

Thermomechanical Behavior of Shape Memory Alloys

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Abstract

The overall thermomechanical behavior of Shape Memory Alloys is described from a microphysical point of view. Results obtained in that way are in good agreement with uniaxial tension test experiments performed on a Cu - Zn - Al Shape Memory Alloy.

Introduction

Typical properties like Shape Memory Effect, Two-Way Shape Memory, Pseudoelasticity and very good damping capacity occur in metallic alloys which present a Thermoelastic Martensitic Transformation. These inelastic behaviors result from microstructural changes associated with this transformation, like the reversible formation of martensite plates or the interfacial motion between martensite variants [1,5].

But the different approaches proposed to describe these behaviors are not based on these physical mechanisms [6,9]. This paper presents a micromechanical simulation of the thermomechanical behavior due to stress-induced martensitic transformation.

In this scheme, the phase transition mechanism is described by the phenomenological theory of Wechsler-Lieberman and Read (W.L.R.) [10]. The habit plane orientation and the macroscopic distortion associated with the formation of each variant are then determined from the crystallographic parameters of parent and product phase.

At first, the different contributions to the overall deformation are detailed and the elementary mechanisms responsible for them described. After that, the local constitutive relation associated with the formation of stress-induced martensitic plates is determined from the study of the local energy balance. Results obtained in that way are in very good quantitative agreement for the single crystal case [11,12].

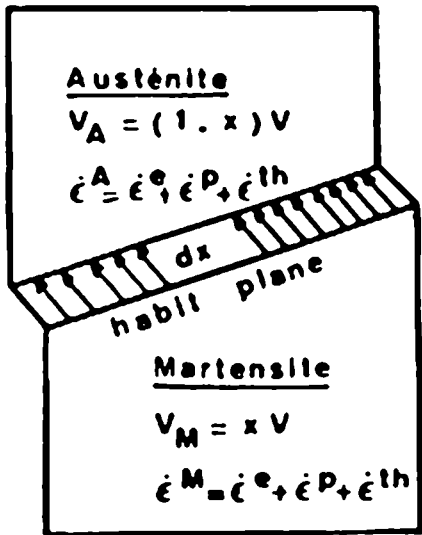
The polycrystalline thermomechanical behavior is deduced from this local behavior by using a self-consistent scheme. Numerical results are in good agreement with uniaxial tension test experiments performed on a Cu - Zn - Al Shape Memory Alloy.

Local Behavior

Let us consider a volume V of parent phase which transforms into martensite (Fig. 1). The macroscopic total strain E_{ij}^T is obtained by an averaging relation

$$E_{ij}^T = \frac{1}{V} \int_V \epsilon_{ij}^T(r) dV = (1-x) \epsilon_{ij}^A + x \epsilon_{ij}^M \quad (1)$$

where ϵ^A and ϵ^M denote the average total strain in austenite and martensite and x the volumic fraction of martensite. This total strain is caused by both the deformation in the two phases



(elastic, plastic...) and the deformation associated with the transformation. Thus, the strain rate equation is [13,14] :

$$\dot{\epsilon}_{ij}^T = (1-x) \dot{\epsilon}_{ij}^A + x \dot{\epsilon}_{ij}^M + \epsilon_{ij}^{AM} \dot{x} \quad (2)$$

ϵ^{AM} denotes the transformation strain, it is the only term directly associated with the transformation mechanism. The average strain rates in the two phases are composed of three terms of different physical meanings : an elastic strain rate $\dot{\epsilon}^e$, associated with local stresses, a thermal strain rate $\dot{\epsilon}^{th}$, and a plastic one $\dot{\epsilon}^p$. These last two contributions could be neglected for the study of the Shape Memory behavior.

Fig.1: Transformation of a volume V of austenite into martensite. If we consider that the elastic properties of the two phases are assumed to be equal, the total strain rate is expressed by :

$$\dot{\epsilon}_{ij}^T = \dot{\epsilon}_{ij}^e + \epsilon_{ij}^{AM} \dot{x} = \dot{\epsilon}_{ij}^e + \dot{\epsilon}_{ij}^{PT} \quad (3)$$

$\dot{\epsilon}^{PT}$ is then the only inelastic contribution. It could be characterized by the Bain's strain, an invariant lattice strain and a lattice rotation (Fig. 2) that are necessary to realize the existence of an invariant plane [10] (the habit plane). The macroscopic strain ϵ^{AM} produced by this mechanism results from a shear along the habit plane and an extension normal to it (Fig. 3). From the knowledge of the crystallographic parameters

