Ni-Mn-Ga single crystal Shape Memory Alloy magneto-thermo-mechanical modeling

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Abstract. In the frame of Thermodynamics of irreversible process, a model describing the thermomagneto-mechanical behavior of a single crystal of Ni-Mn-Ga is built. The choice of internal variables is linked to the physics of the problem (fraction of martensite variants, fraction of Weiss domains, magnetization angle). The simulations permit to describe the paths in the space (stress, temperature, magnetic field) in agreement with experimental tests. A special attention will be devoted to the control laws required to use these functional materials as sensors or actuators.

1 Introduction

The interest of Magnetic Shape Memory Alloys (MSMAs) compared with the classical Shape Memory Alloys (SMAs) is their possible activation not only by stress and temperature actions but also by magnetic field. A model of rearrangement process of martensite platelets in a non-stoichiometric Ni_2MnGa MSMA single crystal under magnetic field and (or) stress actions has been proposed by the same authors in [1]. The aim of this following paper is to extend these works purpose to the anisothermal behavior when including the process of martensite platelets reorientation and phase transformation austenite $\rightleftharpoons$ martensite.

Firstly, MSMA present the same properties as classical shape memory alloys but with the addition of a magnetic field sensibility. Several models are then devoted to the variant reorientation process. Some relatively old models are based on simple energy function [2], energy minimization [3,4] or using a magnetic stress to disconnect mechanical and magnetic behaviours [5]. One of the first thermodynamic approaches was built in [6] and the addition of internal variables in the thermodynamics of irreversible processes was proposed in [7,8] A very interesting experimental study concerning the shape memory and martensitic deformation response of Ni_2MnGa single crystals is performed by Callaway et al. [9]. Few papers relate the global modeling of MSMA including temperature, stress and magnetic field effects in the same formalism. The thermodynamical approach proposed in this paper is a relevant way to model the complex behaviour of MSMA in a global and macroscopic form.

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2 Gibbs free energy expression associated with a magneto-thermo-mechanical loading

The Gibbs free energy G expression can be split into four parts : the chemical one G_{chem} (generally associated with the latent heat of the phase transformation), the thermal one G_{therm} (associated with the heat capacity), the mechanical one G_{mech} and the magnetic one G_{mag}.

$$\begin{aligned} G(\underline{\Sigma}, T, \mathbf{H}, z_o, z_1, \ldots, z_n, \alpha, \theta, \alpha_A) = G_{chem}(T, z_o) + G_{therm}(T) \\ + G_{mech}(\underline{\Sigma}, z_o, z_1, \ldots, z_n) + G_{mag}(\mathbf{H}, z_o, \ldots, z_n, \alpha, \theta, \alpha_A) \end{aligned} \quad (1)$$

where the state variables are:

- $\underline{\Sigma} = \mathrm{diag}(0, \sigma, 0)$ the applied stress tensor,
- $\mathbf{H} = H \cdot \mathbf{x}$ the magnetic field,
- T the temperature.

The internal variables are:

- z_o the austenite volume fraction,
- z_k the volume fraction of martensite variant Mk ($k = 1 \ldots n$, i.e. the martensite presents n different variants),
- α the Weiss domain proportion inside a martensite variant (see figure 1),
- α_A the Weiss domain proportion inside the austenite phase A,
- θ the rotation angle of the magnetization vector $\mathbf{M}$ under the magnetic field $\mathbf{H}$.

The coupling between mechanic and magnetism is made by the choice of internal variables, for instance z_i, and not by the addition of an interaction term $G_{mech-mag}$ in the free energy.

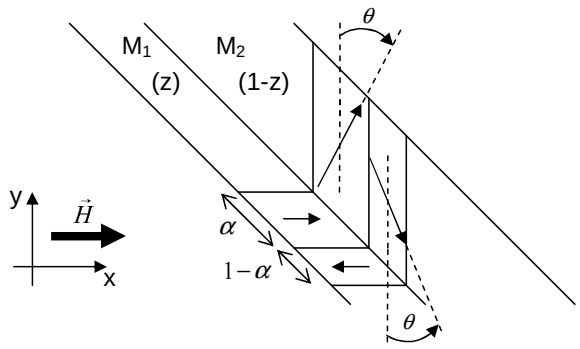

Fig. 1. Representative Elementary Volume (REV) when the sample is composed by only two martensite variants M_1 and M_2 ($z = z_1$ and $1 - z = z_2$).

