CONSTITUTION OF INTERACTION MATRIX BETWEEN MARTENSITIC VARIANTS IN THE SHAPE MEMORY ALLOYS

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ABSTRACT
From a kinematic study of the martensitic transformation, we propose an interaction matrix between martensitic variants, whose terms can be classified in to two types:
- Terms representing the weak interactions which exist between the compatible variants, without internal stress (self-accommodating variants).
- Terms representing the strong interactions between incompatible variants with internal stress source and associated elastic energy.

By using a new technique allowing the constitution of interaction matrix between variants, based on experimental data, and the results obtained by application on the alloys of Cu.Zn.Al which experiments were performed by Delaey and Devos.

Keywords: Thermomechanic / interaction / martensitic variants.

1. INTRODUCTION
The martensitic transformation is a transition of first order phase, which implies the coexistence of the mother phase (austenite) and the transformed phase (martensite), as well as the presence of an interface between these two phases known as habitat plan.
The martensitic transformation can be caused either by a temperature variation or by the application of sufficient macroscopic stress [1, 2].
From the crystallographic point of view, the crystalline symmetry of the mother phase presents the several equivalent variants.
Many studies described by a semi-quantitative or qualitative way [3, 4] these martensitic variants and their possibilities of interaction for simple loading.
We can take for example the works of J.Devos et al. [5] on the self-accommodated variants, those of Delaey et al. [6] on the various situations of interactions between the variants observed under the microscope and the works of O.Fassi.Fehri [7] which describe the remote interaction between variants via the solution of the problem of the pair of flattened ellipsoidal inclusions.
E.Patoor et al. proposed an energy assessment, based on Gibbs reversible thermodynamics, allowing elastic energy term of interaction between the martensitic variants whose role is prevailing on the material behavior as well as on the mechanism of the transformation.
If we limit ourselves to the case of the perfect transformation plasticity (traditional absence of plasticity), the elementary mechanisms are then of two types:
- Formation (reversible) of the martensitic variants starting from austenite.
- Migration of the interfaces between the different already formed martensitic variants and modification of the corresponding voluminal fractions.
The two mechanisms can intervene separately (T>Ms or T<Mf) or simultaneously (Mf<T<Ms).

2. PSEUDOELASTIC POTENTIAL OF THE SINGLE CRYSTAL AT THE TIME OF THE TRANSFORMATION
We use a thermodynamic approach to describe the evolution of the martensitic transformation under isothermal conditions. Experimentally we observe that there is a limit beyond which the martensite appears and from which the voluminal fraction increases with the macroscopic stress.
The variation of the free Gibbs energy $\Delta G$ associated with the formation of the various martensitic variants I of volume $V_I$ in an austenitic matrix of volume $V$ in the presence of external constraints is defined by [8-10]:

$$\Delta G = \Delta^c G(T) \sum_{I=1} V_I + GS + E_{ext} + E_{int}$$ (1)
Where
\( \Delta^c G(T) \) designates the variation of chemical free energy [11], as a function of the temperature and is equivalent to the difference in free energy between martensite and austenite. (\( \Delta^c G(T) \) is equal to zero at the thermochemical temperature of equilibrium).

\( \Gamma_S \) correspond to the surface energy associated with the austenite martensite interface. For thermoelastic materials, this term is negligible.

\( E_{\text{ext}} \) indicates the mechanical energy of interaction with the applied stress field [12]. \( \Sigma_{ij} \) is obtained according to the relation of Eshelby [9] under the form:

\[
E_{\text{ext}} = -\int \sum_{j} e_{ij}^*(r)dv
\]

with

\[
e_{ij}^*(r) = \sum_{t=1}^{n} e_{ij}^t \theta_t(r) = \sum_{t=1}^{n} g R_{ij}^t \theta_t(r)
\]

\( R_{ij}^t \) : Orientation factor for variant I, knowing that \( \mathbf{m}^i \) and \( \mathbf{n}^i \) are respectively the displacement direction and the normal at the habitat plan of variant I.

\( g \) : Amplitude of displacement.

\( \theta_t(r) \) : Indicator function egal 1 in volume \( V \) of variant I and 0 to the outside.

This gives us, taking into account (2) and (3):

\[
E_{\text{ext}} = -\sum_{I=1}^{n} \Sigma_{ij} g R_{ij}^1 V_I
\]

The term \( E_{\text{int}} \) describes the elastic energy associated to the internal stresses of the incompatibility of the transformation. The origin of these internal stresses is multiple and is associated with:

- The presence of martensitic plates in an austenitic matrix.
- Interactions between the martensitic variants.
- The creation of dislocations in the austenite or in the formed martensite.

We limit ourselves in this work to the interaction between the martensitic variants which has an important aspect, particularly in the case of non radial triaxial constraints.