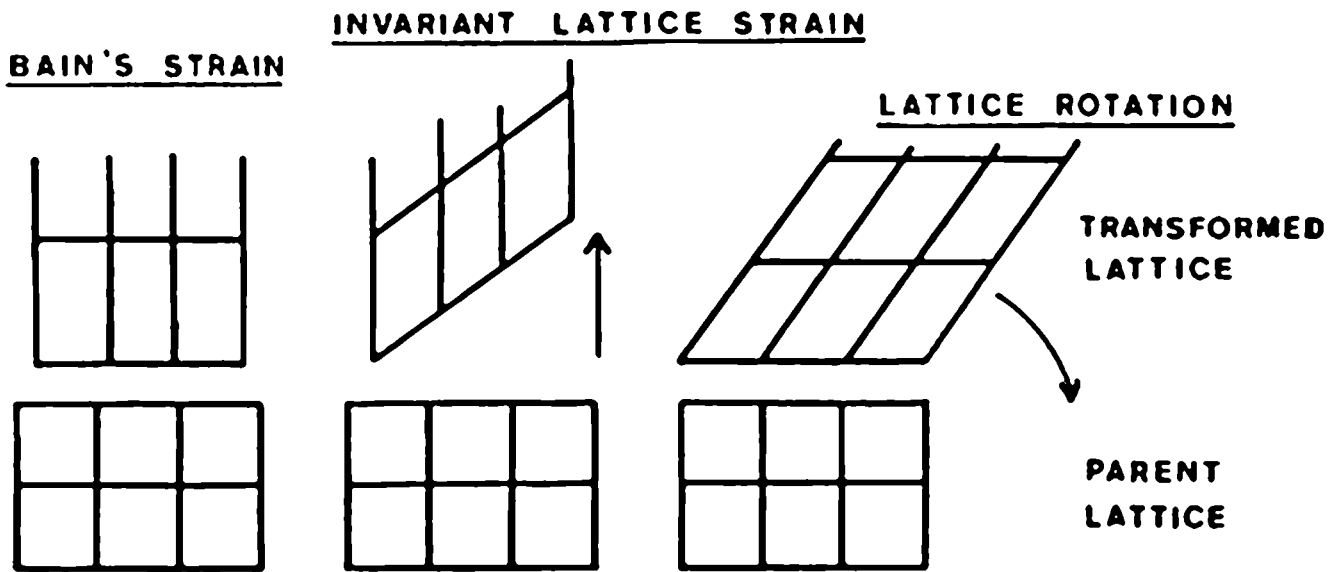


Fig.2: Characterisation of the transformation strain ϵ^{PT} , by the Bain's strain and invariant lattice strain and lattice rotation.

of the two phases, the W.L.R. phenomenological theory allows to determine the habit plane normal \vec{n} , the magnitude g and the direction \vec{m} of the crystallographic shear.

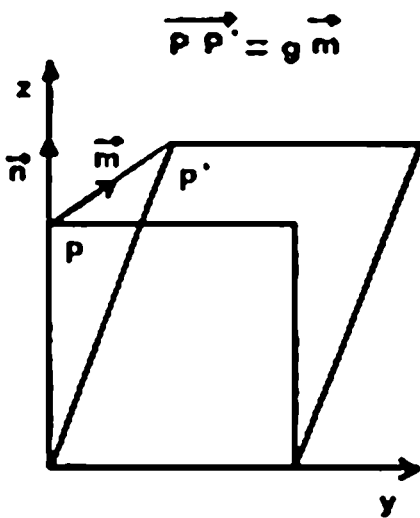


Fig.3: Deformation of an unit volume V by martensitic transformation.

From a kinematical analysis, the transformation strain ϵ^{AM} associated with the formation of one variant is expressed as [11,13] :

$$\epsilon_{ij}^{AM} = \frac{1}{2} (n_i m_j + n_j m_i) g = R_{ij} g \quad (4)$$

This result could be extended in the polyvariant case by summation over all the variant n :

$$\epsilon_{ij}^{PT} = \sum_n R_{ij}^n g x^n \quad (5)$$

The local constitutive relation is now determined with a thermodynamical approach. Thermoelastic Martensitic Transformation, which is a first order phase transition, involves the existence of a local energy balance between driving and resistive

forces [4], [15,18]. The variation of the Gibb's Free Energy is expressed by :

$$\Delta G = \Delta G_{ch}(\theta) V_M + \Gamma S + E_{ext} + E_{incl} \quad (6)$$

where

- | | | |
|---|-------------------------|--|
| { | $\Delta G_{ch}(\theta)$ | is the variation of chemical free energy between the two phases, it is a linear function of the temperature θ ; |
| | ΓS | is the interfacial energy, it could be neglected ; |
| | E_{ext} | denotes the interaction energy with the applied stress σ ; |
| | E_{incl} | is the stored elastic energy due to the transformation. |