For a Ni-Mn-Ga single crystal presenting three variants of martensite and a mother phase (cubic austenite $\rightleftharpoons$ tetragonal martensite), under thermal, magnetic loading and mechanical one, the Gibbs free energy expression can be:

$$\begin{aligned} &\rho G(H, \sigma, T, z_0, z_1, z_2, z_3, \alpha, \theta, \alpha_A) = u_o^M - T s_o^M + z_o(\Delta U - T \Delta S) \\ &+ C_p \left[(T - T_o) - T \cdot \log\left(\frac{T}{T_o}\right) \right] - \frac{\sigma}{2} \left((z_1 + z_3)\left(\beta_a^2 - 1\right) + z_2 \left(\beta_c^2 - 1\right) \right) \\ &- \frac{1}{2}\frac{\sigma^2}{E} + A z_o (1 - z_o) + K(z_1 z_2 + z_1 z_3 + z_2 z_3) - \mu_0 m_s(T) \left[z_1 \left((2\alpha - 1)H - \frac{m_s(T)}{2\chi_a}(2\alpha - 1)^2 \right) \right. \\ &\left. + (z_2 + z_3)\left(\sin(\theta) H - \frac{m_s(T)}{2\chi_t}(\sin(\theta))^2 \right) + z_0 \left((2\alpha_A - 1)H - \frac{m_s(T)}{2\chi_A}(2\alpha_A - 1)^2 \right) \right] \end{aligned} \quad (2)$$

with $\sum_{k=0}^{3} z_k = 1$, u_O^M and s_O^M the internal and entropy of martensite. $\frac{m_s(T)}{m_0} = \tanh\left[\frac{T_c m_s(T)}{m_O T}\right]$.

C_p is the heat capacity, E the Young modulus, $\beta_a = \frac{a}{a_0}$, $\beta_c = \frac{c}{a_0}$. a_0 lattice parameter of A. a and c lattice parameters of M; A and K constant belonging to the mechanical part of free energy G. T_c is the Curie temperature and m_0 the magnetisation at 0K. In order to simplify the model, m_0 and T_c parameters are considered as the same for austenite and martensite. μ_0, χ_a and χ_t are the vaccum magnetic permeabilty, the magnetic susceptibilities in the easy and transverse axis.

3 Clausius-Duhem inequality

In the classical frame of Thermodynamics of Irreversible Process, the total strain in **y** direction, the magnetization in **x** direction, and the entropy can be written as:

$$\varepsilon = -\frac{\partial \rho G}{\partial \sigma} \qquad \mu_o m = -\frac{\partial \rho G}{\partial H} \qquad s = -\frac{\partial \rho G}{\partial T} \tag{3}$$

A magneto-thermal effect takes place in the entropy expression due to the temperature dependence of m_s. This effect will be neglected in the present paper. The thermodynamical forces associated with the progression of the Weiss domains widths α, α_A and rotation angle θ are:

$$\frac{\partial \rho G}{\partial \alpha_A} = 0 \qquad \frac{\partial \rho G}{\partial \alpha} = 0 \qquad \frac{\partial \rho G}{\partial \theta} = 0 \tag{4}$$

The choice of the free energy expression confirms that the pure magnetic behavior is considered as reversible. Actually, the magnetization curves of the two martensite variants have no hysteresis on the figure 2 taken from [10].

