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# Thermo-mechanical description of phase transformation in Ni-Ti Shape Memory Alloy

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**Abstract**

The pseudo-elasticity of Shape Memory Alloys is due to a change in volumetric fraction between the high temperature phase (Austenite) and the low temperature phase (Martensite) under a mechanical loading. When a tensile loading is considered, transformation bands occur leading to strong localization of the deformation and a strong local heating. The modeling of this strongly coupled phenomenon is discussed for a polycrystalline specimen in a multiaxial mechanical framework. Three different scales are considered: the variant scale (or phase scale), the single-crystal scale and the polycrystalline scale. The free energy of each variant is first computed from the loading and the geometrical lattice transformations associated to each variant. The volumetric fraction of each phase is then defined at the grain scale as function of their free energy. A simple averaging operation allows to estimate the deformation at the grain scale. The polycrystalline scale is not considered at present.

## 1. Introduction

Shape Memory Alloys (SMAs) are useful for several industrial applications. They exhibit a specific behavior, called pseudo-elasticity, which is the ability to deform into large proportion (up to 8% in tension) in a reversible manner, ie without residual deformation after unloading [1]. The pseudo-elasticity is associated to a nucleation of a phase called martensite (M) inside a parent phase called austenite (A). It is a martensitic solid-to-solid phase transformation, so called by analogy with the martensitic transformation of steel. This transformation can be induced either by thermal or multiaxial mechanical loading [2] . For the design of SMA structures, the development of efficient thermo-mechanical models for the Representative Volume Element (RVE) is necessary. Many models are available in the literature for describing the behavior of SMAs. Two different approaches can be highlighted. The

phenomenological models are interested in the behavior at a macro-scale using observations done at the same scale [3,4]. These approaches are based on continuum thermodynamics, and so able to describe the thermo-mechanical phenomena such as thermal emission and diffusion associated to the phase transformation [5]. They are usually restricted to uniaxial mechanical loadings and microstructural informations are not reachable. For micromechanical approaches, internal variables are defined at the microstructure scale [6, 7]: the phase transformation corresponds to a geometrical modification of the crystal lattice. This kind of modeling requires a large number of experimental data at the micro-scale and/or microstructural observations [8, 1]. Calculations usually involve a minimization of a functional that is highly time consuming.

The development of micro-macro multiaxial model where the full thermo-mechanical coupling is taken into account is relevant. The development of such approach relies on two key points. The first one is the definition of transition scale rules, depending on the microstructure of the studied material, and allowing estimating fluctuation of the local fields for a given macroscopic loading. The second one is an appropriate description of the behavior of constituents. Our proposition is to use simplifying hypotheses allowing a fast estimation for the thermo-mechanical behavior. Several scales can be chosen to define this behavior, leading to a multiscale calculation strategy. The first scale for which homogeneous chemical and mechanical state can be considered is the variant scale. The next scale is the single crystal scale. Averaging operations allow calculating the macroscopic quantities at the polycrystalline RVE final scale.

The particular behavior of a TiNi shape memory alloy is described in the first part. Thermo-mechanical measurements have been carried out thanks to full fields measurement performed during different tensile tests. The second part describes the key points of the multiscale multiaxial model (called "multivariant model"). The single-crystal model is applied to simulate a tensile/compressive uniaxial loading and to foresee the variant production and the deformation transformation. We observe a good agreement between experimental results and the modeling.

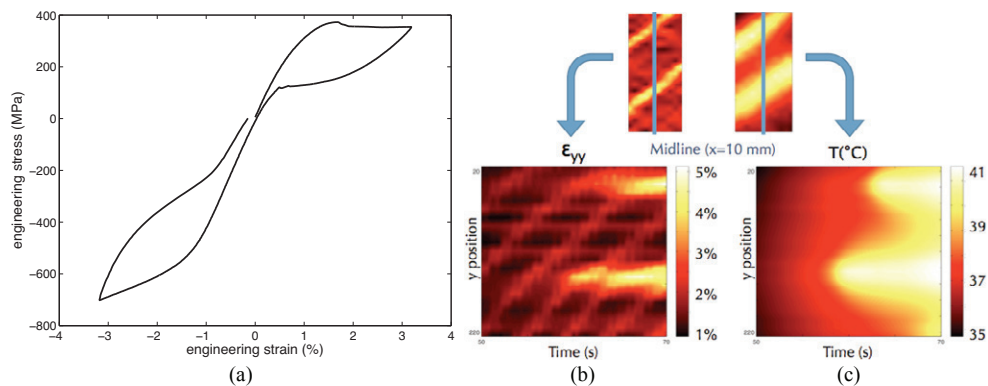## 2. Macro-scale behavior of a Ni- 49.6 at% Ti shape memory alloy



Fig. 1 : (a) Stress-strain curve of tensile-compressive test performed on Ni-Ti wire shape specimen at 28°C with a constant macro-strain rate $1.1 \times 10^{-4} s^{-1}$. Spacio-temporal maps of (b) longitudinal strain and (c) temperature measured by InfraRed Image Correlation (IRIC [11] ) during a tensile test on a flat specimen (section 2x20mm) at a macro-strain rate of $4.2 \times 10^{-4} s^{-1}$. The loading axis is vertical here.