The interaction energy is obtained by the use of Eshelby's relation [19]

$$E_{ext} = - \int_V \sigma_{ij} \epsilon_{ij}^{PT} dV = - \sum_n \sigma_{ij} R_{ij}^n g V^n \quad (7)$$

The elastic energy depends on the interactions existing between the different variants. Its accurate evaluation needs the knowledge of shape and spatial positions of the variants. Nevertheless, indirect evaluations may be realized by using the solution of the problem of the plastic inclusion pair [20,21] or by the calculation of the elastic energy associated with the interface between two compatible or incompatible variants [22]. These two methods give the same expression for E_{incl}

$$E_{incl} = V \left[\sum_n g^2 \epsilon^n x^n + \sum_{n,m} g^2 H^{nm} x^n x^m \right] \quad (8)$$

E^n denotes the interaction energy between martensite inclusion and parent phase, it is equal to zero for an infinitely thin inclusion with a plate shape [19]. The interactions between martensite variants are described by matrix H^{nm} [22].

From this analysis, a local criterion for the stress-induced transformation start is established :

$$\sigma_{ij} R_{ij}^n = \frac{1}{q} \Delta G_{ch}(0) = \frac{h}{q} (0 - H_s) \quad (9)$$

and the local constitutive relation is derived [11,13] :

$$\dot{\epsilon}_{ij}^T = S_{ijkl} \dot{\sigma}_{kl} + \sum_n R_{ij}^n \sum_m (H^{nm})^{-1} (R_{kl}^m \dot{\sigma}_{kl} - \frac{h}{q} \dot{\sigma}) \quad (10)$$

where tensor S is the elastic stiffness.

Single crystal behavior

This local analysis is extended to the single crystal case by considering the stress field as uniform inside the crystal.

Relations (9) and (10) could then be considered as the single crystal constitutive relations during a stress-induced martensitic transformation.

Experimental results for uniaxial tension are presented in previous papers [11,12]. They are in excellent agreement with these relations.

Polycrystalline behavior

In a polycrystal, the individual grains deform heterogeneously and large internal stresses are generated by incompatibilities between the grains. This leads to a more complex problem than in the single crystal case. In order to take into account the internal structure evolution a homogenization method based on the self-consistent scheme is used [23,25].

In the homogenization process, the local behavior is supposed to be known, and the overall behavior is described from the evolution of microphysical parameters by the means of localisation equations (Fig. 4).

OVERALL VARIABLES

$\dot{\Sigma}$
 \dot{E}^T
 $\dot{\sigma}$



LOCAL VARIABLES

$\dot{\sigma}^i$
 $\dot{\epsilon}^i$
 $\dot{\sigma}^i$

Fig.4: Overall and local variables in a polycrystal.

The determination of these relations needs to solve a thermomechanical integral equation which is established from the local stress equilibrium condition [23,26]. This equation could be solved in different ways, in this work a self-consistent scheme is used.

The polycrystalline local behavior is described by relation (10) previously established. In this relation, the local stress rate tensor is now resulting to the superposition of an external applied stress rate and an internal stress rate generated by the polycrystalline effects. It is assumed that the temperature is uniform through the material. Local relation (10) could be written as :

$$\dot{\epsilon}_{ij}^T(r) = g_{ijkl}(r) \dot{\sigma}_{kl}(r) + n_{ij}(r) \dot{\theta} \quad (11)$$

or in a dual form :

$$\dot{\sigma}_{ij}(r) = l_{ijkl}(r) \dot{\epsilon}_{kl}^T(r) - m_{ij}(r) \dot{\theta} \quad (12)$$

The localisation equations between the overall variables and the local one have the following form :

$$\dot{\sigma}_{ij}(r) = B_{ijkl}(r) \dot{\Sigma}_{kl} + b_{ij}(r) \dot{\theta} \quad (13)$$

$$\dot{\epsilon}_{ij}^T(r) = A_{ijkl}(r) \dot{E}_{kl}^T + a_{ij}(r) \dot{\theta} \quad (14)$$

where $\dot{\Sigma}$ and \dot{E}^T denote the overall variables with respect to :

$$\dot{E}_{ij}^T = \frac{1}{V} \int_V \dot{\epsilon}_{ij}^T(r) dV \quad (15)$$

$$\dot{\Sigma}_{ij} = \frac{1}{V} \int_V \dot{\sigma}_{ij}(r) dV \quad (16)$$

If the overall relationships are postulated with the same form as the local one

$$\dot{E}_{ij}^T = G_{ijkl} \dot{\Sigma}_{kl} + N_{ij} \dot{\theta} \quad (17)$$

$$\dot{\Sigma}_{ij} = L_{ijkl} \dot{E}_{kl}^T - M_{ij} \dot{\theta} \quad (18)$$

the overall tensors G , L , N and M could be expressed as [26] :