The elastic energy can then be written:

\[
E_{\text{int}} = \frac{1}{2} \int \sigma_{ij}^t(r)e_{ij}^*(r)dv = -\frac{1}{2} \int \sigma_{ij}^t(r)e_{ij}^*(r)dv
\]

\[
= -\frac{1}{2} \sum_{I=1}^{n} V_I \sigma^I_{ij} e_{ij}^I = -\frac{1}{2} \sum_{I=1}^{n} V_I \sigma^I_{ij} g R_{ij}^I
\]

\[
\bar{\sigma}^I_{ij} = \frac{1}{V_I} \int \sigma_{ij}^t(r)dv
\]

\( \bar{\sigma}^I_{ij} \) : Average stress in variant I.

According to [7] the average stress can be expressed in the form:

\[
\bar{\sigma}^I_{ij} = \sum_{I} T_{ijkl}^u V^I_{kl} e_{ij}^I
\]
Taking into account (6) and (8), one can formally write that:

$$E_{\text{int}} = g^2 V \left( \sum_i E^i f^i + \frac{1}{2} \sum_{i,j} H^{ij} f^i f^j \right)$$

(9)

Where $f^i$ and $f^j$ are respectively the volume fractions of the variants (I) and (J).

The term $E^i$ comes from the interaction of one variant I with the austenite and can be evaluated starting from the solution of the plastic inclusion of Eshelby.

$H^{ij}$ represents the interaction matrix between the martensitic variants.

The evaluation of $H^{ij}$ requires like the fine knowledge of the microstructure (form and spatial distribution of the variants).

$$\Delta G = \Delta^c G(T) \sum_i V^i - \sum_i g^2 \sum_j R_{ij}^i V^i + g^2 V \left( \sum_i E^i f^i + \frac{1}{2} \sum_{i,j} H^{ij} f^i f^j \right)$$

(10)

Thus for a unit volume:

$$\frac{\Delta G}{V} = \Delta^c G(T) \sum_i f^i - \sum_i g^2 \sum_j R_{ij}^i f^i + g^2 \sum_i E^i f^i + \frac{1}{2} g^2 \sum_{i,j} H^{ij} f^i f^j$$

(11)

The thermodynamic potential $\frac{\Delta G}{V}$ then describes the state of the system austenite martensite starting from the variables $T$ (which intervenes only in $\Delta^c G(T)$ ), $\Sigma_i$, and from the internal variables $g f^i$.

The thermodynamic forces $t^i$ associated with the internal variables $g f^i$ are obtained from the traditional relation [9]:

$$t^i = \frac{1}{g} \frac{\partial (\Delta G/V)}{\partial f^i}$$

(12)

At the thermodynamic equilibrium, $t^i = 0$, which leads to:

$$\Sigma_i R_{ij}^i = \frac{\Delta^c G(T)}{g} + g E^i + \frac{1}{2} g \sum_j H^{ij} f^j$$

(13)

$\Sigma_i R_{ij}^i$ represents the reduced stress on the variant I.

The relation (13) means that the variant I can be active only if the resolved stress on this variant equal to breaking value dependent on the temperature $\Delta^c G(T)$, [13], on the morphology of the variant $g f^i$, on the voluminal fraction of the other already formed variants and on the interaction between the active variants.

3. TECHNIQUE OF CONSTITUTION OF INTERACTION MATRIX STARTING FROM EXPERIMENTAL DATA

In this paragraph we will present a technique of constitution of interaction matrix starting from experimental data such as $H_1$ and $H_2$, respectively the value of the weak interaction and the strong interaction between the martensitic variants.

This matrix is generally made up of two terms of which one characterizes the weak interactions and the other; the strong interactions, these values are determined experimentally, which restricts the classes of interactions into two (weak and strong).

The new approach will enable us to constitute the interaction matrix not only from two coefficients but of coefficients which will as much as possible reflect the difference in the degree of interaction between the variants.

$$H^{ij} = \mu / S^{ij} \quad \text{(I, J=1..24)}$$

(14)

With $\mu$ : the shearing modulus
\[ S^{ij} = A K^{ij} + B \]  
(15)

Where A and B are determined by linear interpolation between \( H_1 \) and \( H_2 \) (respectively weak and strong experimental interactions).

\[ A = \mu \left( \frac{1}{H_2} - \frac{1}{H_1} \right) \]  
(16)

\[ B = \frac{\mu}{H_1} \]  
(17)

For the determination of \( K^{ij} \) we propose the following procedure: We calculate the vector product between the directions of transformation of two variants, and then we calculate the module of the vector result of the product, which enables us to have a coefficient making it possible to determine the degree of interaction.

From what preceded we can express \( K^{ij} \) in the following form:

\[ K^{ij} = \sqrt{\varepsilon_{ijk} \varepsilon_{i\ell n} m^i_{jk} m^j_{k\ell} m^\ell_n} \]  
(18)

(Without summation on I and J) \( i, j, k, \ell, n = 1,3 \)

\( \varepsilon_{ijk} \) : Orientation Tensor of order 3.

\( m^i_j \) is the \( j^{th} \) component of the direction of transformation for variant I of the martensite.

