. Introducing the derived Lagrangian (18) and using (7)

as well as equations (4), (5), (21), (23) and (24), the equation (19) becomes:

$$\begin{aligned}
& \left(\mathbf{S} - 2\mathbf{F}_{ine}^{-1} \frac{\partial \mathfrak{S}}{\partial \mathbf{C}_{el}} \mathbf{F}_{ine}^{-T} \right) : \frac{1}{2} \dot{\mathbf{C}} + \left(2\mathbf{C}_{el} \frac{\partial \mathfrak{S}}{\partial \mathbf{C}_{el}} \right) : (\dot{\chi} \bar{\boldsymbol{\varepsilon}}_{max}^{tr} \mathbf{N}^{tr} + (1 - \chi) \dot{\gamma} \mathbf{N}^{pl}) \\
& + \left[\bar{\boldsymbol{\varepsilon}}_{max}^{tr} \mathbf{F}_{ine} \frac{\partial G_g(\mathbf{E}^{ine})}{\partial \mathbf{E}^{ine}} \mathbf{F}_{ine}^T : \mathbf{N}^{tr} - B(T - T_0) - \frac{\partial G_v}{\partial \chi} + G_s - \frac{\partial G_{sv}}{\partial \chi} + \ell_1 - \ell_2 \right] \dot{\chi} \\
& + \left[(1 - \chi) \left(\mathbf{F}_{ine} \frac{\partial G_g(\mathbf{E}^{ine})}{\partial \mathbf{E}^{ine}} \mathbf{F}_{ine}^T : \mathbf{N}^{pl} - \frac{\partial G_s}{\partial \gamma} \right) - \frac{\partial G_{sv}}{\partial \gamma} \right] \dot{\gamma} + \left[c_v \ln \left(\frac{T}{T_0} \right) - \chi B - \xi \right] \dot{T} \geq 0
\end{aligned} \tag{25}$$

210 where \mathbf{N}_{tr} and \mathbf{N}_{pl} are the flow direction vectors, for phase transformation and plasticity
211 respectively, obtained as follows (Khalil et al., 2012); (Cissé et al., 2017):

$$\mathbf{N}_{tr} = \begin{cases} \frac{3}{2} \frac{\mathbf{S}^D}{S^{eq}} & \text{if } S^{eq} \neq 0 \\ \frac{\mathbf{E}_{tr}}{E_{tr}^{eq}} & \text{if } S^{eq} = 0 \end{cases}; \quad \mathbf{N}_{pl} = \begin{cases} \frac{3}{2} \frac{\mathbf{S}^D}{S^{eq}} & \text{if } S^{eq} \neq 0 \\ \frac{\mathbf{E}_{pl}}{E_{pl}^{eq}} & \text{if } S^{eq} = 0 \end{cases} \tag{26}$$

212 where \mathbf{S}^D denotes the second Piola-Kirchhoff stress deviator, S^{eq} is the equivalent second
213 Piola-Kirchhoff stress in the von Mises sense, and E_{α}^{eq} denotes the equivalent Green-Lagrange
214 strain, with $\alpha = [tr, pl]$:

$$\mathbf{S}^D = \mathbf{S} - \frac{1}{3} tr(\mathbf{S}) \tag{27}$$

$$S^{eq} = \sqrt{\frac{3}{2} \mathbf{S}^D : \mathbf{S}^D} \tag{28}$$

$$E_{\alpha}^{eq} = \sqrt{\frac{2}{3} \mathbf{E}_{\alpha} : \mathbf{E}_{\alpha}} \tag{29}$$

217 As the elastic behavior and the heating-cooling process are reversible and occur without
218 dissipation, the second principle of thermodynamics leads to:

$$\mathbf{S} = 2\mathbf{F}_{ine}^{-1} \frac{\partial \mathfrak{S}}{\partial \mathbf{C}_{el}} \mathbf{F}_{ine}^{-T} \tag{30}$$

$$\xi = c_v \ln \left(\frac{T}{T_0} \right) - \chi B \tag{31}$$

220 The residual inequality leads to:

$$\Lambda_{dr}^{\chi} \dot{\chi} + \Lambda_{dr}^{\gamma} \dot{\gamma} \geq 0 \tag{32}$$

with Λ_{dr}^χ and Λ_{dr}^γ being the phase transformation and the plastic thermodynamic driving forces, respectively, defined as:

$$\Lambda_{dr}^\chi = \bar{\varepsilon}_{\max}^{tr} (\mathbf{M} + H_g(\mathbf{E}_{ine} : \mathbf{E}_{ine})^{n_g} \mathbf{F}_{ine} \mathbf{E}_{ine} \mathbf{F}_{ine}^T) : \mathbf{N}^{tr} - B(T - T_0) - H_v \chi^{n_v} + \frac{H_s}{(n_s + 1)} \gamma^{n_s + 1} - H_{sv} \gamma (\chi \gamma)^{n_{sv}} + \ell_1 - \ell_2 \quad (33)$$

$$\Lambda_{dr}^\gamma = (1 - \chi) (\mathbf{M} + H_g(\mathbf{E}_{ine} : \mathbf{E}_{ine})^{n_g} \mathbf{F}_{ine} \mathbf{E}_{ine} \mathbf{F}_{ine}^T) : \mathbf{N}^{pl} - (1 - \chi) H_s \gamma^{n_s} - H_{sv} \chi (\chi \gamma)^{n_{sv}} \quad (34)$$

221 whereas the symmetric Mandel Tensor \mathbf{M} (The coaxiality of \mathbf{C}_{el} and $\frac{\partial \mathfrak{S}}{\partial \mathbf{C}_{el}}$ involving the
222 symmetry of \mathbf{M}) written as:

$$\mathbf{M} = 2\mathbf{C}_{el} \frac{\partial \mathfrak{S}}{\partial \mathbf{C}_{el}} \quad (35)$$

223 To ensure the positivity of the dissipation of plastic slip and phase transformation, either
224 for forward or reverse phase transformation, indicated in (32), the ensuring evolution equa-
225 tions are built with respect to the accumulative plastic strain γ and the volume fraction of
226 martensite χ , respectively, and are given as:

$$\begin{aligned} \dot{\gamma} &= \dot{\kappa}^\gamma \\ \dot{\chi} &= \dot{\kappa}^\chi Sgn(\Lambda_{dr}^\chi) \end{aligned} \quad (36)$$

227 with $\dot{\kappa}^\chi$ and $\dot{\kappa}^\gamma$ being non negative-multipliers. The function $Sgn(\cdot)$ is used to express the
228 sign of Λ_{dr}^χ . This function is exploited to distinguish the forward and the reverse phase
229 transformation.

230 The yield forces for forward phase transformation, reverse phase transformation, and
231 plastic slip are defined, respectively, as follows:

$$\Lambda_y^{tr,m} = \sigma_y^m \bar{\varepsilon}_{tr}^{\max} + \zeta_m (T_0 - M_s) - H_\gamma \gamma^2 \quad (37)$$

$$\Lambda_y^{tr,a} = \sigma_y^a \bar{\varepsilon}_{tr}^{\max} + \zeta_a (T_0 - A_s) - H_\chi \chi \quad (38)$$

$$\Lambda_y^{pl} = \sigma_y^\gamma - K_T T \quad (39)$$

234 with ζ_a and ζ_m being control parameters (Cissé et al., 2017). M_s is the start forward
 235 martensitic transformation temperature, A_s is the start reverse martensitic transformation,
 236 σ_y^m , σ_y^a , and σ_y^γ are, respectively, the yield stress of forward and reverse phase transformation
 237 and plasticity. $\bar{\varepsilon}_{tr}^{\max}$ is the equivalent maximal transformation strain for saturation (for $\chi =$
 238 1) and K_T represents the evolution of slope of the yield plastic stress with the temperature.
 239 The determination of the activated process needs the introduction of three loading surfaces:
 240 Υ_{tr}^m for forward transformation, Υ_{tr}^a for reverse transformation, and Υ_{pl}^a for plasticity. They
 241 correspond to the difference between driving and yield forces as follows:

$$\Upsilon_{tr}^m = \Lambda_{dr}^\chi - \Lambda_y^{tr,m} \quad (40)$$

242

$$\Upsilon_{tr}^a = -\Lambda_{dr}^\chi - \Lambda_y^{tr,a} \quad (41)$$

243

$$\Upsilon_{pl}^a = \Lambda_{dr}^\gamma - \Lambda_y^{pl} \quad (42)$$

244 These loading functions have to satisfy the Kuhn–Tucker conditions for forward and
 245 reverse phase transformation and plasticity:

$$\left\{ \begin{array}{l} \Upsilon_{tr}^m \leq 0, \quad \dot{\chi} \geq 0, \quad \dot{\chi} \Upsilon_{tr}^m = 0 \\ \Upsilon_{tr}^a \leq 0, \quad -\dot{\chi} \geq 0, \quad -\dot{\chi} \Upsilon_{tr}^a = 0 \\ \Upsilon_{pl}^a \leq 0, \quad \dot{\gamma} \geq 0, \quad \dot{\gamma} \Upsilon_{pl}^a = 0 \end{array} \right. \quad (43)$$

246 Therefore, Table 1 summarizes the constitutive equation system to be solved in order to
 247 predict the thermomechanical behavior for a given loading. The next section describes how
 248 this system is solved with an implicit integration scheme.

249 4. Constitutive equations: Resolution algorithm

250 The constitutive equations are solved with the Newton-Raphson method combined to the
 251 return mapping technique (elastic predictor-inelastic corrector procedure) using the Matlab
 252 software. An exponential integration scheme is adopted to update the inelastic deformation
 253 gradient.

$$\mathbf{F}_{ine}^{n+1} = \exp(\Delta \mathbf{D}_{ine}^{n+1}) \mathbf{F}_{ine}^n \quad (44)$$

Table 1: Summary of the constitutive equations

Deformation gradients

$$\mathbf{F} = \mathbf{F}_{el} \mathbf{F}_{ine}$$

$$\mathbf{F}_{ine} = \mathbf{F}_{tr} \mathbf{F}_{pl}$$

Strain quantities

$$\mathbf{C} = \mathbf{F}^T \mathbf{F}$$

$$\mathbf{C}_{ine} = \mathbf{F}_{ine}^T \mathbf{F}_{ine}$$

$$\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I})$$

$$\mathbf{E}_{ine} = \frac{1}{2}(\mathbf{C}_{ine} - \mathbf{I})$$

$$\mathbf{H} = \frac{1}{2} \ln(\mathbf{C})$$

Stress quantities

$$\mathbf{S} = \mu \mathbf{C}_{ine}^{-1} + (\lambda \ln(J) - \mu) \mathbf{C}^{-1}$$

$$\mathbf{M} = \frac{\mu}{2} \mathbf{C}_{ine}^{-1} \mathbf{C} \mathbf{C}_{ine}^{-1} + \frac{1}{2} (\lambda \ln(J) - \mu) \mathbf{C}_{ine}^{-1}$$

$$\boldsymbol{\sigma} = \frac{1}{J} \mathbf{F} \mathbf{S} \mathbf{F}^T$$

Loading functions

$$\Upsilon_{tr}^m = \Lambda_{dr}^\chi - \Lambda_y^{tr,m}$$

$$\Upsilon_{tr}^a = -\Lambda_{dr}^\chi - \Lambda_y^{tr,a}$$

$$\Upsilon_{pl}^a = \Lambda_{dr}^\gamma - \Lambda_y^{pl}$$

Kuhn-Tucker conditions on the loading functions

$$\Upsilon_{tr}^m \leq 0, \quad \dot{\chi} \geq 0, \quad \dot{\chi} \Upsilon_{tr}^m = 0$$

$$\Upsilon_{tr}^a \leq 0, \quad -\dot{\chi} \geq 0, \quad -\dot{\chi} \Upsilon_{tr}^a = 0$$

$$\Upsilon_{pl}^a \leq 0, \quad \dot{\gamma} \geq 0, \quad \dot{\gamma} \Upsilon_{pl}^a = 0$$

