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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 1. Introduction

Conventional materials have long been used for their structural properties. However, con-2 tinuous technological innovation in advanced fields such as aeronautics, bio-medical, energy 3 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 5 such as sensing, actuation, etc. In this category of so-called functional, adaptive or intelligent 6 materials, the most widely used materials are those having electrical/mechanical (piezo-7 electric), magnetic/mechanical (magnetostrictive) or thermal/mechanical (shape memory 8 allovs) coupling (e.g. Kim and Kwon (2015); Ojha and Schitoglu (2016); Lookman et al. 9 (2017); Xue et al. (2018); Jella et al. (2019)). 10

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 microstucture, 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, 18 etc.), Nickel-Titanium-based SMAs (Ni-Ti, Ni-Ti-Nb, etc.) and Iron-based SMAs (Fe-Mn-19 Si, Fe-Ni-Co, etc.). In particular, Iron-based SMAs (Fe-SMAs) are distinguished from other 20 SMAs by their thermomechanical coupling between martensitic transformation and plastic 21 slip. Koval et al. (1979) noticed a shape memory effect on Fe-Ni-Co-Ti steel. The discovery 22 of this new material was better recognized after the research of Sato et al. (1982) on Fe-Mn-23 Si that reveals the same shape memory effect. Since then these new materials have been 24 recognized by the name Iron-based SMAs. Fe-SMAs drew a lot of attention for their use of 25 various applications due to their low cost and their good mechanical properties. The shape 26

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

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

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.

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

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

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

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

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

135 2. Kinematic framework

136 2.1. Deformation gradient

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

$$\mathbf{F} = \mathbf{F}_{el}\mathbf{F}_{ine} = \mathbf{F}_{el}\mathbf{F}_{tr}\mathbf{F}_{pl} \tag{1}$$

The phase transformation-plasticity evolution diagram of yield stresses as a function of temperature (Olson and Cohen, 1972); (Bouraoui et al., 2008), describes the behavior of Fe-SMAs. Two domains are differentiated by the temperature T_0 (labeled Ms^{σ} in Bouraoui et al. (2008)) as shown in figure 1-(b). If the temperature of the material is lower than the temperature T_0 , the phase transformation of the austenite to martensite has priority. Otherwise, the activation of the plasticity in the austenite takes place, preventing the nucleation 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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The inelastic behavior of Fe-SMAs is induced by phase transformation and plastic slip for
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:

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

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

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

179

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

180

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

181

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

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

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:

$$0 \le \chi \le 1 \tag{15}$$

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:

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

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

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

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

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

¹⁹⁵ 3.2. Inelastic driving and yield forces

At this step, the second law of thermodynamics is taken into account. It asserts that the entropy production rate ξ is always greater than or equal to the heating rate (heat flux vector \mathbf{q} multiplied by the temperature gradient grad T) divided by the temperature T. As a result, the Clausius-Duhem inequality takes the following form:

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

with S being the second Piola-Kirchhoff tensor. The temperature is assumed homogeneous
on the RVE.

$$\operatorname{grad} T = 0 \tag{20}$$

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

$$\mathbf{C}_{el}\frac{\partial\mathfrak{F}}{\partial\mathbf{C}_{el}} = \frac{\partial\mathfrak{F}}{\partial\mathbf{C}_{el}}\mathbf{C}_{el} \tag{21}$$

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

$$\mathbf{D}_{ine} = \mathbf{D}_{tr} + \mathbf{D}_{pl} \tag{22}$$

208

$$\mathbf{D}_{tr} = \dot{\chi} \bar{\varepsilon}_{\max}^{tr} \mathbf{N}^{tr} \tag{23}$$

209

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

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:

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

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

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

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

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

215

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

216

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

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

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

219

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

²²⁰ The residual inequality leads to:

$$\Lambda^{\chi}_{dr}\dot{\chi} + \Lambda^{\gamma}_{dr}\dot{\gamma} \ge 0 \tag{32}$$

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

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

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

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

$$\mathbf{M} = 2\mathbf{C}_{el} \frac{\partial \Im}{\partial \mathbf{C}_{el}} \tag{35}$$