$$L_{ijkl} = \frac{1}{V} \int_V l_{ijmn}(r) A_{mnkl}(r) dV \quad (19)$$

$$N_{ij} = \frac{1}{V} \int_V B'_{ijkl}(r) n_{kl}(r) dV \quad (20)$$

$$\text{with } \left. \begin{aligned} M_{ij} &= L_{ijkl} N_{kl} \\ G_{ijkl} &= L_{ijkl}^{-1} \end{aligned} \right\} \quad (21)$$

$$\text{and } A_{ijkl}(r) = l_{ijmn}^{-1}(r) B_{mnpq}(r) L_{pqkl} \quad (22)$$

The localisation tensor $A(r)$ is then determined from the solution of an integral equation [26] which described the thermomechanical behavior of the material :

$$\dot{\epsilon}_{ij}^T(r) = \dot{\epsilon}_{ij}^* + \int_V \Gamma_{ijkl}(r-r') [\delta_{klmn}(r') \dot{\epsilon}_{mn}^T(r') - m_{kl}(r') \dot{\theta}] dV' \quad (23)$$

where :

$$\left\{ \begin{array}{ll} \dot{\epsilon}^* & \text{is the solution of the homogeneous equivalent problem ;} \\ \Gamma(r-r') & \text{is an operator derived from the Green tensor of the infinite homogeneous equivalent medium ;} \\ \delta l(r') & = l(r') - L^* \\ L^* & \text{is the modulus of the homogeneous equivalent medium.} \end{array} \right.$$

Different methods could be used to solve relation (23). Zero range approximation leads to the Taylor-Lin model :

$$\dot{\epsilon}^T(r) = \dot{\epsilon}^* = \dot{\epsilon}^T \quad (24)$$

In this paper a particular approximation of the exact solution of integral equation (23) is realized by using a self-consistent scheme [23,26]. In a homogeneous medium with a modulus L^* equal to the effective modulus L^{eff} , let us consider an inclusion of volume V^I where the local variables are assumed to be uniform (Fig. 5). The Eshelby's solution of this inclusion problem gives for local tensor $A(r)$ the following expression :

$$A_{ijkl}(r) = A_{ijkl}^I = [\delta_{ij} \delta_{kl} - T_{ijmn}^{II} (l_{mnkl}^I - L_{mnkl}^*)]^{-1} \quad (25)$$

where T^{II} is the Eshelby's tensor [19].

EFFECTIVE MEDIUM

INCLUSION IN HOMOGENEOUS EQUIVALENT MEDIUM

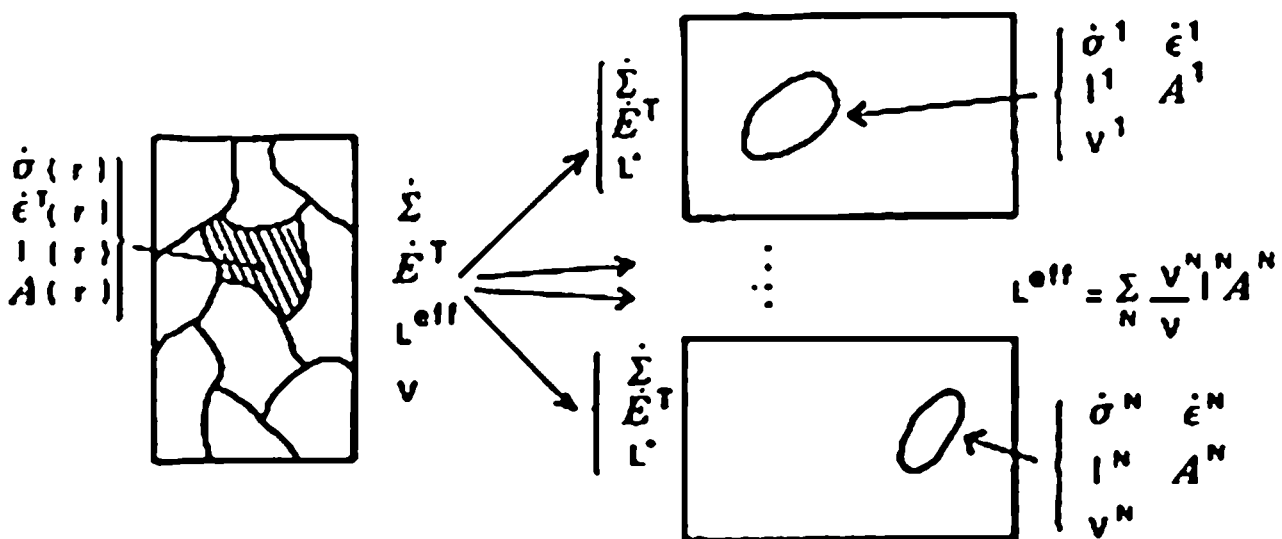


Fig. 5: Self-consistent method - Basic scheme.