Kuhn-Tucker conditions on the state variables

$$\ell_1 \geq 0, \quad \ell_1 \chi = 0$$

$$\ell_2 \geq 0, \quad \ell_2 (1 - \chi) = 0$$

Flow rules

$$\mathbf{D}_{ine} = \mathbf{D}_{tr} + \mathbf{D}_{pl}$$

$$\mathbf{D}_{tr} = \dot{\chi} \bar{\boldsymbol{\varepsilon}}_{\max}^{tr} \mathbf{N}^{tr}$$

$$\mathbf{D}_{pl} = (1 - \chi) \dot{\gamma} \mathbf{N}^{pl}$$

254 where $\Delta \mathbf{D} = \mathbf{D} \Delta t$. Reminding that for any invertible matrix \mathbf{B} , the tensor exponential
 255 satisfies $\exp(\mathbf{B})^{-1} = \exp(-\mathbf{B})$. Using this latter relation along with equations (1) and (44)
 256 leads to:

$$\mathbf{F}_{el}^{n+1} = \mathbf{F}_{el}^{trial} \exp(-\Delta \mathbf{D}_{ine}^{n+1}) \quad (45)$$

257 where $\mathbf{F}_{el}^{trial} = \Delta \mathbf{F} \mathbf{F}_{el}^n$, and $\Delta \mathbf{F}$ is an incremental deformation gradient, for a local pertur-
 258 bation. The incremental form of the global deformation gradient can be given as:

$$\mathbf{F}^{n+1} = \Delta \mathbf{F} \mathbf{F}_{el}^n \mathbf{F}_{tr}^n \mathbf{F}_{pl}^n \exp(-\Delta \mathbf{D}_{ine}^{n+1}) \quad (46)$$

259 The incremental form for the temperature evolution is defined as follows:

$$T^{n+1} = T^n + \Delta T \quad (47)$$

260 Using Matlab software, the first step defines the known initial states. In the second step,
 261 iterative scheme based on the return mapping procedure allows to identify which mechanisms
 262 are activated and to determine the increment for χ and γ solutions of the system in table
 263 1. If the trial state is admissible, the step is elastic. Otherwise, the step is inelastic and
 264 internal variables for phase transformation and/or plasticity have to be updated. To solve
 265 the constitutive equations, time-discrete incremental equations are rewritten over a discrete
 266 time intervals $[t_n; t_{n+1}]$ where n indicates the n th kinematic time instant. For the first
 267 increment, all these gradients of deformation are isochoric ($\mathbf{F}_{el}^0 = \mathbf{F}_{tr}^0 = \mathbf{F}_{pl}^0 = \mathbf{I}$) with
 268 \mathbf{I} being the identity second order tensor. Also an initializing form for the volume fraction
 269 of martensite and the accumulative plastic strain to be zero ($\chi^0 = \gamma^0 = 0$), i.e., the Fe-
 270 SMA is purely austenitic and there are no initial or residual solicitations. Then, using
 271 the incremental form of the deformation gradient in equation (46) to quantify all model
 272 constitutive equations, an exponential mapping method updates the phase transformation
 273 and plastic gradient deformations as follows:

$$\begin{aligned} \mathbf{F}_{tr}^{n+1} &= \exp(\Delta \mathbf{D}_{tr}^{n+1}) \mathbf{F}_{tr}^n \\ \mathbf{F}_{pl}^{n+1} &= \exp(\Delta \mathbf{D}_{pl}^{n+1}) \mathbf{F}_{pl}^n \end{aligned} \quad (48)$$

274 The computation of the total and the inelastic right Cauchy Green tensors, \mathbf{C} and \mathbf{C}_{ine} ,
 275 respectively, allows to determine the second Piola-Kirchhoff, \mathbf{S} , and Mandel, \mathbf{M} , stresses

276 quantities which are used to calculate the different loading functions. Based on the loading
 277 functions values, the typical of behavior of the Fe-SMA (Elasticity, Forward Phase Trans-
 278 formation, Reverse Phase Transformation, Plastic Slip, coupling form between Forward
 279 Phase Transformation/Plastic Slip and coupling form between Reverse Phase Transforma-
 280 tion/Plastic Slip) can be determined and it allows to quantify the evolution of the internal
 281 variables. An implicit integration scheme based on the Newton-Raphson method used to
 282 extract the internal variables multipliers. Since the internal variables multipliers are calcu-
 283 lated, the evolution equation of the martensite volume fraction and the accumulative plastic
 284 strain can be rewritten using the backward Euler approximation as follows:

$$\chi^{n+1} = \chi^n + \Delta\kappa^X Sgn(\Lambda_{dr}^X) \quad (49)$$

285

$$\gamma^{n+1} = \gamma^n + \Delta\kappa^\gamma \quad (50)$$

286 with $\Delta\kappa^X = \dot{\kappa}^X \Delta t$ and $\Delta\kappa^\gamma = \dot{\kappa}^\gamma \Delta t$ are respectively the phase transformation and plasticity
 287 increments at time t_{n+1} .

288 After the determination of the internal variables, they are inserted in the function which
 289 defines the strain rate for phase transformation and plasticity as:

$$\Delta\mathbf{D}_{tr}^{n+1} = \Delta\kappa^X \bar{\varepsilon}_{\max}^{tr} \mathbf{N}_{tr}^n \quad (51)$$

290

$$\Delta\mathbf{D}_{pl}^{n+1} = (1 - \chi^{n+1}) \Delta\kappa^\gamma \mathbf{N}_{pl}^n \quad (52)$$

291 Remembering that the total strain rate is the sum of the phase transformation and the
 292 plastic one as:

$$\Delta\mathbf{D}_{ine}^{n+1} = \Delta\mathbf{D}_{tr}^{n+1} + \Delta\mathbf{D}_{pl}^{n+1} \quad (53)$$

293 Introducing (53) into the equation defining the elastic predictor (45) allows to predict the
 294 next increment. The same procedure is repeated until reaching the desired level of strain.
 295 Figure (3) illustrates the algorithm adopted to solve the finite strain problem in a given
 296 material point.

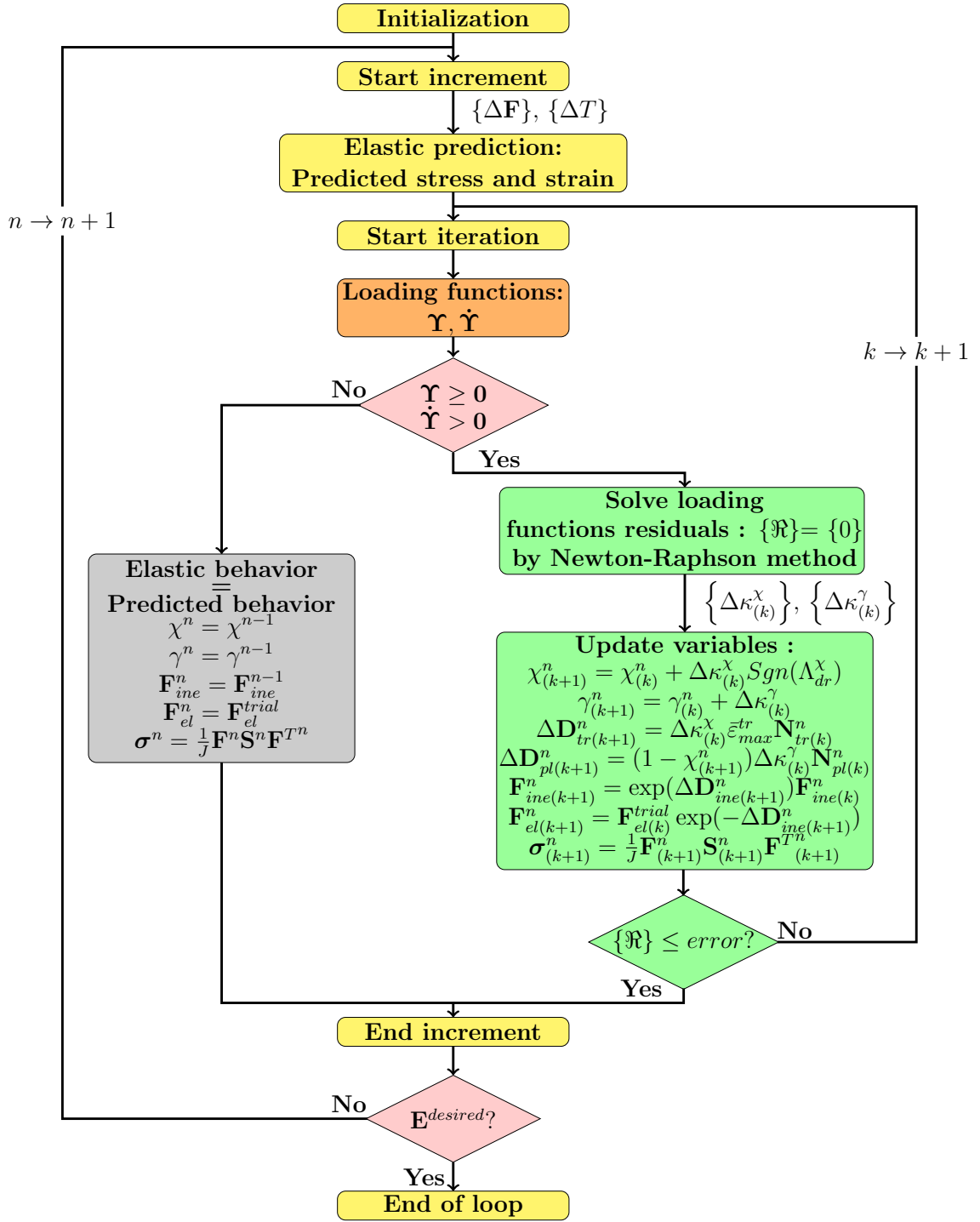


Figure 3: Solution algorithm

Table 2: Model parameters for Fe-Mn_{31.6}-Si_{6.45}-C_{0.018}(wt%)

Parameter	Value	Parameter	Value
σ_y^m (MPa)	137.7	A_s (°C)	96
σ_y^a (MPa)	125.2	T_0 (°C)	79.4
σ_y^γ (MPa)	210	H_v (MPa)	27.2
ν	0.3	H_s (MPa)	632.5
μ (MPa)	65385	H_{sv} (MPa)	1000
λ (MPa)	98077	H_g (MPa)	627
$\bar{\epsilon}_{\max}^{tr}$	0.048	n_v	0.44
ζ_m (MPa/°C)	0.086	n_s	0.55
ζ_a (MPa/°C)	0.036	n_{sv}	0.45
B (MPa/°C)	0.104	n_g	3.07
K_T (MPa/°C)	0.45	H_γ (MPa)	500
M_s (°C)	-25	H_χ (MPa)	-3

5. Results and discussion

In order to verify the developed model, small and finite strain simulations are carried out and compared with the experimental data of Khalil et al. (2013) and the numerical results of Khalil et al. (2012) at different tension loading levels followed by a heating-cooling process. Then, finite strain uni-axial simulations for higher strain level are carried out to predict the corresponding Fe-SMA behavior. In the case of a uni-axial tension test, $\Delta\mathbf{F}$ is defined as:

$$\Delta\mathbf{F} = \begin{bmatrix} \varrho & 0 & 0 \\ 0 & \frac{1}{\sqrt{\varrho}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{\varrho}} \end{bmatrix}; \quad \varrho = 1 + \frac{\Delta u_1}{\Delta X_1} = 1 + 10^{-6} \quad (54)$$

The material parameters considered for small strain simulations are gathered in table 2. They were identified starting from experimental results in Khalil et al. (2013).

