Phase transformation yield surface of anisotropic shape memory alloys

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Abstract. Two theoretical investigations i.e. a phenomenological macroscopic one and a "micro-macro" are developed for modelling the experimental surfaces of initiation of phase transformation in shape memory alloys. The eventual initial anisotropy of the materials is taken into account.

1. INTRODUCTION

Pseudoelasticity associated to the stress induced phase transformation between the mother phase called austenite A and the product phase called martensite M is very useful for several industrial applications.
For the design of SMA structures, the development of efficient models for the representative elementary volume (REV) is necessary. As for classical plasticity models, the definition of a yield surface of initiation of phase transformation (A → M) under multiaxial proportional loadings at first, is a key point. In this aim, one can built phenomenological models with efficient internal variables choice [1]. An alternative way can be the use of the Crystallographical Theory of Martensite (CTM) performed by Ball, James [2,3], Bhattacharya [4] and others to know precisely the microstructure.
Therefore a homogenization process permits the prediction of the yield surfaces of phase transformation.
Moreover, modelling must take into account the fact that the martensitic transformation does not proceed in a symmetrical way in the stress space [5] and particularly the asymmetry between tension and compression is obvious [6,7].
At last, an another feature to consider is the initial texture of the austenitic sample which can be random, drawn or rolled.

2. STUDIED TEXTURES [8]

A polycrystalline material is represented by 1000 grains defined by their crystallographic orientations. Isotropic, rolled and drawn textures are defined. Each of them is characterized by the orientation of the different grains given by the three Euler's angles (φ_1, Ø, φ_2). Isotropic texture corresponds to a random distribution of the grain orientation. In order to obtain other textures an elastoplastic model based on a self-consistent approach [9] is used. A rolling loading up to a strain of 0.5 was simulated starting from an initial isotropic texture for a FCC Cu Zn Al.
The three textures (isotropic, rolled, drawn) are now used as initial texture to describe the pseudoelastic behaviour of a Cu Al Zn or a Cu Al Be alloy and the loading transformation surface associated.

3. PHENOMENOLOGICAL MODELLING FOR MARTENSITIC TRANSFORMATION YIELD SURFACE AT MACROSCOPIC SCALE

3.1 Experimental characterization of SMA yield surfaces

<table>
<tr><td rowspan="2">Mechanical tests</td><td>Polycrystals Alloy</td><td colspan="3">Composition at (%)</td><td colspan="4">Transformation temperatures °C</td></tr>
<tr><td></td><td>Cu</td><td>Al</td><td>Be</td><td>M_s^0</td><td>M_F^0</td><td>A_s^0</td><td>A_F^0</td></tr>
<tr><td>Bi-compression on cubes</td><td>Cu Al Be n° 1</td><td rowspan="2">74.44</td><td rowspan="2">22.63</td><td rowspan="2">2.93</td><td>21</td><td>-7</td><td>19</td><td>32</td></tr>
<tr><td rowspan="2">Tension-(compression) internal pressure or torsion on tubes</td><td>Cu Al Be n° 2</td><td>14</td><td>-13</td><td>12</td><td>26</td></tr>
<tr><td>Cu Al Zn</td><td>66.84</td><td>23.73</td><td>9.4</td><td>14</td><td>5</td><td>17</td><td>20</td></tr>
<tr><td rowspan="2">Tension (compression) torsion on tubes</td><td rowspan="2">Ni-Ti</td><td>Ni</td><td colspan="2">Ti</td><td rowspan="2">-4</td><td rowspan="2">-29</td><td rowspan="2">-2,6</td><td rowspan="2">21</td></tr>
<tr><td>50.7</td><td colspan="2">49.3</td></tr>
</table>

Table 1

In Figure 1 which deals with an isotropic Cu Al Be alloy, one can observe (i) the asymmetry between tension and compression, (ii) the symmetry towards the equibiaxial axis $\sigma_1 = \sigma_2$, (iii) the scalar value obtained under equibiaxial tension seems higher than the one observed under tension and compression, (4i) pure shear symmetry, (5i) the strain rate $\dot{\varepsilon}^{tr}$ seems perpendicular to the yield surface and one can refer to the same normality rule as in classical plasticity. The transverse isotropy property of Cu Al Be induces that under tension (compression)-torsion the alloy behaves as an anisotropic material (figure 2). The figure (3) reveals that it is not the case for Ni Ti under the same loading.