By combining the relations (13), (15), (16), (17) and (18) we can express the interaction matrix in the following form:

\[ H^{ij} = \frac{H_1 H_2}{(H_1 - H_2) \sqrt{\varepsilon_{ijk} \varepsilon_{i\ell n} m^i_{jk} m^j_{k\ell} m^\ell_n} + H_2} \]  
(19)

3.1. Application and discussion

We can apply our new technique to the case of the Cu.Zn.Al alloys whose chemical compositions as well as the various characteristics are as follows; the shearing modulus \( \mu = 30 \) GPa, the term of weak interaction and that of strong interaction are respectively \( H_1 = \mu/1000 \) and \( H_2 = \mu/200 \) [14].

The alloys are transformed completely into martensite at constraints lower than the elastic limit, and are thus very close to the conditions of plasticity of pure transformation.

The habitat plan is located by its: normal unit \( \vec{n} \), transformation of deformation \( \vec{m} \) and amplitude \( g \) [14,15].

\( n_1 = -0.182, n_2 = 0.669, n_3 = 0.721 \)

\( m_1 = -0.165, m_2 = -0.165, m_3 = 0.655 \)
3.1. Results

<table>
<thead>
<tr>
<th>Variant</th>
<th>Normal of habit plane</th>
<th>Direction of transformation</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>n₁ n₂ n₃</td>
<td>m₁ m₂ m₃</td>
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<tr>
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<td>n₁ n₃ n₂</td>
<td>m₁ m₃ m₂</td>
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<td>4</td>
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<td>-m₁ m₃ m₂</td>
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<td>5</td>
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<tr>
<td>6</td>
<td>-n₁ n₁ n₂</td>
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<td>7</td>
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<tr>
<td>24</td>
<td>n₁ n₁ n₂</td>
<td>m₁ m₂ m₃</td>
</tr>
</tbody>
</table>

3.1.1. Results

**Interaction matrix \( H^{(n)} \) (Novel approach)**

\[
\begin{pmatrix}
0.03 & 0.04 & 0.04 & 0.03 & 0.11 & 0.13 & 0.14 & 0.10 & 0.15 & 0.15 & 0.14 & 0.15 & 0.10 & 0.07 & 0.07 & 0.07 & 0.09 & 0.10 & 0.08 & 0.12 & 0.10 & 0.09 & 0.12 \\
0.04 & 0.03 & 0.04 & 0.07 & 0.09 & 0.10 & 0.06 & 0.15 & 0.14 & 0.15 & 0.15 & 0.12 & 0.10 & 0.09 & 0.13 & 0.11 & 0.13 & 0.14 & 0.10 & 0.10 & 0.07 & 0.07 \\
0.04 & 0.02 & 0.02 & 0.04 & 0.07 & 0.10 & 0.11 & 0.07 & 0.14 & 0.15 & 0.15 & 0.13 & 0.12 & 0.10 & 0.12 & 0.14 & 0.12 & 0.13 & 0.09 & 0.09 & 0.07 & 0.06 & 0.13 \\
0.03 & 0.04 & 0.06 & 0.03 & 0.10 & 0.12 & 0.13 & 0.09 & 0.15 & 0.15 & 0.14 & 0.14 & 0.13 & 0.12 & 0.10 & 0.12 & 0.14 & 0.12 & 0.13 & 0.09 & 0.07 & 0.06 & 0.13 \\
0.11 & 0.07 & 0.07 & 0.10 & 0.03 & 0.04 & 0.03 & 0.04 & 0.04 & 0.04 & 0.04 & 0.04 & 0.04 & 0.04 & 0.04 & 0.04 & 0.04 & 0.04 & 0.04 & 0.04 & 0.04 & 0.04 & 0.04 \\
0.13 & 0.09 & 0.10 & 0.10 & 0.06 & 0.07 & 0.09 & 0.04 & 0.03 & 0.03 & 0.04 & 0.09 & 0.13 & 0.12 & 0.10 & 0.11 & 0.07 & 0.11 & 0.11 & 0.11 & 0.11 & 0.11 & 0.11 \end{pmatrix}
\]

3.1.2. Discussion
The matrix obtained to obey the principle of six groups of four martensitic variants:
- Group 1: V1, V2, V3 and V4.
- Group 2: V5, V6, V7 and V8.
- Group 4: V13, V14, V15 and V16.
- Group 5: V17, V18, V19 and V20.
The weak interactions which exist between the compatible variants (self-accommodating variants), lie between 0.03 and 0.04 and the strong interactions which exist between the incompatible variants lie between 0.06 and 0.15. It is noticed that the interactions between the compatible variants are included in an interval of 0.01 (angle between directions of displacement exist between 0 and 20°) on the other hand, between the incompatible variants we have a significant interval of 0.09 (angle between directions of displacement exist between 40° and 90°) which enabled us to carry out a classification in terms of weak and strong incompatibilities.

4. CONCLUSION

In this work, we proposed a technique which allows the constitution of the interaction matrix between martensitic variants starting from experimental data. The results obtained by this technique were compared successfully with the literature in the case of the Cu.Zn.Al alloys. The approach also made it possible to highlight the incompatible classes of interactions. Although the values of KIJ are the result of approximations, the suggested technique constitutes a good approach to the problem of the selection of the martensitic variants.

5. REFERENCES