5.1. Small strain model response

This section deals with a series of uni-axial loadings described by figure 4 with small strain level (tension loading-unloading followed by a heating-cooling). Numerical results are com-

308 pared to the experimental data of [Khalil et al. \(2013\)](#) for the Fe-Mn_{31.6}-Si_{6.45}-C_{0.018}(wt%).
 309 Table 2 illustrates the model parameters. Three different temperatures (20, 50 and 130°C)
 310 were considered for the uni-axial applied loading. Each temperature corresponds to special
 311 behavior of the Fe-SMA (20°C: Only phase transformation; 130°C: Only plasticity; 50°C:
 312 Coupling between phase transformation and plasticity). The applied thermomechanical
 313 loading cycle consists of a mechanical loading / unloading followed by heating to activate
 314 the reverse transformation (figure 4). The heating allows to quantify the part of strain
 315 due to the phase transformation compared to that due to the plasticity. Therefore, all
 316 the martensite created during the mechanical loading can be recovered by heating and the
 317 plastic strain remains permanent.

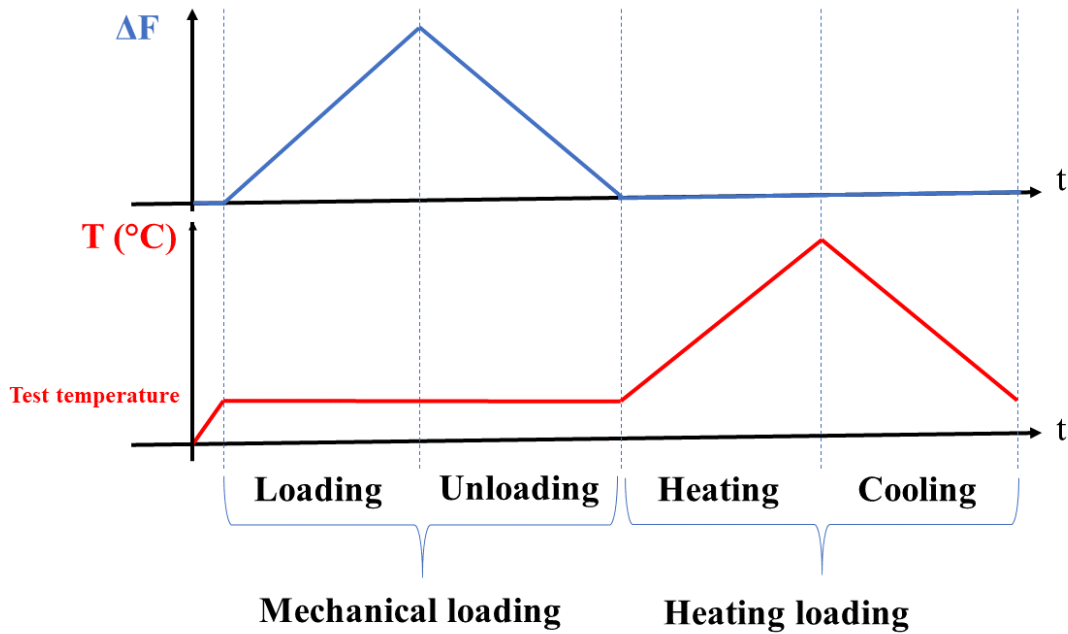


Figure 4: Thermomechanical loading

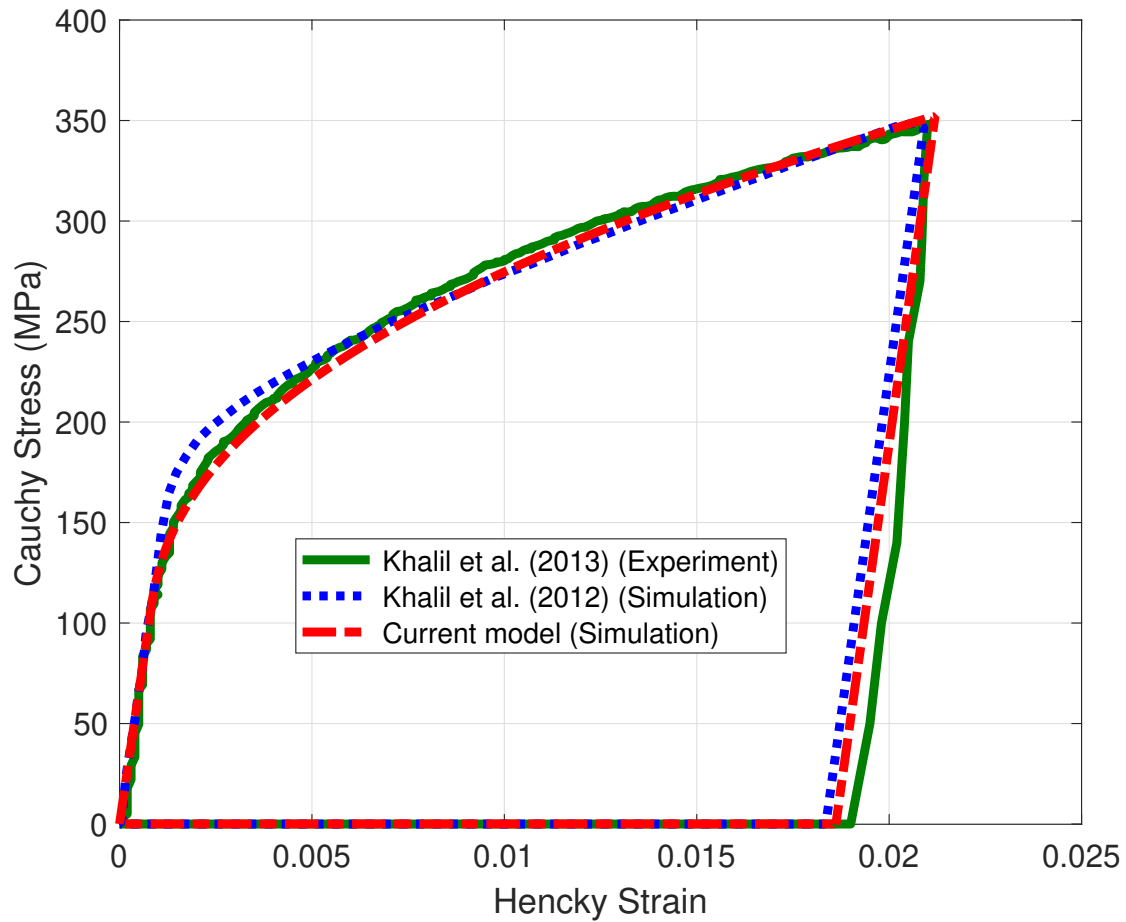


Figure 5: Experimental and simulated stress-strain behavior at 20°C

318 Figure 5 depicts the comparison of present results with those of available experimental,
 319 and numerical data of (Khalil et al., 2012, 2013) based on small strain. The obtained results
 320 here show that the finite-strain model is in a good agreement with experimental data. For
 321 the level of 2.2% of strain at 20°C only phase transformation is activated. As shown in
 322 figure 6 the accumulative plastic strain remains stagnant and only the volume fraction of
 323 martensite increases during mechanical loading and decreases during heating, leading to the
 324 full strain recovery.

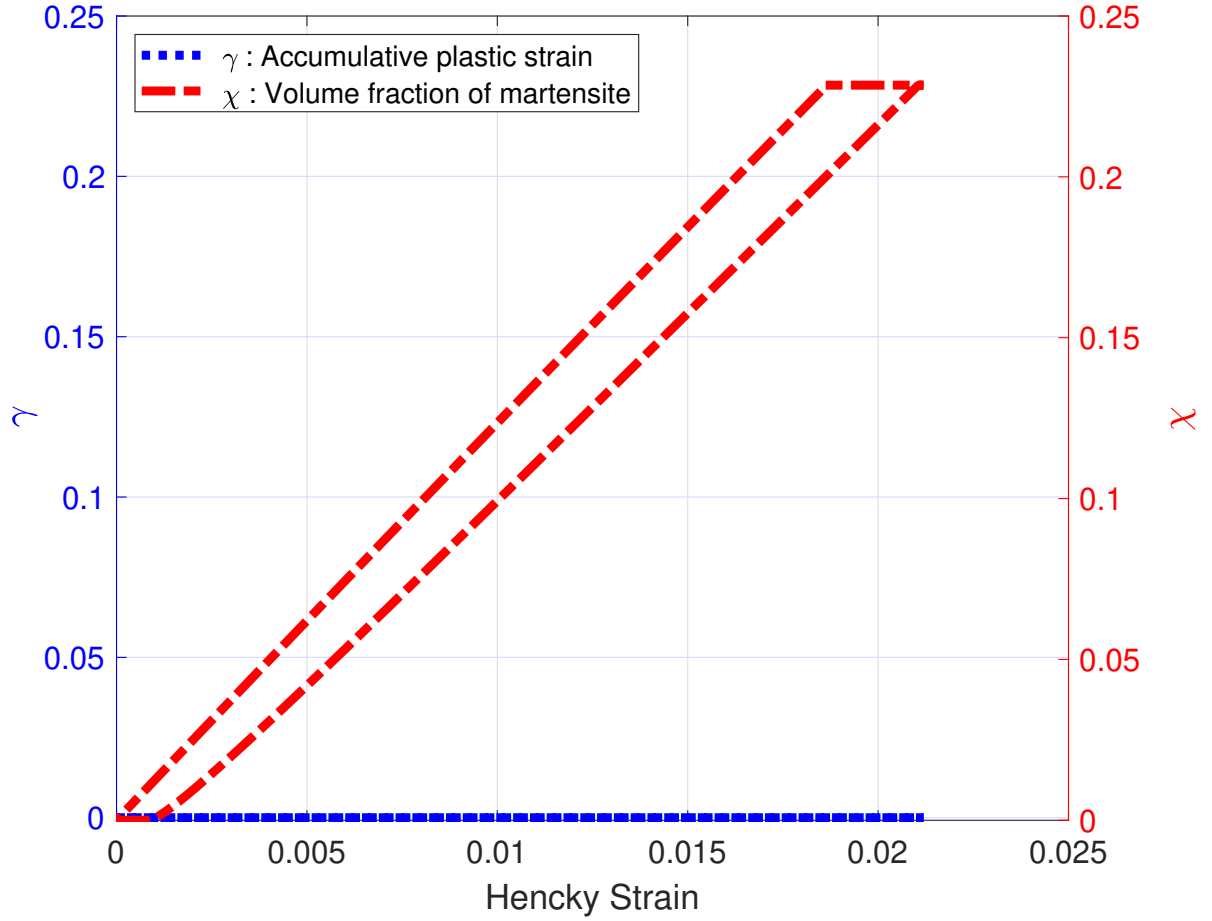


Figure 6: Evolution of the volume fraction of martensite and the accumulative plastic strain function of strain at 20°C

325 Figure 7 shows a comparison between numerical and experimental results at 50°C for
 326 a uni-axial tensile test. The numerical curve is consistent with the experimental one. The
 327 present model describes Fe-SMA hardening compared to that of Khalil et al. (2012). At
 328 this temperature, Fe-SMA behavior exhibits a coupling between phase transformation and
 329 plasticity. After a heating cycle, a part of strain is recovered due to the reverse phase trans-
 330 formation and the other part is irreversible due to the plasticity of austenite. Figure 8 shows
 331 the evolution of the volume fraction of martensite and the accumulative plastic strain as a
 332 function of strain during mechanical loading at 50°C. At first, only the transformation is
 333 activated (only the volume fraction of martensite evolves). Starting from a certain loading
 334 level, plasticity is occurred and the two mechanisms are active simultaneously. The marten-

335 site evolution slope is changed after the start of the plasticity, marking the fact that the
336 activation of the plasticity hinders the development of the phase transformation. For this
337 temperature, the inelastic strain corresponds to the two combined mechanisms, the phase
338 transformation and the plastic slip.