If all the grains are successively considered as an inclusion, all the localisation tensor could be determined in that way, and the effective modulus of the polycrystalline is then expressed by :

$$L_{ijkl}^{eff} = \sum_I F^I l_{ijmn}^I A_{mnkl}^I \quad (26)$$

where F^I denotes the volume fraction of grain I.

In this complete self-consistent scheme there are no assumption on the form of the interaction between the homogeneous matrix and the inclusion. An other self-consistent scheme could be used by postulating the existence of an a-priori interaction law [27] :

$$\dot{\sigma}_{ij} = \dot{\epsilon}_{ij} + \alpha\mu (\dot{E}_{ij}^{PT} - \dot{c}_{ij}^{PT}) + \frac{\alpha\mu}{2} (\dot{E}_{kk}^{PT} - \dot{c}_{kk}^{PT}) \delta_{ij} \quad (27)$$

where μ denotes the elastic shear modulus and α an accommodation parameter. This leads to an easier calculation. Results obtained in that way are presented in figure 6 [12]. They are in good agreement with uniaxial tension tests performed at different temperature levels on a Cu - Zn - Al pseudoelastic alloy.

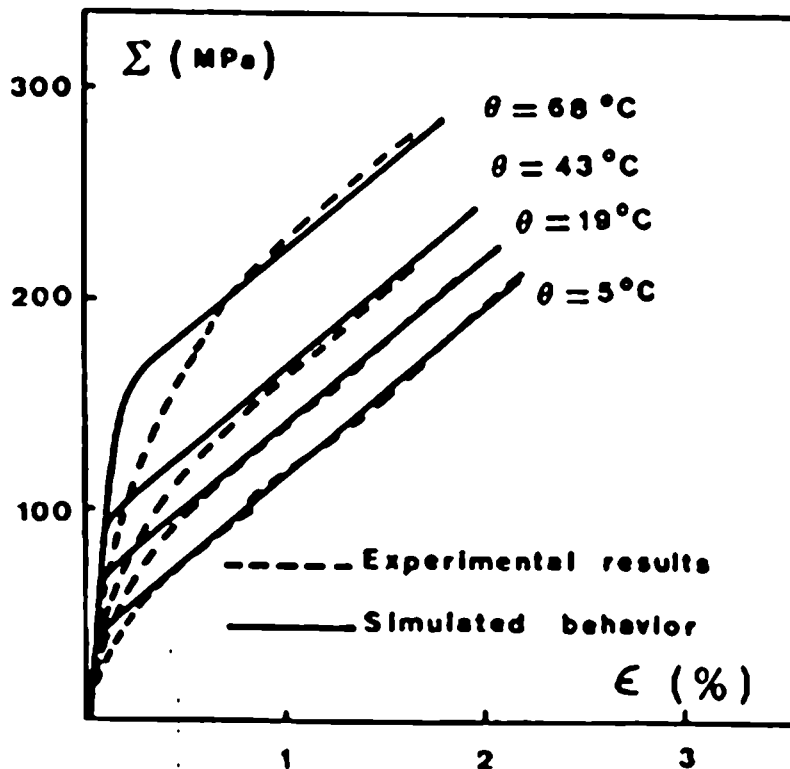


Fig. 6: Uniaxial tensile test curves of a Cu-Zn-Al polycrystalline pseudoelastic alloy. Comparison between experimental results and theoretical predictions which are obtained by using an a-priori self-consistent scheme.

Conclusion

In this work, the thermoelastic behavior associated with stress-induced transformation is completely described from the microphysical mechanisms which controlled the internal structure of the material. Parameters used in this kind of modelling are generally accessible by experiments (habit plane orientation,

intervariant interaction, texture, single crystal transformation point...). A good quantitative agreement is obtained in that way, and it could be expected that this result may be improved by using the complete self-consistent scheme.

The knowledge of the influence of the internal structure evolution on the overall behavior is a major advantage to determine the influence of a previous thermomechanical treatment on the global properties of a specimen (education training, cycling behavior...).

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