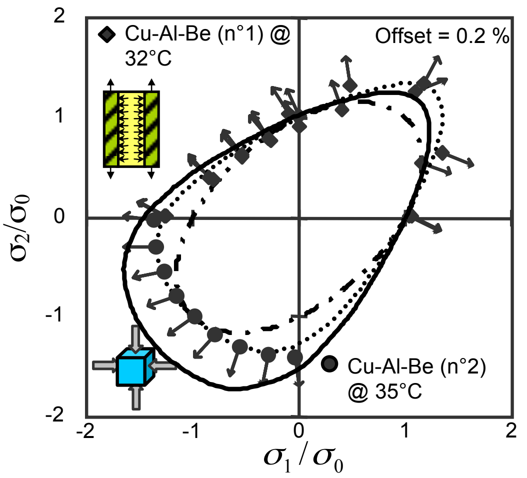

Figure 1 : —— micro-macro simulation, …….. phenomenological simulation $\bar{\sigma}.g(y_\sigma) = cte$, -.-. $\bar{\sigma} = cte$, ♦• experiments

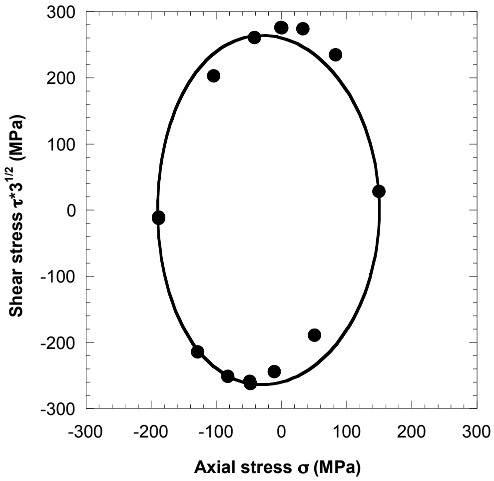

Figure 2 : Tension(compression)-torsion,,textured (drawn) Cu-Al-Be 60°c

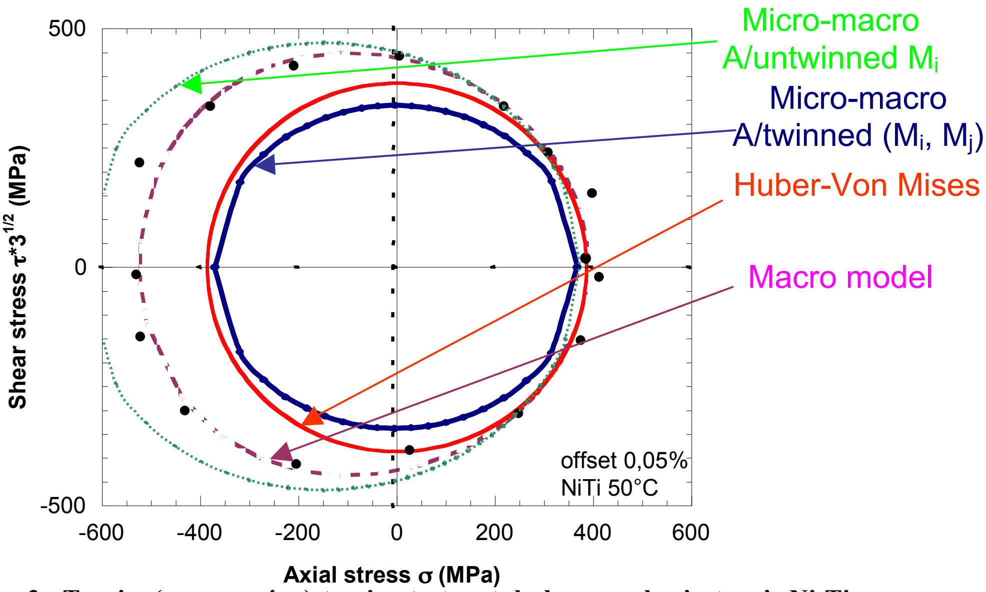

Figure 3 : Tension(compression)-torsion test on tubular sample , isotropic Ni-Ti

3.2 Macroscopic criterion of onset transformation

The main objective of this macroscopic criterion based on experimental results is the description of the boundary of the domain in the stress space. It means that inside the domain, the martensitic transformation is not activated. Moreover, this transformation is considered as volume invariant. For the isotropic case, Bouvet et al [10] have proposed the following equivalent stress $\sigma_{eq} = \sigma_{eq}(\bar{\sigma}, y_\sigma) = \bar{\sigma} g(y_\sigma)$ where $\bar{\sigma} = \sqrt{\frac{3}{2} \underline{\sigma}_D : \underline{\sigma}_D}$

is the Von Mises stress, $y_\sigma = \dfrac{27}{2}\dfrac{\det(\sigma_s)}{\bar{\sigma}^3}$, $\det(\underline{\sigma}_D)$ the third stress invariant of deviatoric stress tensor $\underline{\sigma}_D$ and g is a function defined by $g(y_\sigma) = \cos\left(\dfrac{1}{3}\cos^{-1}(1 - a(1 - y_\sigma))\right)$. The material parameter, a, is taken between 0 and 1 . For anisotropic