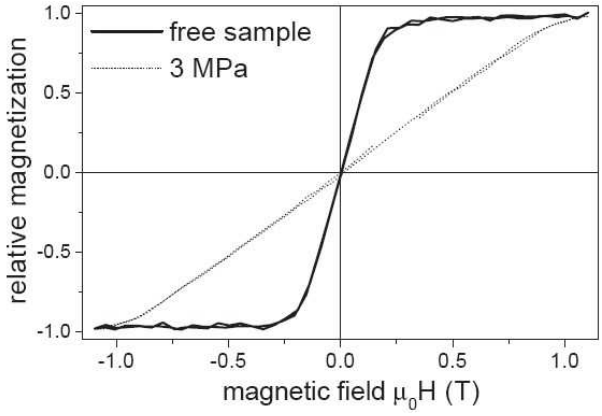

Fig. 2. Magnetization curves measured in easy (free sample) and hard (sample constrained by stress) magnetization directions [10].

Finally, the thermodynamical forces associated with the z_i martensite and austenite fractions are:

$$\pi_i^f = -\frac{\partial \rho G}{\partial z_i} \quad \text{for } i = 0, 1, 2, 3 \tag{5}$$

The mechanical behavior is highly irreversible, hence the Clausius-Duhem inequality has to be written:

$$dD = -\rho dG - \mu_o m dH - \varepsilon d\sigma - s dT \geq 0 \tag{6}$$

where dD is the dissipation increment. This expression can be reduced to:

$$dD = \pi_o^f dz_o + \pi_1^f dz_1 + \pi_2^f dz_2 + \pi_3^f dz_3 \geq 0 \qquad \text{with } \sum_{k=0}^{3} dz_k = 0 \tag{7}$$

3.1 kinetic equations (example with two variants)

In the previous inequality, three of the four variables are independent and the evolution depends on the configuration of the forces. For example, if the sample contains only two variants ($z_o = z_3 = 0$) during the evolution at constant temperature, then $z = z_1 = 1 - z_2$ and the Clausius-Duhem inequality becomes:

$$\begin{aligned} dD &= \pi_1^f dz_1 + \pi_2^f dz_2 \geq 0 \\ dD &= (\pi_1^f - \pi_2^f) dz_1 \geq 0 \end{aligned} \tag{8}$$

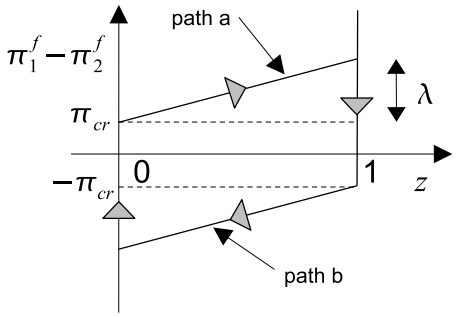

Fig. 3. Thermodynamical force $[\pi_1^f - \pi_2^f](\sigma, \alpha, \theta)$ as a function of the M_1 martensite fraction $z \in [0, 1]$.

An external loop, e.g. a complete rearrangement from $z = 0$ to $z = 1$ (path a) and from $z = 1$ to $z = 0$ (path b), is reported on figure 3. Rearrangement begins when $(\pi_1^f - \pi_2^f) \geq \pi_{cr}(T)$ for the path a and when $(\pi_1^f - \pi_2^f) \leq -\pi_{cr}(T)$ for the path b. After the rearrangement start, the behavior is modeled according to the following kinetic equations:

$$\dot{\pi}_1^f - \dot{\pi}_2^f = \lambda \dot{z} \qquad \text{with:} \qquad \dot{z} = \dot{z}_1 = -\dot{z}_2 \tag{9}$$

λ is considered as a constant value in the present paper. But, in [1], the value of λ was considered depending on the previous strain history. The concept of memorized point was introduced and a difference appears between partial loops and major loops. Moreover, $\pi_{cr}(T)$ is a function of the temperature as it was shown in [11]. A linear dependence is used in this paper as $\pi_{cr}(T) = \pi_{cr}^o + k_{cr}(A_S^o - T)$. Parameters are summarized in the table 1 with $\Delta S = \frac{2\Delta U}{As+Ms}$, $A = \frac{-\Delta S(As-Ms)}{2}$ and $\lambda_A = -\Delta S(Af - Ms)$.