A Nickel-Titanium SMA is considered (Ni- 49.6 at% Ti). Specimens for all experiments are wrought and underwent an annealing treatment at 450°C in salt bath for two minutes. It provides polycrystalline specimen with a mean grain size of about 30μm. At room temperature, the material is full Austenitic [11].

The tensile-compressive stress-strain curve performed on a wire specimen at 28°C is presented in fig.1-(a). In the tensile step, a plateau can be observed associated to a generation of localization bands. Besides, one can notice the clear dissymmetry of transformation threshold and hysteresis loops: martensitic variants produced in traction or compression are different. Tensile tests performed on flat specimen (20x2x120mm) allow the measurement of kinematics and thermal fields (fig. 1 (b) and (c)) [11] . Strain and temperature increase uniformly and simultaneously until strain equals 1% then localization occurs. The strain in the transformation bands rises until 5% before it saturates, and the bands enlarge. At the same step, the front bands temperature rises up to 7°C higher than in homogeneous areas, depending on the thermal condition and loading rate.

## 3. Multivariant model for phase transformation under thermal and multiaxial mechanical loading

The phase transformation described in the previous section involves three different scales: the variant scale (or phase scale), the single-crystal scale and the polycrystalline scale. The polycrystalline medium undergoes both thermal and mechanical loading that can be multi-axial. In a first approach, temperature $T$ is considered as a homogeneous loading over the medium: latent heat associated to the phase transformation and heat exchange are neglected. Since the elastic behavior of the single-crystal is different from the elastic behavior of the polycrystalline aggregate, the stress $\sigma$ is not homogeneous over the polycrystalline medium. Localization and homogenization tools have to be employed following Eshelby and Hill's approaches [9]. Inside the grains, M and A phases exhibit different crystallographic orientations, symmetries and so elastic properties. Stress is consequently heterogeneous too within the grain. Finally we make the common assumption that the transformation strain is homogeneous inside each variant of M phase.

Each phase is denoted $\phi$, considered as a substructure of a single-crystal or a grain denoted $g$ in a polycrystalline medium considered as a representative volume element (RVE). Each phase owns its crystallographic structure and orientation inferred from the parent phase. In the rest of the document a phase is corresponding to any M variant or A parent phase, exhibiting homogeneous elastic and chemical properties. Since the transformation deformation is homogenous in a phase, it can be computed from the transformation matrices for each variant and it is equal to zero for the A phase (reference phase).

The model we propose is a single crystalline model giving the volumetric fraction of each phase as function of their free energy. It is based on the simple fact that the phase (or variant) exhibiting the lowest energy under a specific loading has a higher probability to exist. This energy (that can be seen as Gibbs energy) is the sum of the elastic and chemical energies. In this approach we neglect the role of interfacial energies, assuming that they act in a similar manner on each phase. Another point is that this energy is strongly associated to a specific topography: this information is unknown.

The martensitic transformation corresponds to a deep change of the crystal lattice. This transformation leads to a distortion (shear) and a lattice rotation but the volume is usually constant. A transformation gradient operator can describe the phase transformation. We consider $\phi$ variants of martensite ($\phi=0$ denotes the austenite parent phase). The $U_{\phi, \phi=1...n}$ matrices are the transformation gradient operators. They give the pass from an initial configuration $\vec{r}_0$ to the deformed one $\vec{r}_\phi$ by:

$$\vec{r}_\phi = U_\phi \vec{r}_0$$

The transformation strain is defined as the Green-Lagrange tensor associated to the transformation:

$$\varepsilon_\phi^{tr} = E_\phi = \frac{1}{2}\left(U_\phi^T U_\phi - \underline{\underline{I}}\right)$$

In the following, the phase $\phi$ undergoes uniform thermal $T$ and mechanical $\sigma$, loadings. We consider $w_\phi^T$ the chemical energy and $w_\phi^\sigma$ the elastic energy. Each phase $\phi$ can be associated to a characteristic binding energy associated to the enthalpy $H_\phi$. Entropy $S_\phi$ has to be taken into account since we are

interested in an energy balance between different phases at different temperatures. A and M phases have their own enthalpy and entropy but enthalpy and entropy are supposed the same for all M variants whatever the origin of loading they are the result of (mechanical or thermal). This chemical energy considered in the balance is so the free enthalpy:

$$W_\phi^T = H_\phi - TS_\phi$$

The elastic energy is function of the local stress tensor $\sigma_\phi$ :

$$W_\phi^\sigma = \frac{1}{2}\left(\sigma_\phi : C_\phi^{-1} : \sigma_\phi\right)$$