case, the following extension is proposed [16]: $\sigma_{eq} = \sigma_{eq}(\bar{\tilde{\sigma}}, y_{\tilde{\sigma}}) = \bar{\tilde{\sigma}}\, g(y_\sigma)$, where $\tilde{\sigma}$ is the dilated stress tensor, $\tilde{\sigma}$ is taken such as the Hill's hyper ellipsoid which is dilated by an affine transformation in an hypersphere $\underline{\tilde{\sigma}} = \underline{\underline{D}}\,\underline{\sigma}$. Where $\underline{\underline{D}}$ is the operator of the affine transformation (see figure 2 concerning tension (compression) torsion of drawn Cu Al Be tube).

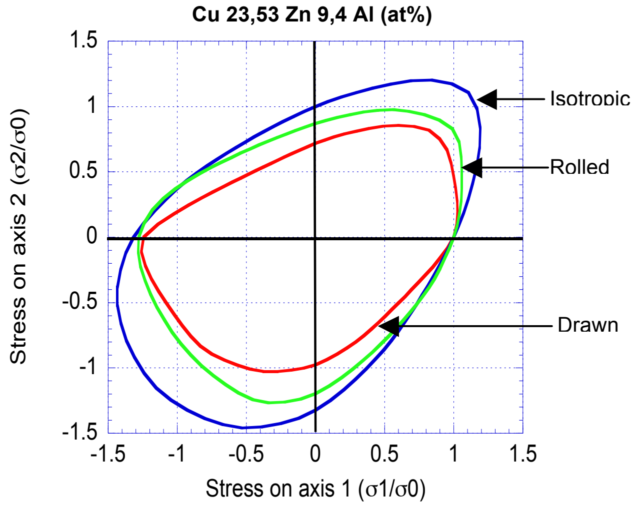

Figure 4 : Influence of texture on transformation yield surfaces

4. CRYSTALLOGRAPHIC THEORY OF MARTENSITE UTILIZATION

4.1 Theory

The CTM used to determine the phase transformation surfaces was developed for isotropic SMA in two publications [11,12]. Here, we extend the investigation for textured SMA. Recalling that the CTM used to construct microstructures is a geometrically non-linear theory of martensite transformation performed by Ball and James [2,3]. These authors formulate a free energy function that would produce the A-M interface and relate it to crystal structure. One of the main results of this CTM is the recognition that some of the common microstructures in SMA are possible (as energy minimizing microstructures) only with exceedingly special lattice parameters.