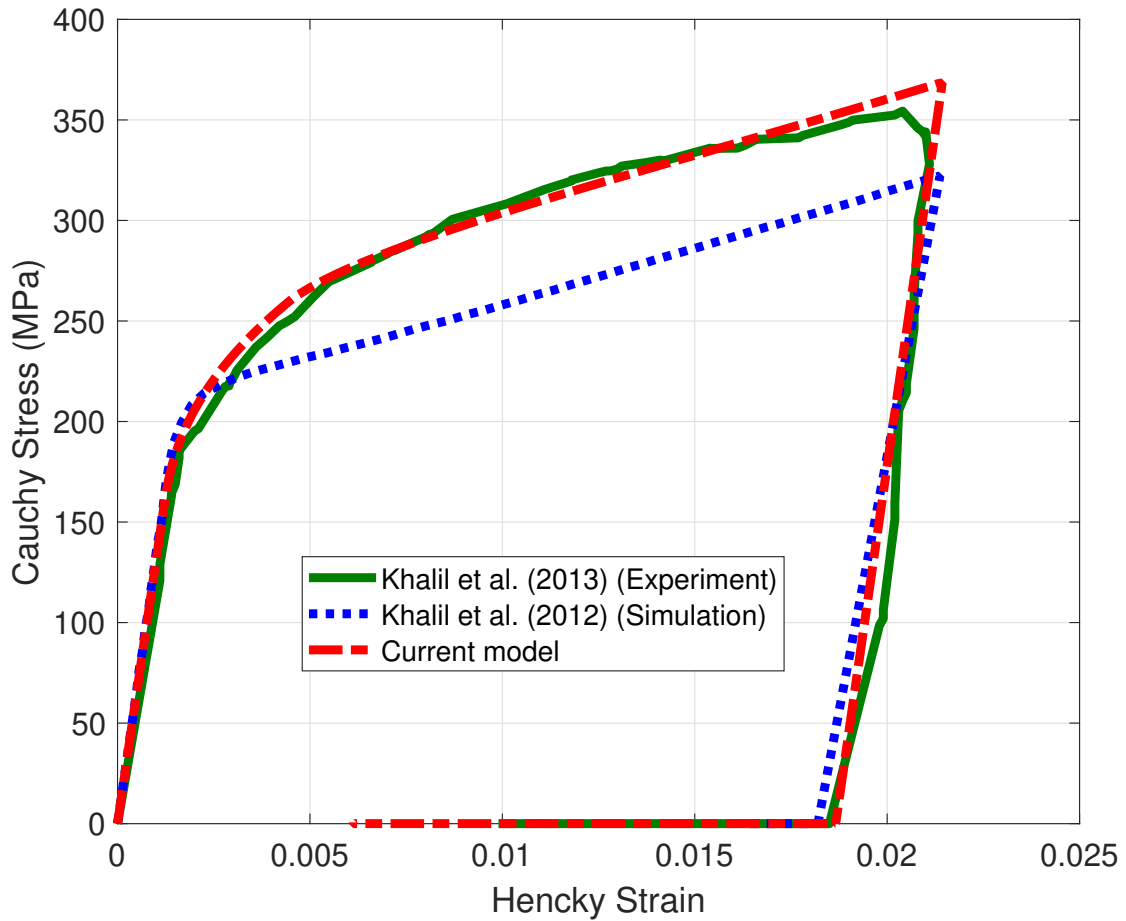


Figure 7: Experimental and simulated stress-strain behavior at 50°C

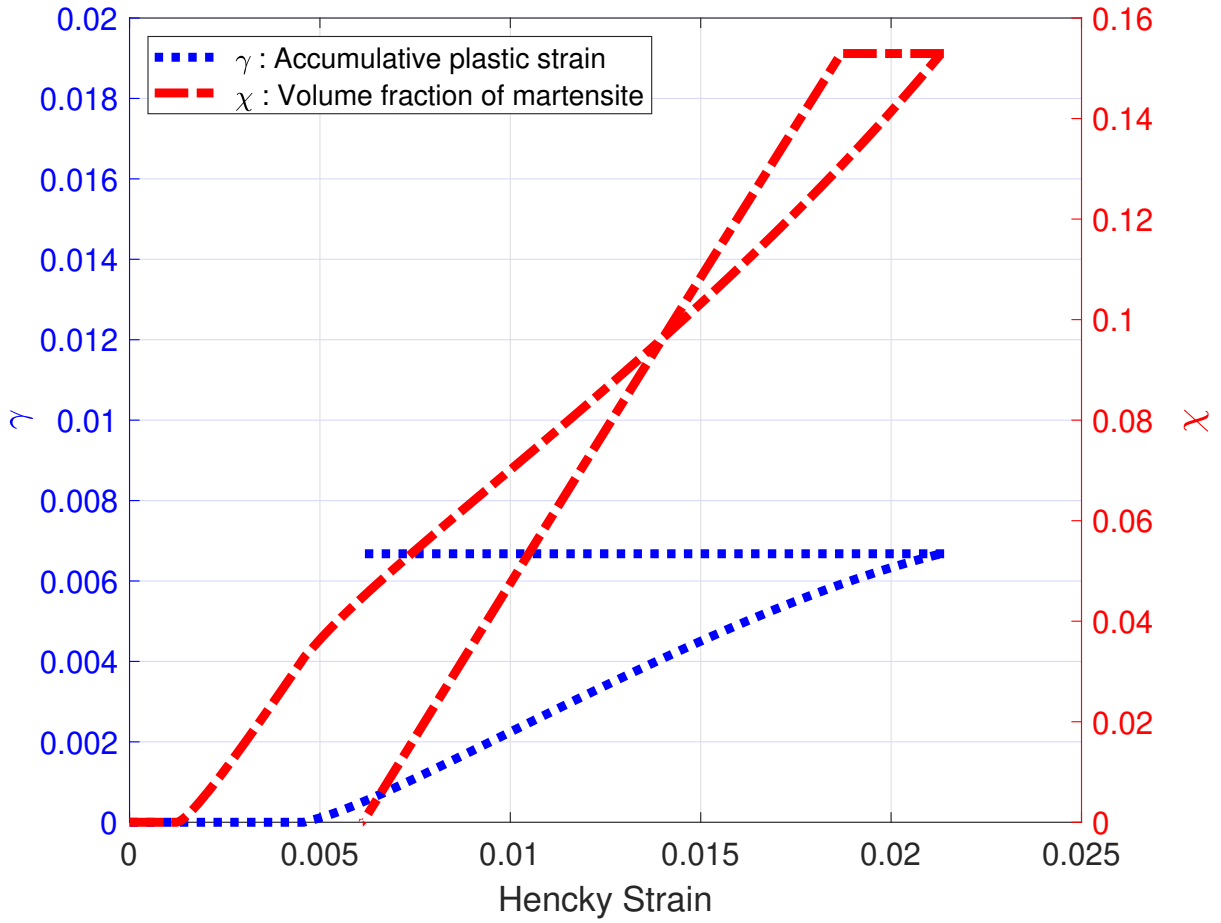


Figure 8: Evolution of the volume fraction of martensite and the accumulative plastic strain function of strain at 50°C

339 Moreover, the comparison between the numerical and experimental results in figure 9
 340 shows that the model is consistent with the experimental results at 130°C. Similarly, the
 341 present model describes the non-linear hardening more accurately than those of Khalil et al.
 342 (2012). Even after a heating cycle, the Fe-SMA maintains the same deformed configuration.
 343 Next, the study is focused on the evolution of the volume fraction of martensite and the
 344 accumulative plastic strain. Figure 10 shows only the presence of plasticity and the strain
 345 is irreversible denoting the behavior is purely plastic.