$C_\phi$ denotes the stiffness tensor of a phase $\phi$. $C_\phi$ is different from one phase to another. In this expression the coupling with the phase transformation does not explicitly appear since the local stress is a complex function of the applied stress and internal stresses associated to the deformation transformation. The original formulation of stress localization is due to Hill [9] :

$$\sigma_\phi = \sigma_g + C^* : (\varepsilon_g - \varepsilon_\phi)$$

$\sigma_g$ is the stress tensor defined at the grain scale. $\varepsilon_\phi$ and $\varepsilon_g$ are the total deformation tensor at the phase and grain scale. C* is the so-called Hill's constraint tensor. It has been shown [10] using an hypothesis of uniform deformation that the elastic energy reduces to :

$$W_\phi^\sigma = W_g^\sigma - \sigma_g : \varepsilon_\phi^{tr}$$

$W_g^\sigma$ is an energetic term constant over the grain. This term does not participate to the energetic balance. It is taken as zero. The total free energy considered at the phase scale is given by:

$$W_\phi = H_\phi - T.S_\phi - \sigma_g : \varepsilon_\phi^{tr}$$

This general expression is completed by an energetic term allowing to model the delay associated to the germination of a phase (latent heat), depending of the history of loading. It is denoted $L_\phi$.

To each phase $\phi$, it is now possible to attribute a volume fraction $f_\phi$ function of its free energy and the free energy of the other phases. We use the Boltzmann probabilistic formula already applied to magneto-mechanical problems [10] :

$$f_\phi = \frac{\exp\left(-A_s.W_\phi\right)}{\sum_{\phi=0}^{n}\exp\left(-A_s.W_\phi\right)}$$

Parameter $A_s$ permits to adjust the fraction ratio comparing to the energy changes. The single-crystal transformation strain tensor is computed by a simple averaging of the transformation strain tensors:

$$\varepsilon_g^{tr} = \left\langle\varepsilon_\phi^{tr}\right\rangle = \sum_{\phi=0}^{n} f_\phi \varepsilon_\phi^{tr}$$

The modeling of the polycrystalline aggregate behavior is available since it can be described by an orientation distribution function (ODF). A first important step is to compute the stress at the grain scale as function to the stress applied at macro-scale thanks to a localization procedure [9]. A self-consistent method can be applied. The second step is the homogenization procedure, allowing reaching the deformation transformation at the macro-scale.

## 4. Simulation of a tensile-compressive test on a single-crystalline Ni- 49.6 at% Ti SMA

The martensitic transformation occurring in the Ni- $49.6\%_{at}$ Ti corresponds to a change of the cubic A parent phase into 24 monoclinic M variants exhibiting 12 distinct geometrical transformations [1]. If the A phase is considered as the reference lattice, the axes of monoclinic symmetry correspond to the $<110>_{Austenite}$ directions. The transformation tensors can be computed from the lattice parameters and the

orientation (see ref. [1, 2, 8]). The austenite parameter of the alloy is $a_0=3.014\text{Å}$, the martensite parameters are $a=2.889\text{Å}$, $b=4.12\text{Å}$, $c=4.622\text{Å}$, and angle $\beta=96.8°$ [8, 2]. The material constants used for the multivariant modeling are detailed in table 1.
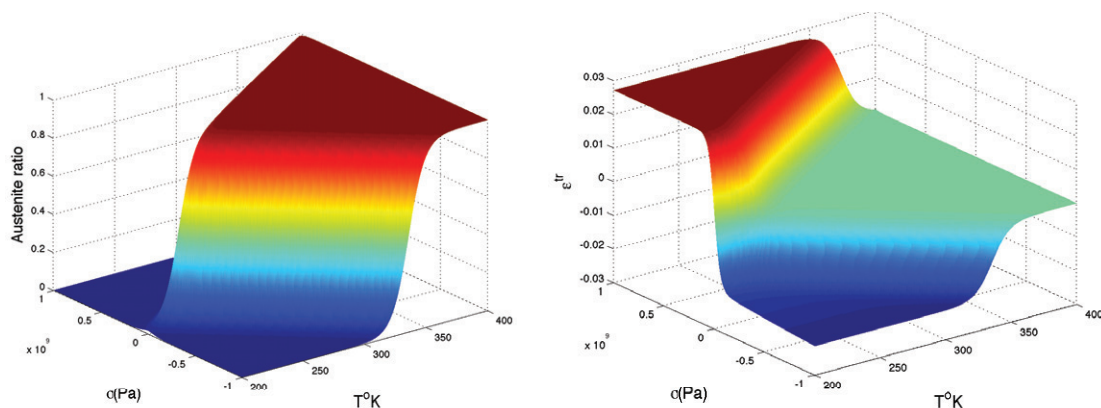