As a summary, there are two cases

(1) certain alloys such as Cu Al Ni, Cu Al Zn, Cu Al Be (cubic → monoclinic type I) exhibit an undeformed interface between austenite and a single variant of martensite [13]

(2) a region consisting of fine twins of two martensite variants i and j can give a coherent interface with the austenite. It works for Cu Al Ni (cubic → orthorhombic), Ni Ti (cubic → monoclinic type II) [14].

Using the theorems of [2,3], if the Hadamard equation (or compatibility condition) between austenite and a single variant of martensite are fulfilled, the microstructure (1) is obtained. If it's not the case, one has to solve the Hadamard equation at first between all the martensite variants (i) and (j) and choose all compatible twins (i,j). In a second step, the resolution of the compatibility equation between A and compatible twins (i,j) delivers the situation (2). However, in any case, the microstructure is viewed at stress free state and the elastic strains are neglected in comparison with the transformation strains. But the CTM permits to solve the problem for "dead loads" i.e. no change of stress or displacement in time. As it was underlined by Lexcellent and Blanc [12], the microstructure change under continuous loading or unloading is in the author's knowledge, still an opened problem (except the important fact that the austenite delivers martensite variants under stress or and temperature action). From the knowledge of lattice parameters a_o of the cubic austenite, (a,b,c,θ) of the monoclinic martensite, the calculations deliver the microstructure of each investigated alloys : an exact interface between A and a single variant Mi for copper based alloys and a twinned martensite (Mi, Mj) along with A for Ni Ti alloys. In both cases, the phase transformation strain tensor $\underline{E}_t$ is obtained

$$\underline{E}^T = \frac{1}{2}(\underline{U}^2 - \underline{1}) \quad \text{with} \quad \underline{U}^2 = {}^T\underline{F}\,\underline{F} \tag{1}$$

with

$$\underline{U} = \underline{U}_i \ (i = 1, ..., 12) \ \text{for} \ A/Mi \tag{2}$$
$$\underline{U} = (1-\lambda)\underline{U}_i + \lambda\underline{U}_j \quad (i, j = 1, ..., 12) \ \text{for} \ A/(Mi, Mj)$$

$\underline{F}$ represents the gradient of transformation $(d\vec{x}_0(A) \xrightarrow{F} d\vec{x}(Mj)$ and $\underline{U}$ is designed as the Bain strain.

4.2 Micro-macro integration process of onset transformation surface for isotropic or textured SMA

If we consider a biaxial loading, the stress tensor will be expressed in the sample reference configuration as

$$\underline{\sigma} = \sigma_1 \vec{e}_1 \otimes \vec{e}_1 + \sigma_2 \vec{e}_2 \otimes \vec{e}_2 \tag{3}$$

For each grain, the first variant appears when a thermodynamical force associated to the phase transformation is equal to zero

$$\underline{\sigma} : \underline{\varepsilon}^t - K(T) = 0 \quad , \quad \underline{\varepsilon}^t = {}^T\underline{R}\,\underline{E}^t\,\underline{R} \tag{4}$$