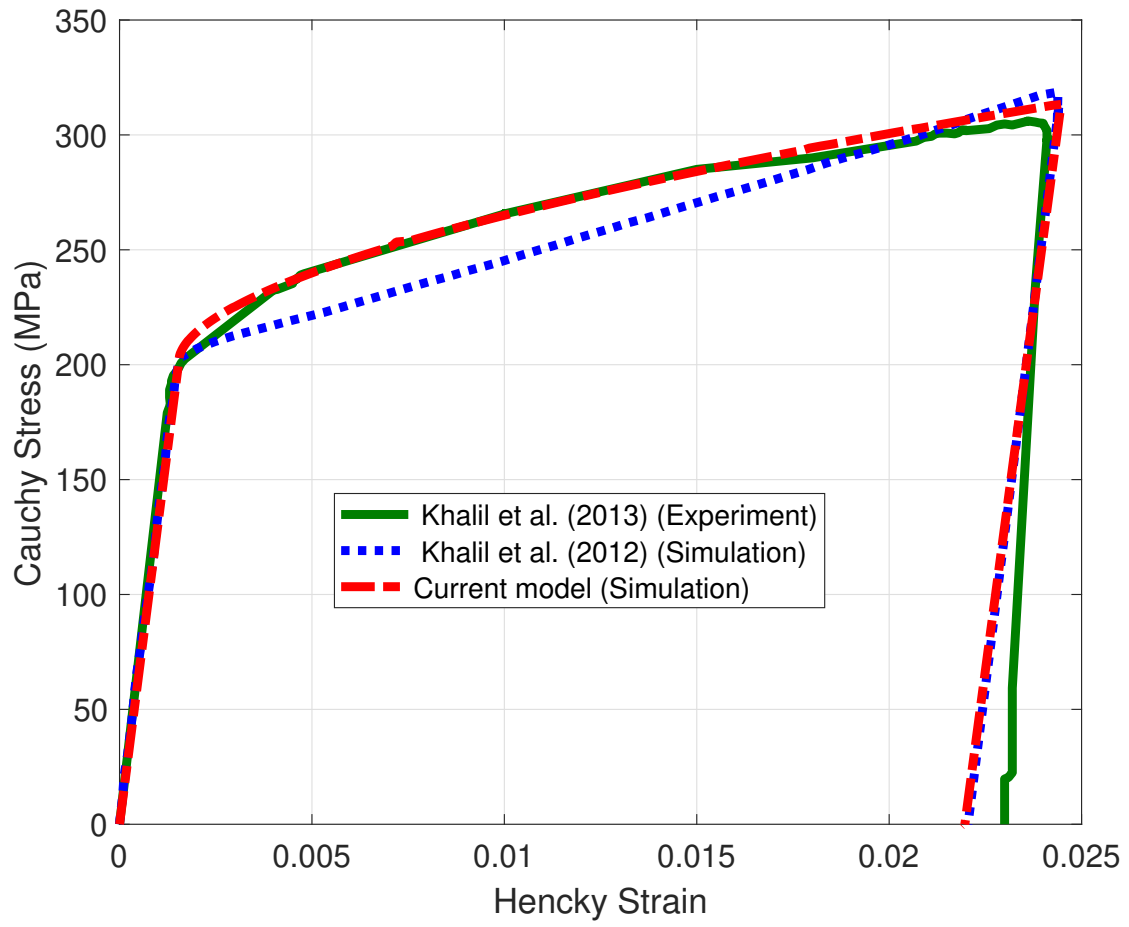


Figure 9: Experimental and simulated stress-strain behavior at 130°C

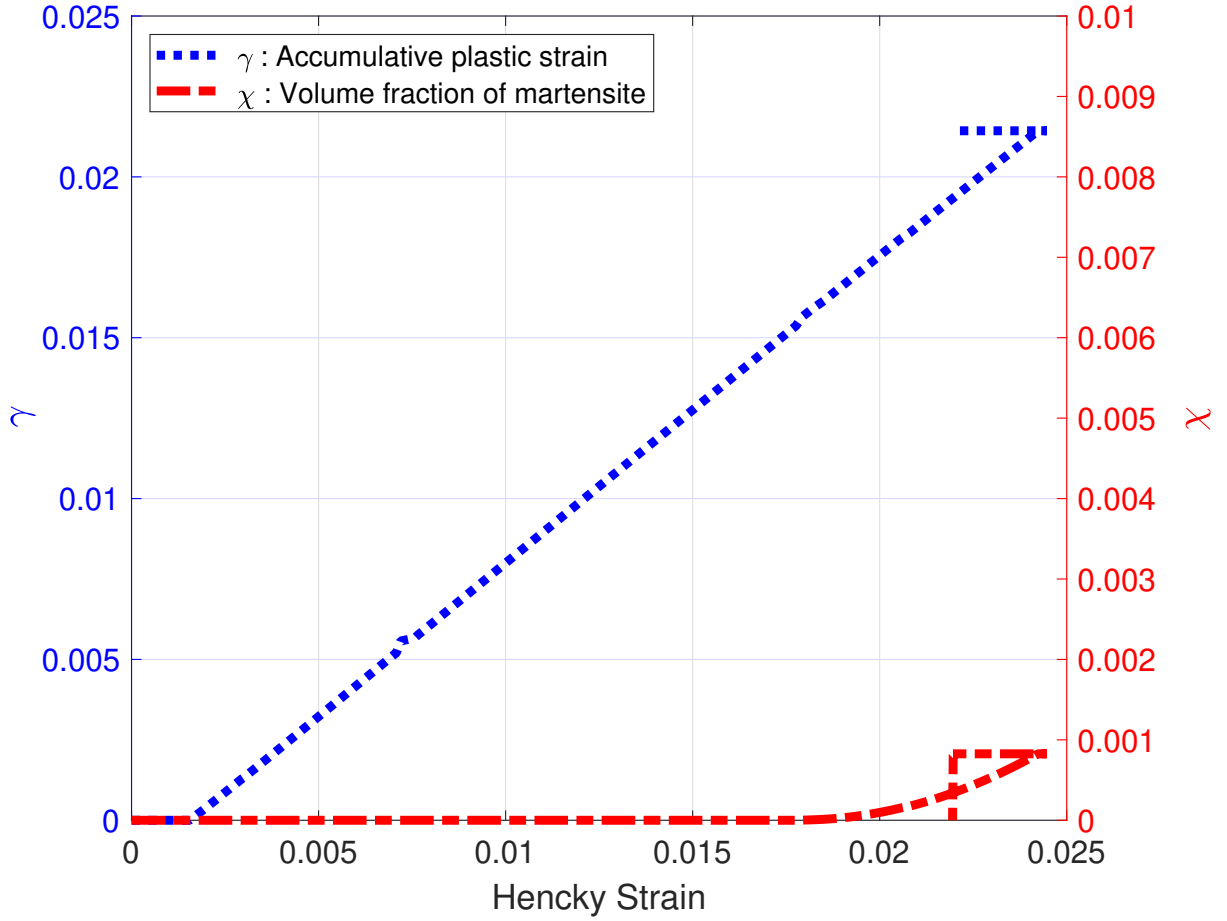


Figure 10: Evolution of the volume fraction of martensite and the accumulative plastic strain function of strain at 130°C

346 Figure 11 presents the 3D stress-strain-temperature diagram for the applied tensile load-
347 ing at three constant temperatures. This diagram shows that the Fe-SMA behavior is af-
348 fected by the sample's temperature. By going further from the M_s temperature, the plastic
349 behavior becomes dominant. Figure 12 shows the corresponding curves in the temperature-
350 strain diagram. It is given that, after a loading-unloading cycle, the elastic strain is recovered
351 for each temperature. After heating, the strain is fully recovered at 20°C and only partially
352 recovered at 50°C. This behavior brings out that the inelastic strain has a reversible part
353 induced by phase transformation and a remnant part induced by plasticity. At 130°C tem-
354 perature, the Fe-SMA behavior is purely plastic with a very low recovered strain during
355 heating. It appears that the present model predicts well the Fe-SMA behavior for small

356 strains. The next subsection presents the predicted Fe-SMA behavior for higher strain
357 levels.

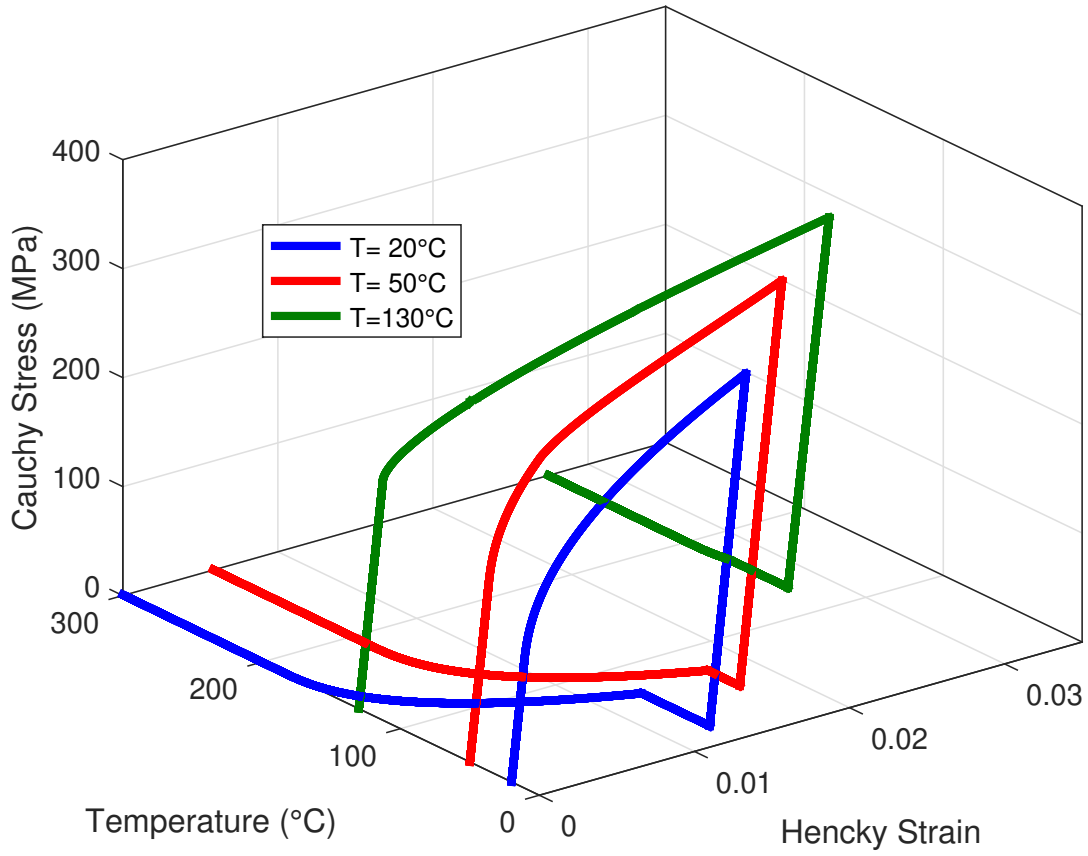


Figure 11: Small strain 3D stress-strain-temperature diagram

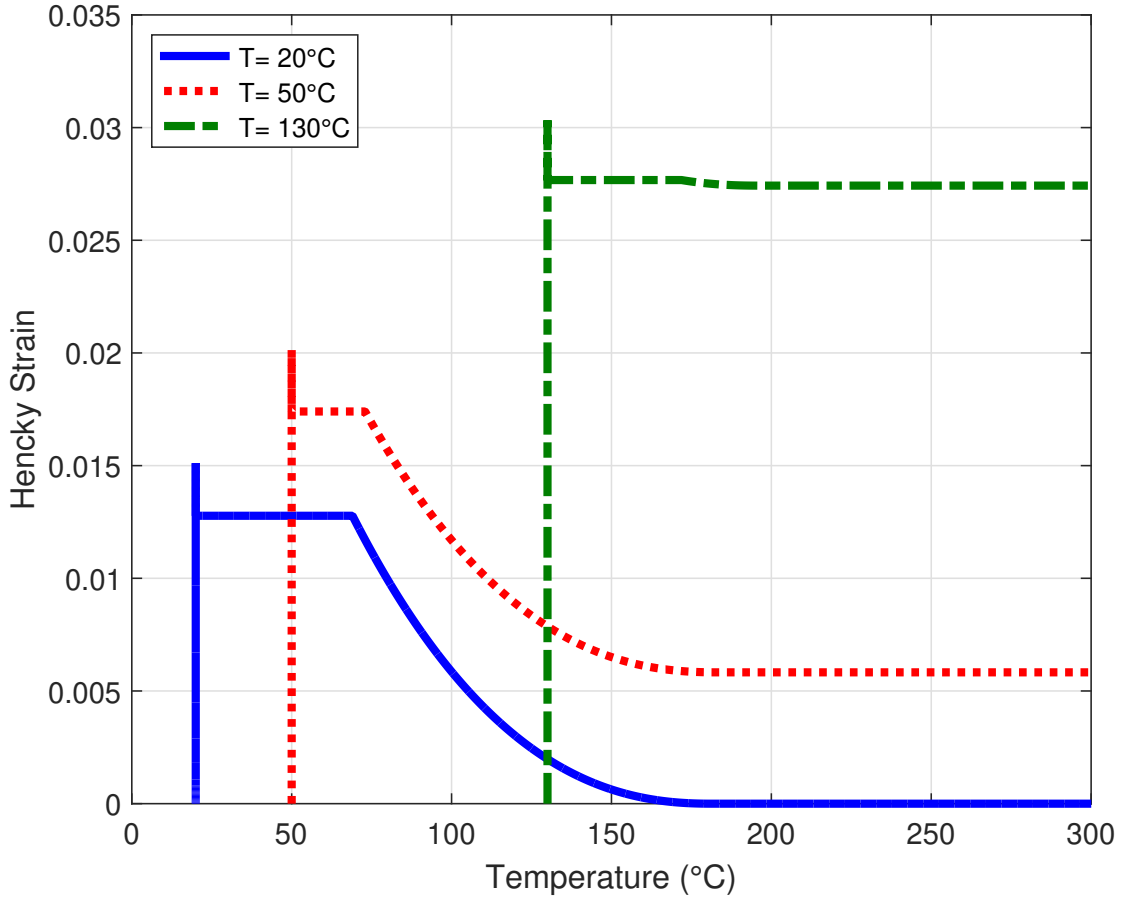
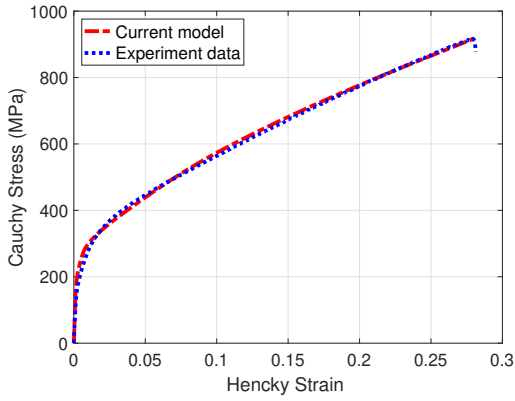


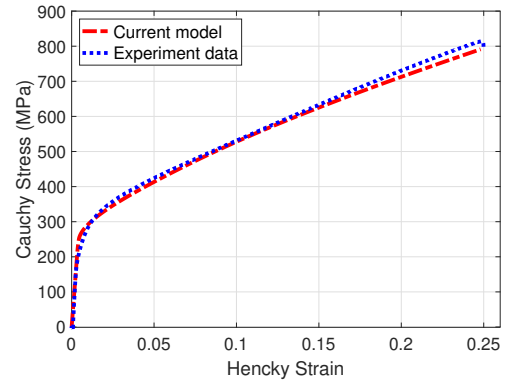
Figure 12: Shape memory effect of an Fe-SMA response in small strain

358 *5.2. Results for uni-axial tensile tests with higher strain levels*

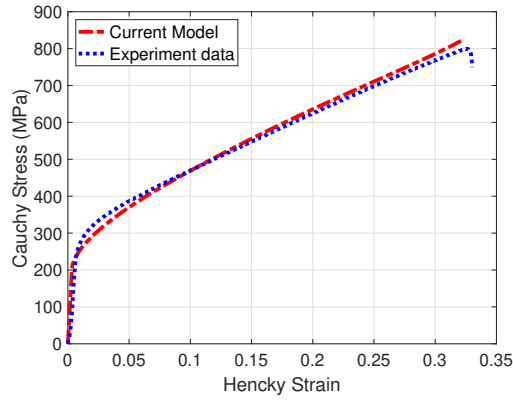
359 The Fe-SMAs can reach high level strains due to their ductility. Hence, destructive quasi-
 360 static tensile tests for Fe-SMA type Fe-Mn₃₀-Si₆-Cr₅(wt%) is performed on a Dynamic Me-
 361 chanical Analysis (DMA) machine type LTM1 Zwick/Roell at 3 different temperatures (20,
 362 50 and 130°C). The capacity of the machine is ± 1 KN on loading and a temperature range of
 363 -80 to +250°C. The specimen used here has the following dimensions (35 mm \times 1.25 mm \times 1
 364 mm). The model is adjusted with the obtained curves (figure 13). Table 3 shows the
 365 material corresponding new parameters of the Fe-Mn₃₀-Si₆-Cr₅(wt%).