Fig. 2 : (a) Austenite ratio matrix for the explored $(\sigma,T)$ couples and (b) Macro transformation strain along the loading axis, both for the direct transformation (A→M).

| $\Delta H_{transformation}$ $(J/m^3)$ | $\Delta S_{transformation}$ $(J/m^3/K)$ | $L_M$ $(J/m^3)$ | $L_A$ $(J/m^3)$ | As (Adjustment) |
|---|---|---|---|---|
| $80 \times 10^6$ | $0.38 \times 10^6$ | $10 \times 10^6$ | $5 \times 10^6$ | $4 \times 10^{-7}$ |

Tab. 1 : Material and numerical parameters used for the multivariant modeling.

For obvious concision requirements, a simple simulation of a tensile-compressive test is presented. A perfectly oriented single-crystalline specimen is considered. Stress is applied along a *[100]* axis of the parent phase. The volume fraction of each phase is first computed as function of stress and temperature. Because of the difference between direct and reverse transformation, two sets of volume fractions are calculated. Figure 2.a plots for example the volume fraction of A phase as function of stress and temperature for a direct transformation (A => M). The transformation strain tensor at the single-crystal scale can then be computed by averaging. Figure 2.b gives the deformation obtained in the direction of the applied stress (*[100]* axis). When latent heat is considered (delay between A=>M and M=>A transformations) direct and reverse transformations give a different set of volume fraction leading to transformation hysteresis loop. Such a simulated uniaxial test in quasi-isothermal conditions (law rate) is represented in figure 3. It is a simple tensile compressive test between 1000MPa and -1000MPa. The tension/compression dissymmetry is clearly highlighted (fig.3.a). Figure 3.b shows that this dissymmetry is associated to a dissymmetry in the M variants production.

According to these preliminary results, the model gives a good qualitative description of the different behaviors depending on the loading conditions and valuable information regarding the phase partition. Besides, the multi-axial nature of the model allows us to test many loading stories in many thermal conditions. Extension to polycrystalline media is going on.
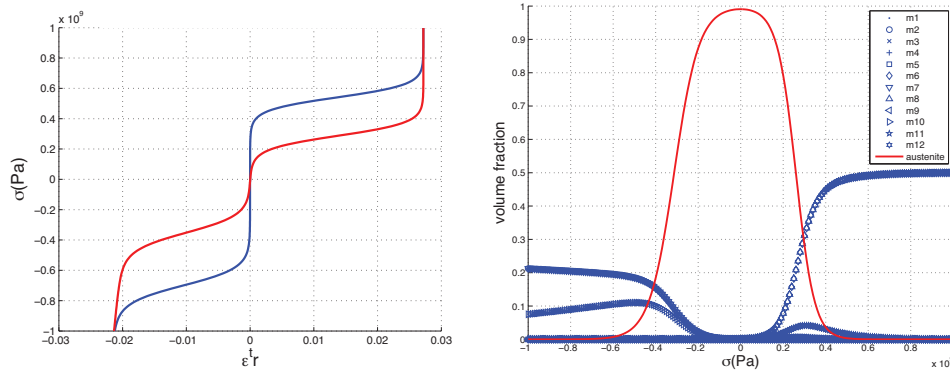
Fig 3: (a) stress versus macroscopic transformation strain  (elasticity is not considered) (b) volume fraction evolution for each phase during the tensile test.

## 5. Conclusion and outlooks

In this paper, a micro-macro multi-axial model has been proposed in order to take into account the full thermo-mechanical coupling in SMA. At the micro-scale, the model is based on the geometrical modification of the crystal lattice, with respect to temperature and mechanical loading. The volumetric fraction of phase is calculated thanks to Boltzmann type statistical energy considerations. Numerical estimation of single-crystal indicators such as prediction of variants or transformation strain are in qualitative good agreement with experimental observations. The next step is the introduction of the single-crystal modeling in a polycrystalline framework. Prediction of localization bands and heat diffusion for a specimen submitted to a uniaxial tensile strengthening requires -1- the introduction of the RVE constitutive law in a finite element code -2- the real-time resolution of the heat diffusion equation.

For now, numerous parameters have been chosen arbitrary. We plan to perform experimental campaigns in order to measure some material parameters (e.g. lattice parameters, enthalpies and entropies). Peculiar in-situ tests instrumented with full thermal and kinematics fields measurement will allow to identify the thermal local and structural parameters, and the numerical adjustment variable $A_s$.

The scientific approach developed here can be applied to others SMA systems than TiNi.

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