A_S^o = 309.4 K	M_S^o = 301.7 K	$A = 5.48.10^5$ J/m^3
a_o = 5.84 Å	a = 5.95 Å	c = 5.60 Å
$E = 5.10^9$ Pa	$\lambda_M = 4.10^5$	$K = 0$
$\chi_a = 5$	$\chi_t = 1.05$	$\chi_A = 1.76$
T_c = 370 K	m_{S0} = 710 kA/m	$\lambda_A = 1.26.10^6$ J/m^3
$\pi_{cr}^o = 12.10^3$ J/m^3	k_{cr} = 800 Pa/K	

Table 1. Selected material parameters.

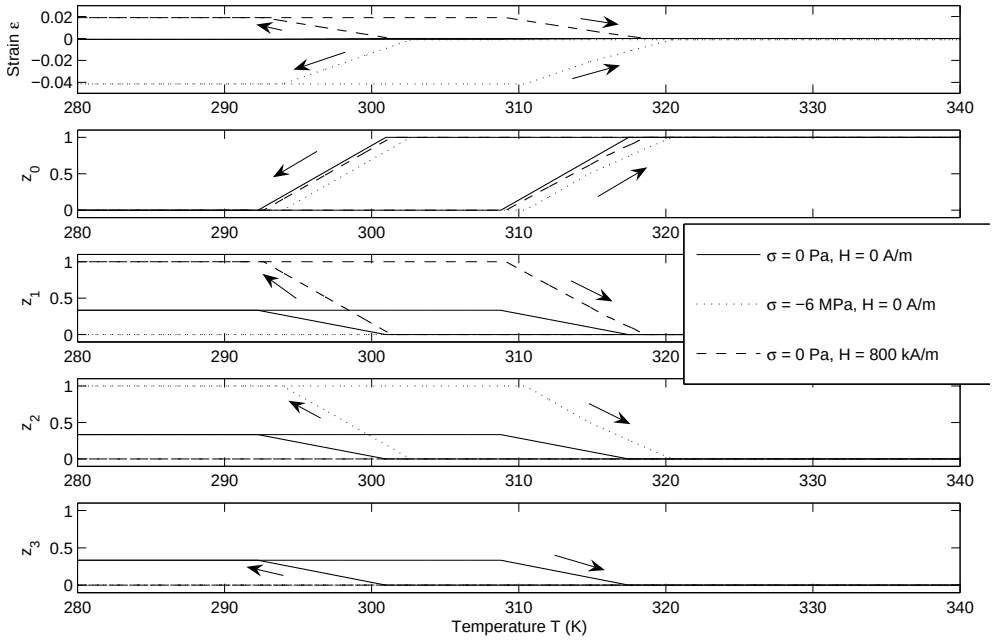

Fig. 4. Simulation results of thermal action with or without magnetic field and mechanical stress.