(a) $T=20^{\circ}\text{C}$



(b) $T=50^{\circ}\text{C}$



(c) $T=130^{\circ}\text{C}$

Figure 13: Experimental and simulated stress strain behavior at: (a) 20°C , (b) 50°C and (c) 130°C

366 Simulations are carried out to predict Fe-SMA behavior for different temperature under
 367 uni-axial tensile tests at large strain. Figure 14 highlights a simulation tensile test for 15,
 368 20 and 25% of strain at 20, 50 and 130°C , respectively. After a loading-unloading-heating
 369 cycle, a part of strain is recovered due to the reverse phase transformation.

Table 3: Model parameters of Fe-Mn₃₀-Si₆-Cr₅(wt%)

Parameter	Value	Parameter	Value
σ_y^m (MPa)	117.7	A_s (°C)	96
σ_y^a (MPa)	100.2	T_0 (°C)	79.4
σ_y^γ (MPa)	210	H_v (MPa)	30.7
ν	0.3	H_s (MPa)	632.5
μ (MPa)	46154	H_{sv} (MPa)	2000
λ (MPa)	69231	H_g (MPa)	1254
$\bar{\epsilon}_{\max}^{tr}$	0.05	n_v	0.45
ζ_m (MPa/°C)	0.086	n_s	0.55
ζ_a (MPa/°C)	0.036	n_{sv}	0.45
B (MPa/°C)	0.104	n_g	3.07
K_T (MPa/°C)	0.45	H_γ (MPa)	500
M_s (°C)	-25	H_χ (MPa)	-9

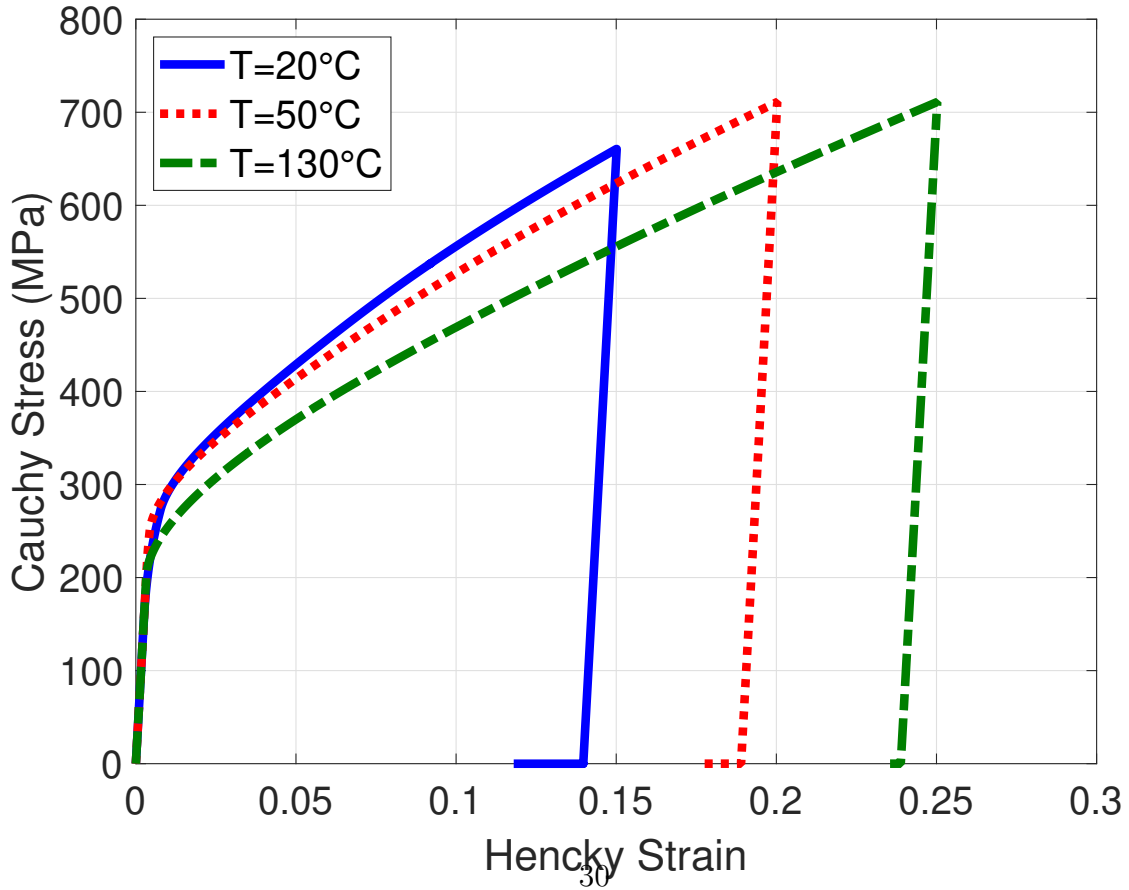


Figure 14: Finite strain current model response at different temperatures

370 Looking at the evolution of the internal variables in figure 15, the activation of the
 371 plasticity initially reduced the slope of the volume fraction of martensite. Then, the stable
 372 trend started when reaching 52% of the martensite. This is due to the trapped martensite
 373 variants (unlike the classical SMA which can be totally transformed). At this level, the
 374 accumulative plastic strain slope increased until reaching the desired strain.

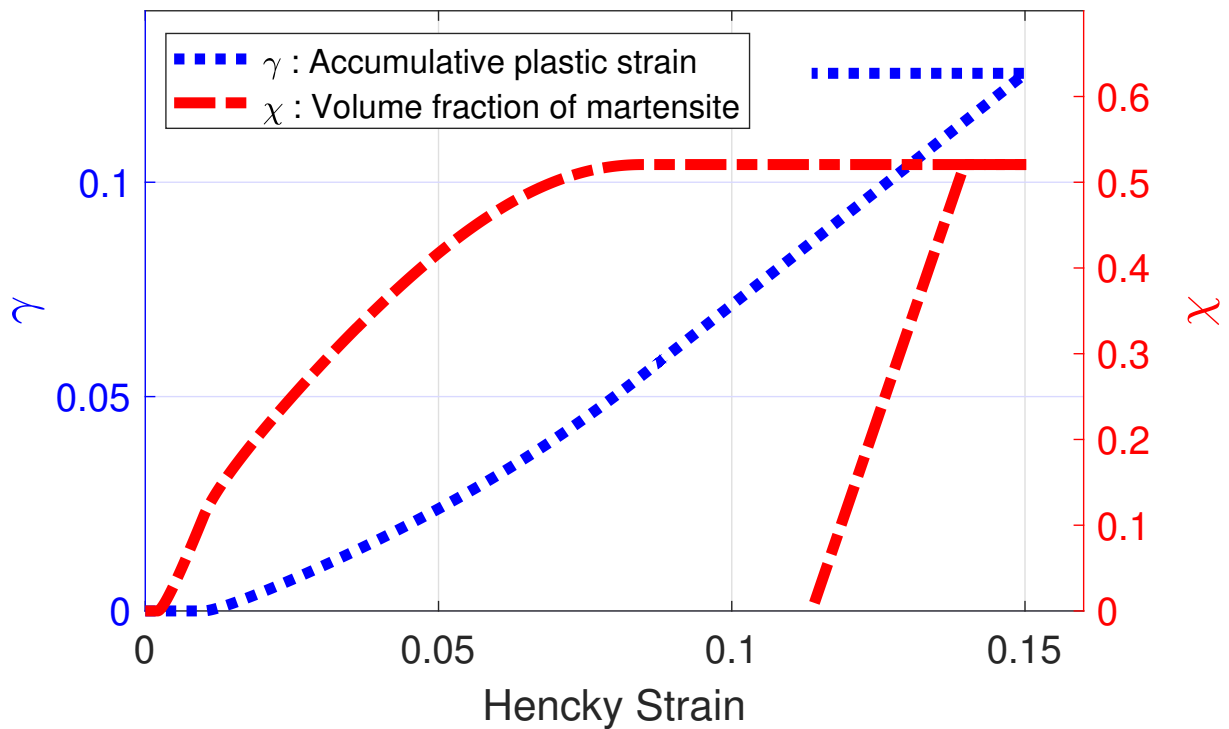


Figure 15: Evolution of the volume fraction of martensite and the accumulative plastic strain function of strain at 20°C

375 For the 50°C temperature, only 27 % of martensite is created (figure 16), which decreases
 376 the recovered strain (figure 14).

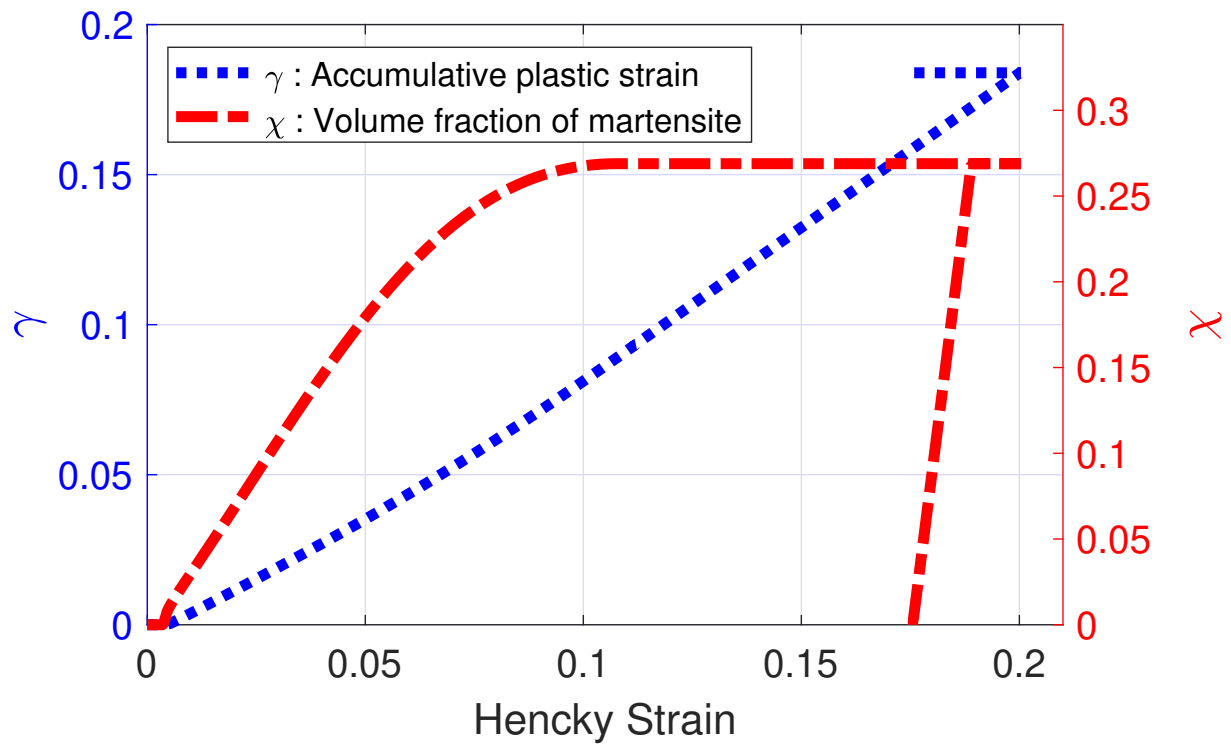


Figure 16: Evolution of the volume fraction of martensite and the accumulative plastic strain function of strain at 50°C

377 At the 130°C temperature, the accumulative plastic strain is activated initially (figure
 378 17), and then, the martensite appears in consistency with the experimental observations on
 379 the temperature dependence of yield stresses outlined in the work of Bouraoui et al. (2008).
 380 This created martensite is in the order of 6.6 %, which recovers a small part of the strain
 381 (figure 14).