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

$$\dot{\gamma} = \dot{\kappa}^{\gamma}$$

$$\dot{\chi} = \dot{\kappa}^{\chi} Sgn(\Lambda_{dr}^{\chi})$$
(36)

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

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

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

232

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

233

$$\Lambda_y^{pl} = \sigma_y^{\gamma} - K_T T \tag{39}$$

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

$$\Upsilon^m_{tr} = \Lambda^{\chi}_{dr} - \Lambda^{tr,m}_y \tag{40}$$

242

$$\Upsilon^a_{tr} = -\Lambda^{\chi}_{dr} - \Lambda^{tr,a}_y \tag{41}$$

243

$$\Upsilon^a_{pl} = \Lambda^\gamma_{dr} - \Lambda^{pl}_y \tag{42}$$

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

$$\begin{split} \Upsilon^m_{tr} &\leq 0, \qquad \dot{\chi} \geq 0, \qquad \dot{\chi}\Upsilon^m_{tr} = 0\\ \Upsilon^a_{tr} &\leq 0, \qquad -\dot{\chi} \geq 0, \qquad -\dot{\chi}\Upsilon^a_{tr} = 0\\ \Upsilon^a_{pl} &\leq 0, \qquad \dot{\gamma} \geq 0, \qquad \dot{\gamma}\Upsilon^a_{pl} = 0 \end{split}$$
(43)

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

249 4. Constitutive equations: Resolution algorithm

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

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

$$\mathbf{S} = \mu \mathbf{C}_{ine}^{-1} + (\lambda \ln (J) - \mu) \mathbf{C}^{-1}$$
$$\mathbf{M} = \frac{\mu}{2} \mathbf{C}_{ine}^{-1} \mathbf{C} \mathbf{C}_{ine}^{-1} + \frac{1}{2} (\lambda \ln (J) - \mu) \mathbf{C}_{ine}^{-1}$$
$$\boldsymbol{\sigma} = \frac{1}{4} \mathbf{F} \mathbf{S} \mathbf{F}^{T}$$

Loading functions

$$\Upsilon^m_{tr} = \Lambda^{\chi}_{dr} - \Lambda^{tr,m}_y$$

 $\Upsilon^a_{tr} = -\Lambda^{\chi}_{dr} - \Lambda^{tr,a}_y$
 $\Upsilon^a_{pl} = \Lambda^{\gamma}_{dr} - \Lambda^{pl}_y$

Kuhn-Tucker conditions on the loading functions

$$\begin{split} \Upsilon^m_{tr} &\leq 0, \qquad \dot{\chi} \geq 0, \qquad \dot{\chi} \Upsilon^m_{tr} = 0 \\ \Upsilon^a_{tr} &\leq 0, \qquad -\dot{\chi} \geq 0, \qquad -\dot{\chi} \Upsilon^a_{tr} = 0 \\ \Upsilon^a_{pl} &\leq 0, \qquad \dot{\gamma} \geq 0, \qquad \dot{\gamma} \Upsilon^a_{pl} = 0 \end{split}$$

Kuhn-Tucker conditions on the state variables

$$\ell_1 \ge 0, \ \ell_1 \chi = 0$$

 $\ell_2 \ge 0, \ \ell_2 (1 - \chi) = 0$

Flow rules

$$\mathbf{D}_{ine} = \mathbf{D}_{tr} + \mathbf{D}_{pl}$$
$$\mathbf{D}_{tr} = \dot{\chi} \bar{\varepsilon}_{\max}^{tr} \mathbf{N}^{tr}$$
$$\mathbf{D}_{pl} = (1 - \chi) \dot{\gamma} \mathbf{N}^{pl}$$

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

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

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

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

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

$$T^{n+1} = T^n + \Delta T \tag{47}$$

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

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

$$\mathbf{F}_{pl}^{n+1} = \exp(\Delta \mathbf{D}_{pl}^{n+1}) \mathbf{F}_{pl}^{n}$$
(48)

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

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

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

285

$$\gamma^{n+1} = \gamma^n + \Delta \kappa^\gamma \tag{50}$$

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

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

$$\Delta \mathbf{D}_{tr}^{n+1} = \Delta \kappa^{\chi} \bar{\varepsilon}_{\max}^{tr} \mathbf{N}_{tr}^{n} \tag{51}$$