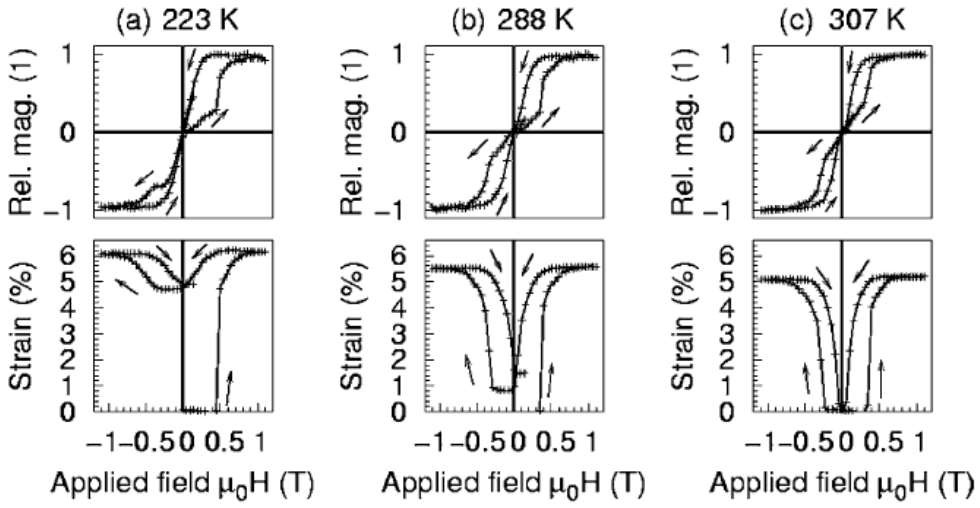

Fig. 5. Experimental results of strain and magnetization under magnetic action and constant stress ($\sigma = -1$ MPa) at different temperature levels (taken from [12]).

A numerical simulation was done with the help of the Matlab/Simulink® software. The powerful of the modeling approach presented here is that either mechanical (pseudo-elasticity and martensite re-orientation), thermal, and magnetic effects can be taken into account in the same numerical simulation. Some different cases will be considered in this section.

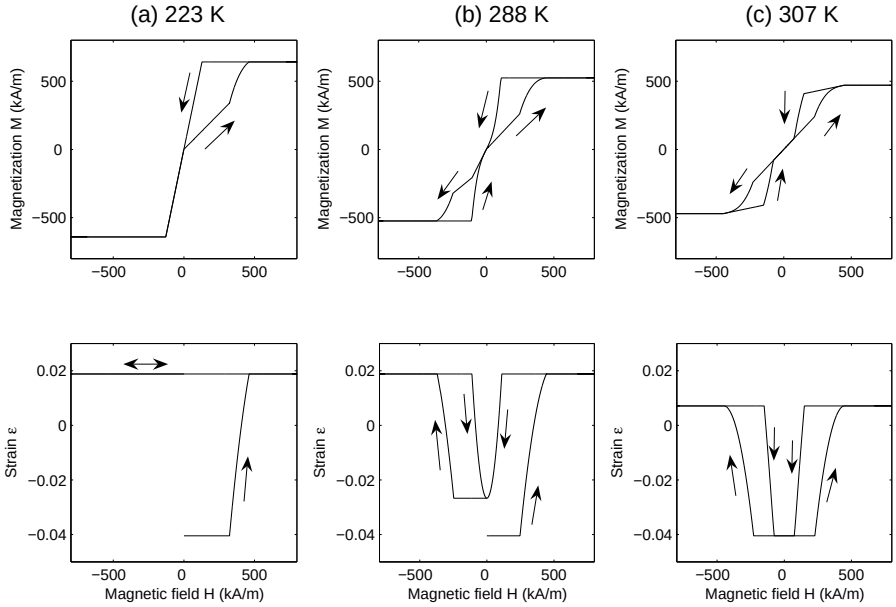

Fig. 6. Simulation results of strain and magnetization under magnetic action and constant stress at different temperature levels ($\sigma = -1$ MPa, experimental results in FIG. 5).

4 Conclusion

The purpose of this paper was to propose a full single crystal modeling of Magnetic Shape Memory alloys including the magneto-thermo-mechanical coupling. In the frame of the thermodynamics of irreversible processes, a model was proposed using a Gibbs free energy expression. As it can be seen in (2), the model is quite complicated and its use may be difficult. Nevertheless in practical applications and for specific conditions, some reductions can be made (isothermal process on 2D motions) and in such a case, the usefulness of the model is shown. For example, in the paper [13], an extension of the quasi-static isothermal model to the dynamical case was made, including the magnetic circuit creating the magnetic field and a dynamical load applied to the MSMA sample. A thermodynamic approach with hamiltonian modeling was used by the authors to design actuators [13] and new control laws [14]. Moreover, the thermodynamical approach proposed in this paper to model a specific MSMA can be easily extended to other materials, such as future MSMA monocristals and polycristals. Finally, this global model can be a basis to model MSMA in a Finite Element Analysis to design new mechanical structures for actuation and sensing applications.

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