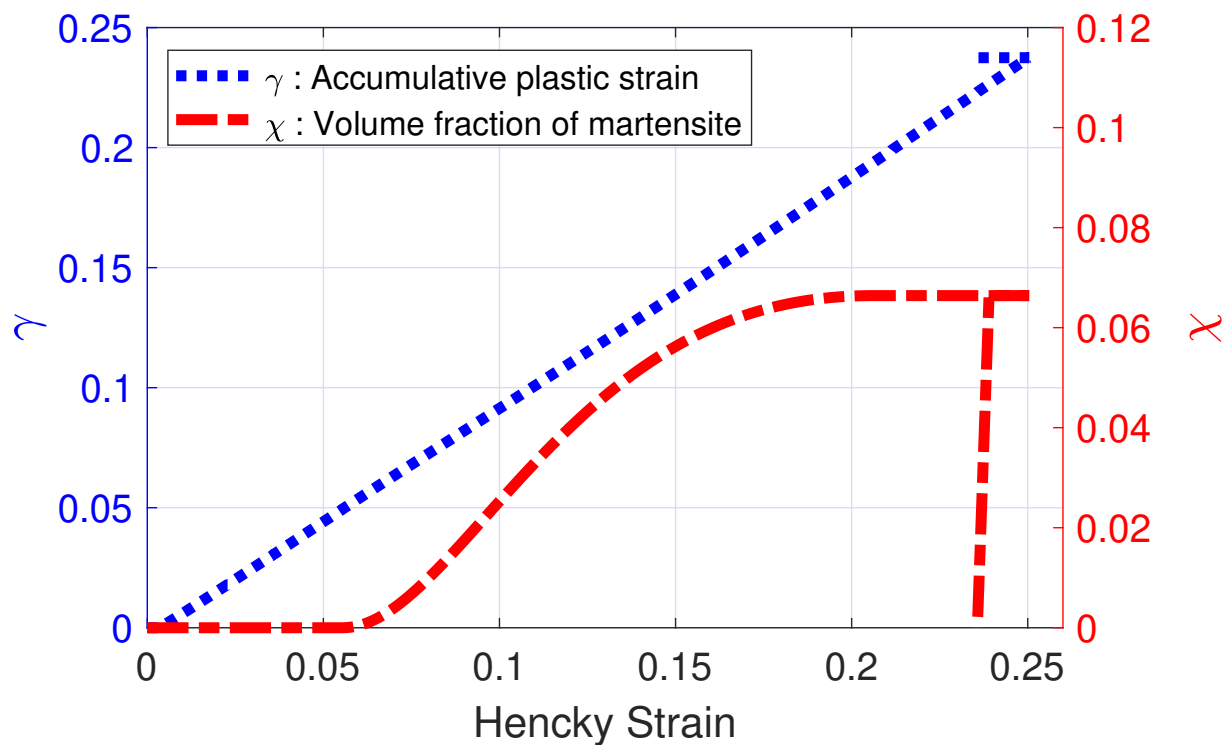


Figure 17: Evolution of the volume fraction of martensite and the accumulative plastic strain function of strain at 130°C

382 For the Fe-SMA, increasing the strain activates the plasticity and prevents the phase trans-
 383 formation activation. This is the reason, in figures 18 and 19, the phase transformation
 384 strain quantities even in the 20°C test are very small compared to the plastic strain.

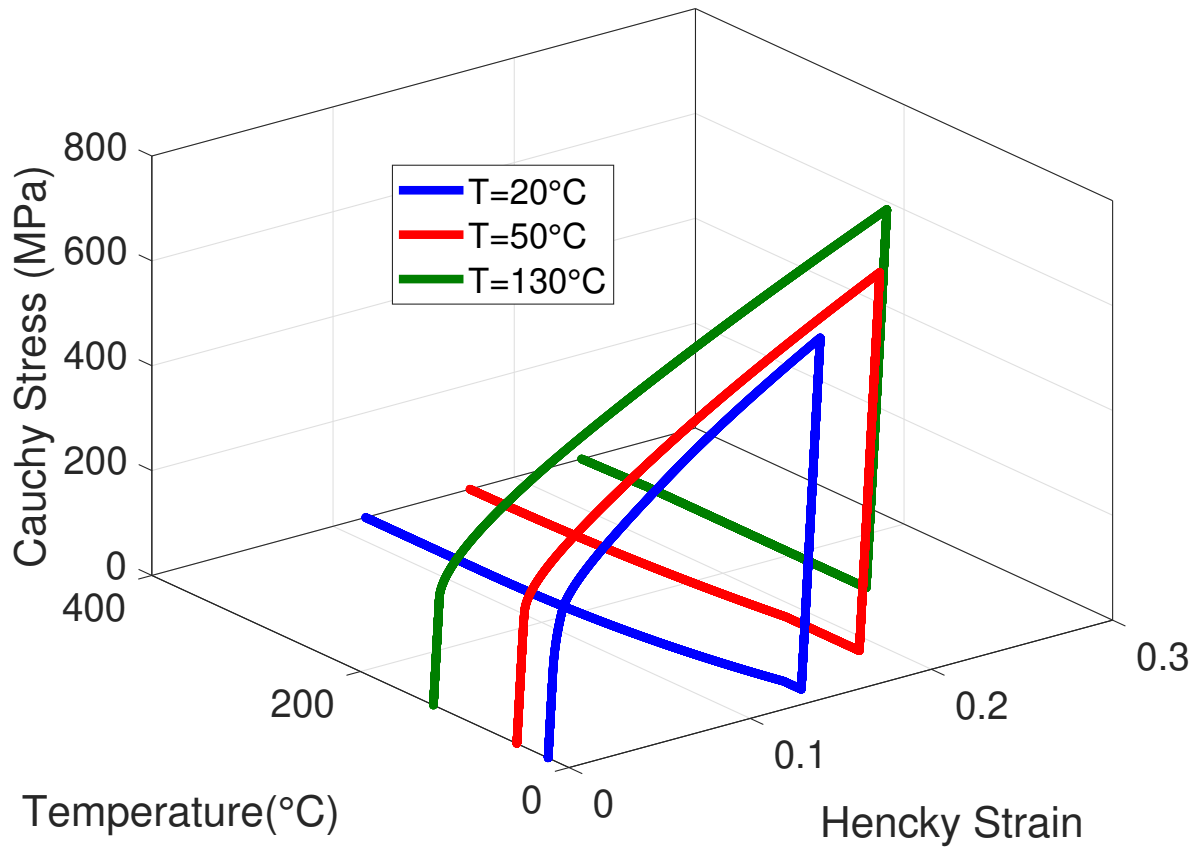


Figure 18: Finite strain 3D stress-strain-temperature diagram

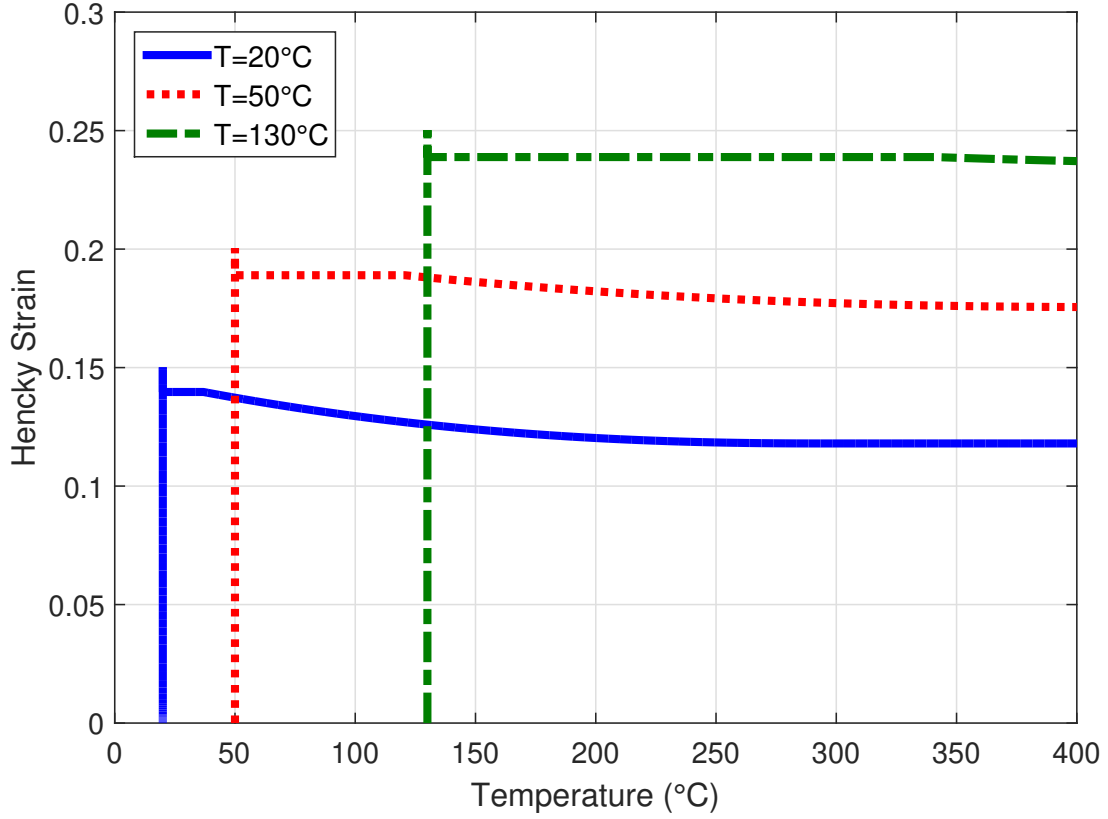


Figure 19: Shape memory effect of an Fe-SMA response in finite strain

385

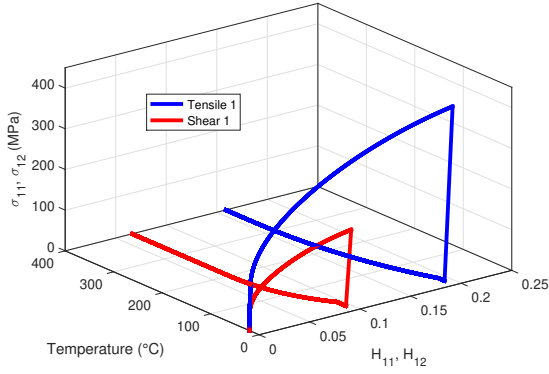
386 5.3. Results for multi-axial loadings with high strain levels

387 In order to show the validity of the proposed model in the case of multi-axial loadings, an
 388 investigation of its prediction range under different complex loading paths (tensile-shear and
 389 bi-axial tensile tests) has been carried out within the large strain framework. The increment
 390 of the deformation gradient in the case of tensile-shear test has been defined as follows:

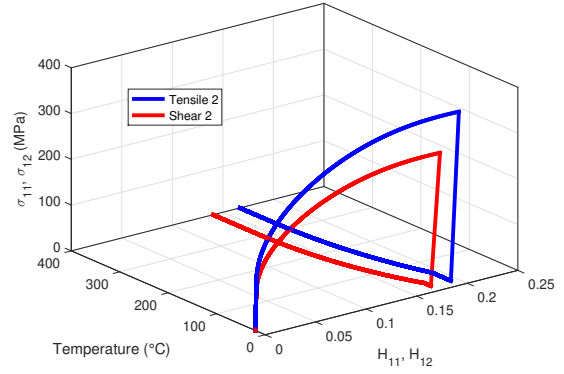
$$\Delta \mathbf{F} = \begin{bmatrix} \varrho & \pi & 0 \\ 0 & \frac{1}{\sqrt{e}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{e}} \end{bmatrix} \quad (55)$$

391 Two different values of the ratio between tension and shear strains have been defined ($\theta =$
 392 $\frac{H_{12}}{H_{11}}$ is equal to 0.5 or 0.9). Figure 20 presents the 3D stress-strain-temperature diagram