290

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

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

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

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



Figure 3: Solution algorithm

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
$ar{arepsilon}_{ m max}^{tr}$	0.048	n_v	0.44
$\zeta_m ~({\rm MPa}/^{\circ}{\rm C})$	0.086	n_s	0.55
$\zeta_a \ ({\rm MPa}/^{\circ}{\rm C})$	0.036	n_{sv}	0.45
$B \ (MPa/^{\circ}C)$	0.104	n_g	3.07
$K_T (\mathrm{MPa}/^{\circ}\mathrm{C})$	0.45	H_{γ} (MPa)	500
M_s (°C)	-25	H_{χ} (MPa)	-3

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

²⁹⁷ 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:

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

305 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-

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



Figure 4: Thermomechanical loading



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

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



Figure 6: Evolution of the volume fraction of martensite and the accumulative plastic strain function of strain at $20^{\circ}C$

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

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

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



Figure 9: Experimental and simulated stress-strain behavior at $130^{\circ}\mathrm{C}$



Figure 10: Evolution of the volume fraction of martensite and the accumulative plastic strain function of strain at $130^{\circ}C$

Figure 11 presents the 3D stress-strain-temperature diagram for the applied tensile load-346 ing at three constant temperatures. This diagram shows that the Fe-SMA behavior is af-347 fected by the sample's temperature. By going further from the M_s temperature, the plastic 348 behavior becomes dominant. Figure 12 shows the corresponding curves in the temperature-340 strain diagram. It is given that, after a loading-unloading cycle, the elastic strain is recovered 350 for each temperature. After heating, the strain is fully recovered at 20°C and only partially 351 recovered at 50°C. This behavior brings out that the inelastic strain has a reversible part 352 induced by phase transformation and a remnant part induced by plasticity. At 130°C tem-353 perature, the Fe-SMA behavior is purely plastic with a very low recovered strain during 354 heating. It appears that the present model predicts well the Fe-SMA behavior for small 355

strains. The next subsection presents the predicted Fe-SMA behavior for higher strainlevels.



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

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



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

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

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
$\lambda ~({ m MPa})$	69231	H_g (MPa)	1254
$ar{arepsilon}_{ m max}^{tr}$	0.05	n_v	0.45
$\zeta_m \ ({\rm MPa}/^{\circ}{\rm C})$	0.086	n_s	0.55
$\zeta_a \ ({\rm MPa}/^{\circ}{\rm C})$	0.036	n_{sv}	0.45
$B (MPa/^{\circ}C)$	0.104	n_g	3.07
$K_T (\mathrm{MPa/^{\circ}C})$	0.45	H_{γ} (MPa)	500
M_s (°C)	-25	H_{χ} (MPa)	-9

Table 3: Model parameters of Fe- Mn_{30} -Si₆- $Cr_5(wt\%)$



Figure 14: Finite strain current model response at different temperatures

Looking at the evolution of the internal variables in figure 15, the activation of the plasticity initially reduced the slope of the volume fraction of martensite. Then, the stable trend started when reaching 52% of the martensite. This is due to the trapped martensite variants (unlike the classical SMA which can be totally transformed). At this level, the 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 $20^{\circ}C$

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



Figure 16: Evolution of the volume fraction of martensite and the accumulative plastic strain function of strain at 50 $^{\circ}{\rm C}$

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



Figure 17: Evolution of the volume fraction of martensite and the accumulative plastic strain function of strain at $130^{\circ}{\rm C}$

For the Fe-SMA, increasing the strain activates the plasticity and prevents the phase transformation activation. This is the reason, in figures 18 and 19, the phase transformation 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

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

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

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

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



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

Another complex loading path is investigated. It corresponds to a bi-axial tensile loading 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:

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

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







(b) T=50°C, θ_3 =0.8



(c) T=130°C, θ_3 =0.8

Figure 21: Bi-axial tensile test: (a) $20^\circ\mathrm{C}$ (b) $50^\circ\mathrm{C}$ and (c) $130^\circ\mathrm{C}$

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

425 6. Conclusions and prospects

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

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

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

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

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