$\underline{R}$ is the rotation matrix from the austenite cell frame to the geometrical sample one.
The procedure used to calculate yield surface of polycrystal is purely phenomenological.
(i) a polycrystal constitutes an aggregate of n grains (n chosen equal to 1000) with a random orientation distribution meaning an isotropic behaviour and the distribution delivered by the calculation in [8] for rolled or drawn textures. The interaction between the grains are not taken into account, (ii) under a given stress condition $\underline{\sigma}^o$ for each grain k (k = 1…n) and among the m possible variants, the one presenting the highest factor K is selected. A set of n factors K_k^{max} is determined by this method, (iii) a new set of K_k^{max} is calculated under different stress loading. $K_{tension,k}^{max}$ stands for the results under uniaxial tension, (iv) a ratio called r and the phase transformation start stress are obtained $r = \dfrac{\Sigma_{k=1...n} K_k^{max}}{\Sigma_{k=1...n} K_{tension,k}^{max}}$ and $\underline{\sigma}^t = \dfrac{1}{r}\underline{\sigma}_o$, (5i) a new stress $\underline{\sigma}_o'$ delivers $\underline{\sigma}_t'$ and so on.

5. COMPARISON BETWEEN EXPERIMENTS AND SURFACE PREDICTIONS

For the Cu Al Be under tension (compression) internal pressure or bicompression (fig. 1), the agreement between experiments and phenomenological and micro-macro model is good except for the equibiaxial elongation prediction for tension-compression (for micro-macro model). For the same alloy, the anisotropy revealed by tension (compression) – torsion tests is fairly taken into account by the macroscopic formulation (fig. 2). Figure 4 revealed that the micro-macro model takes into account the drawn or rolled texture see Cu 23.53 Zn 9.4 Al (at %) in agreement with the prediction of Aleong et al [15]. The surface predictions are very closed for micro-macro and phenomenological models for Cu 15 – Zn 17 Al (at %) (figs. 5,6). At last, the experiments performed on isotropic Ni Ti demonstrate that in this case the CTM prediction e.g. an interface with twinned martensite (A/Mi, Mj) does not work, but the non predicted interface (A/Mi) works [12]. Obviously, the phenomenological macroscopic theory which represents some curve fitting also works in this case (fig. 3).

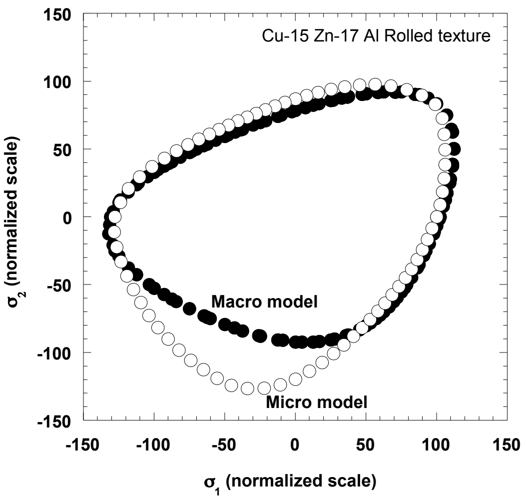

Figure 5 : Cu- 15 Zn-17 Al Rolled texture

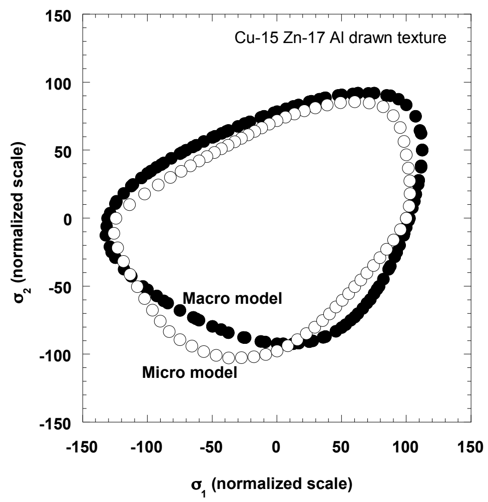

Figure 6 : Cu- 15 Zn-17 Al Drawn texture

6. CONCLUSION

The modelling of yield surfaces of phase transformation is extended from isotropic to textured materials with success by an affine transformation for the phenomenological approach and by an efficient choice of grains orientation distribution. The microstructure predicted by the CTM theory can be extended to continuous loading for Copper based alloys but not for Ni Ti. The determination of microstructure evolution under continuous stress action remains an opened problem.

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