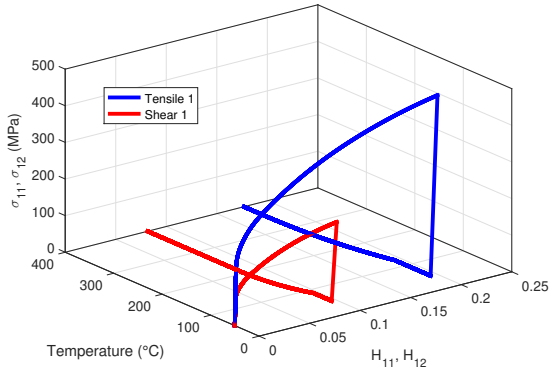
393 for the applied tensile-shear loading at three constant temperatures and under two different
394 loading cases. The obtained results show that by increasing the ratio θ , the shear effect
395 on the global behavior becomes more pronounced. At 20°C (figures 20a, 20b), the normal
396 stress level inducing the transformation or plasticity is lower than the one for pure tension.
397 Indeed, the shear stress component significantly contribute on the driving forces for phase
398 transformation and plasticity. More than that, the ratio ($\theta = \frac{H_{12}}{H_{11}}$) modifies the recovered
399 normal strain component. For the first ratio ($\theta_1 = 0.5$) after heating cycle the recovered
400 normal strain is about 3.4% whereas the second ratio ($\theta_2 = 0.9$) leads to only 2.65% of
401 recovered normal strain. Furthermore, for the second ratio ($\theta_2 = 0.9$), the maximum reached
402 normal stress decreases compared to the loading with the first ratio ($\theta_1 = 0.5$). To remind,
403 this value (the normal stress) is much higher in the case of pure tension. At 50°C (figures
404 20c, 20d), the same effect has been observed. At this temperature and like uni-axial tests,
405 the recovered strain decreases. Additionally, shear loading has an influence on the recovered
406 strain which decreases from 1.64% in the first ratio ($\theta_1 = 0.5$) to 1.31% in the second ratio
407 ($\theta_2 = 0.9$). At 130°C (figures 20e, 20f), for both ratios (θ_1 and θ_2) the transformation strain
408 remains negligible compared to plastic strain. As already seen for other temperatures, the
409 normal stress decreases by increasing the ratio value.



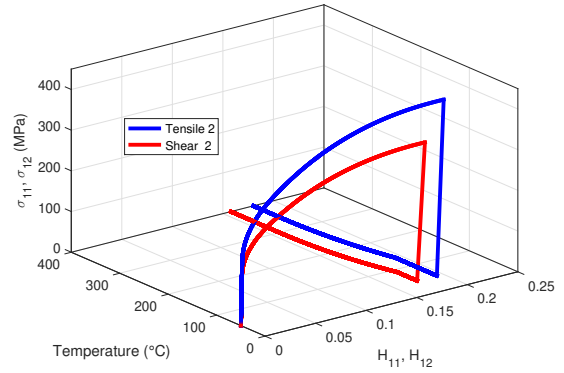
(a) $T=20^{\circ}\text{C}$, $\theta_1=0.5$



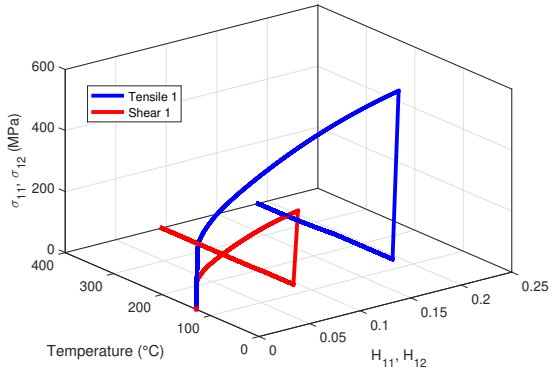
(b) $T=20^{\circ}\text{C}$, $\theta_2=0.9$



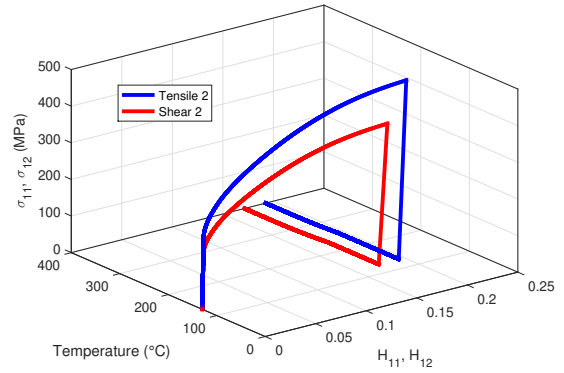
(c) $T=50^{\circ}\text{C}$, $\theta_1=0.5$



(d) $T=50^{\circ}\text{C}$, $\theta_2=0.9$



(e) $T=130^{\circ}\text{C}$, $\theta_1=0.5$



(f) $T=130^{\circ}\text{C}$, $\theta_2=0.9$

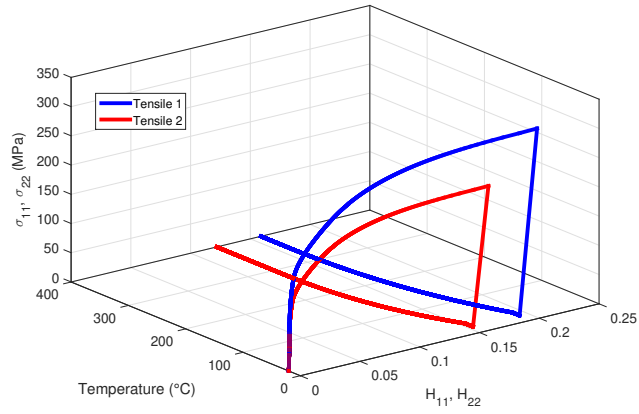
Figure 20: Combined tensile-shear test at different temperature and loading levels: (a-b) 20°C , (c-d) 50°C and (e-f) 130°C

410 Another complex loading path is investigated. It corresponds to a bi-axial tensile loading
 411 with a strain ratio ($\theta_3 = \frac{H_{22}}{H_{11}} = 0.8$) and at different constant temperatures. The increment

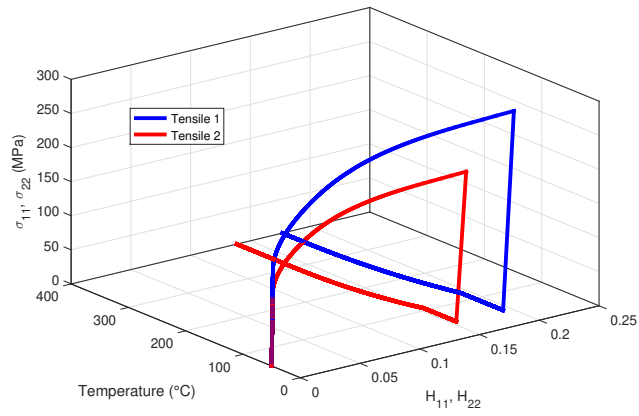
412 of the corresponding deformation gradient has the following expression:

$$\Delta \mathbf{F} = \begin{bmatrix} \varrho_1 & 0 & 0 \\ 0 & \varrho_2 & 0 \\ 0 & 0 & \frac{1}{\varrho_1 \varrho_2} \end{bmatrix} \quad (56)$$

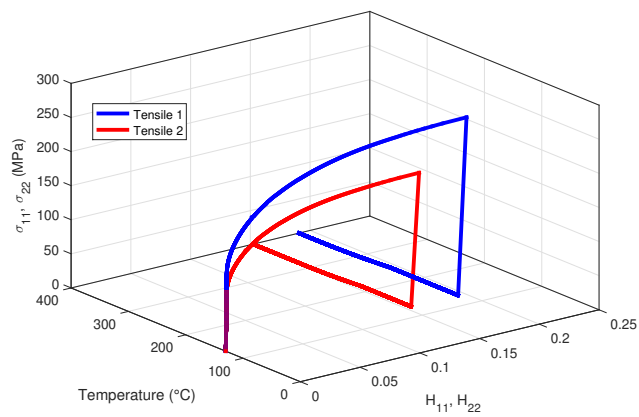
413 Figure 21 presents the 3D stress-strain-temperature diagram. The combined bi-axial test has
414 an influence on the yield stress for phase transformation and plasticity because of changes on
415 the equivalent stress. Figure 21a presents the 20°C bi-axial test. At this temperature, 3.17%
416 of normal strain has been recovered due to the phase transformation compared to 3.92% of
417 strain recovered in the case of pure tension. Furthermore, the maximum reached normal
418 stress decreases compared to the pure tension. Also, at 50°C (figure 21b) the recovered
419 normal strain and the maximum reached stress decrease comparing to pure tension test. At
420 130°C (figure 21c), the plasticity dominates the Fe-SMA behavior. Similar to the previous
421 temperatures, in the bi-axial case the maximum reached normal stress decreases compared
422 to pure tension one.



(a) $T=20^{\circ}\text{C}$, $\theta_3=0.8$



(b) $T=50^{\circ}\text{C}$, $\theta_3=0.8$



(c) $T=130^{\circ}\text{C}$, $\theta_3=0.8$

Figure 21: Bi-axial tensile test: (a) 20°C (b) 50°C and (c) 130°C

423 All the presented results show the capability of the proposed model to predict simple and
424 complex loading paths at large strain levels.

425 6. Conclusions and prospects

426 In this paper, a constitutive finite-strain model for Iron-based SMAs (Fe-SMAs) is devel-
427 oped by generalizing the small-strain model. The finite-strain model is formed based on a
428 multiplicative decomposition of the deformation gradient into elastic and inelastic elements.
429 Furthermore, the inelastic deformation gradient is consists of elements of phase transforma-
430 tion and plasticity. The constitutive equations are derived in a thermodynamically consistent
431 framework involving Clausius-Duhem inequality. The constructed Lagrangien is a combi-
432 nation of a hyper-elastic and an inelastic energies that represent the part of the free energy
433 of Helmholtz. The other part is a corresponding inner potential to introduce the conditions
434 for, the martensite volume fraction. The coupling between the phase transformation and
435 the plastic slip represents the distinguished behavior of the Fe-SMAs. In this model, two
436 internal variables have been defined; the volume fraction of martensite χ and the accumu-
437 lative plastic strain γ . These variables are related to the different gradients of deformation.
438 Furthermore, an exponential scheme is used to update the deformation gradients, and it is
439 adopted to circumvent the singularity problems of the linear method.

440 An implicit integration scheme based on the Newton-Raphson method is applied to quantify
441 the martensite volume fraction and the plastic slip by adopting an elastic predictor-inelastic
442 corrector method for handling the corresponding stress-strain values. After calibration, the
443 algorithm predicts the internal variable increments with respect to discrete-time. The ob-
444 tained results either in small or finite strain simulations fulfill the fact that the internal
445 variables evolve in accordance with the activated behavior. This new model is in good
446 agreement with experimental data. Also, different temperatures simulations are made for
447 higher strain levels to predict an Fe-SMA response.

448 As perspective, this model will be implemented in the finite element code Abaqus via the
449 subroutine UMAT in order to predict the response of an Iron-based SMA with complex
450 geometry and/or under complex loading paths at large strains. Also, large displacements
451 and rotations applications can be simulated with this model in order to check its capacity.
452 Taking the mechanical forming simulation such us (lamination, stamping, ...) can be con-

453 ducted by advantages of this model by comparing it with those developed in small strains.
454 Since the present work does not take into account of the latent heat, as a future work, it
455 will be addressed to model the effect of loading rates on the structure response. Also, the
456 non-Schmid average effect at the macroscopic scale can be integrated in the future work by:
457 i) replacing the scalar interaction parameters by a tensorial ones leading to an anisotropic
458 interactions and hardening, ii) introducing a transformation saturation function taking into
459 account the difference between tension and compression. Finally, larger strain experimental
460 basis data will be required to verify the predicted behavior model response.

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