

Thermomechanical behaviour of shape memory alloys

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THIS work describes the thermomechanical behaviour for both single crystal and polycrystal of metallic alloys during a stress-induced thermoelastic martensitic transformation. A thermodynamical analysis based on Gibb's free energy has shown that the single crystal is a standard material for pseudoelasticity. The transformation criterion and its associated flow rule deduced from the pseudoelastic potential are in good agreement with experiments performed on a Cu Zn Al alloy. The polycrystal behaviour is described by two different approaches: a phenomenological one which extends the single crystal results and a self-consistent scheme used for the micro-macro transitions. Uniaxial tensile test experimental measurements showed that this theoretical simulated behaviour gives very good agreement. The results obtained with the self-consistent scheme are more accurate than those obtained using the phenomenological approach.

W pracy przedstawiono opis termomechanicznego zachowania się pojedynczych kryształów i polikryształów stopów metalicznych podczas martenzytowej przemiany fazowej wywołanej przez naprężenie. Na podstawie analizy termodynamicznej wykazano, że pojedynczy kryształ jest standardowym materiałem w sensie pseudosprężystości. Kryterium przemiany oraz stowarzyszone z nim prawo płynięcia, wyprowadzone przy wykorzystaniu potencjału pseudosprężystego, zweryfikowano doświadczalnie na przykładzie stopu Cu Zn Al, notując dobrą zgodność teorii z eksperymentem. Zachowanie się polikryształu opisano dwiema różnymi metodami. Pierwsza, fenomenologiczna, polegała na uogólnieniu wyników dotyczących pojedynczego kryształu, w drugiej wykorzystano procedurę „self-consistent” do przejścia od poziomu mikro do makro. Porównanie wyników teoretycznych uzyskanych przy użyciu obu metod z wynikami doświadczeń w testach jednoosiowego rozciągania dało bardzo dobrą zgodność. Wskazano, że procedura „self-consistent” prowadzi do lepszych rezultatów niż podejście fenomenologiczne.

В работе представлено описание термомеханического поведения единичных кристаллов и поликристаллов металлических сплавов во время мартензитного фазового превращения, вызванного напряжениями. На основе термодинамического анализа показано, что единичный кристалл является стандартным материалом в смысле псевдоупругости. Критерий превращения, а также ассоциированный с ним закон течения, выведенные при использовании псевдоупругого потенциала, проверены экспериментально на примере сплава Cu, Zn, Al, отмечая хорошее совпадение теории с экспериментом. Поведение поликристалла описано двумя разными методами. Первый, феноменологический, заключается в обобщении результатов, касающихся единичного кристалла, во втором методе использована процедура „self-consistent” к переходу от микро уровня к макро уровню. Сравнение теоретических результатов, полученных при использовании обоих методов, с результатами экспериментов в тестах одноосного растяжения привело к очень хорошему совпадению. Указывается, что процедура „self-consistent” приводит к лучшим результатам, чем феноменологический подход.

1. Introduction

STRESS-INDUCED phase transformation in some metallic alloys shows a typical behaviour called transformation plasticity. Numerous metallurgical studies [1, 2] have described this phenomenon by the quantitative or semi-quantitative method. The formation or the growth of different martensite variants due to thermomechanical loading is the microstructural mechanism responsible for the overall behaviour. Different approaches were

proposed [3, 8] to describe this behaviour in the complex case of the ferrous alloys, where phase transformation and plastic yielding of the parent phase occur simultaneously. In the same way, different schemes are proposed by JAMES [9], TANAKA *et al.* [10] and MÜLLER [11] for the Cu Zn Al or Ni Ti alloys where a thermoelastic martensitic transformation occurs without plastic yielding. Their approaches are not based on the physical mechanism of the transformation which is described by the phenomenological theories of WECHSLER, LIEBERMAN and READ [12], BOWLES and WAYMAN [13] and EBERHARDT and BERVEILLER [14]. In these theories the parent phase behaviour is taken into account more or less directly. For the general case of transformation plasticity in ferrous alloys, numerous elementary mechanisms interact, so this case is very complex. In the special case of thermoelastic martensitic transformation only two elementary mechanisms could exist:

- (i) reversible formation of martensite variants from the parent phase;
- (ii) interfacial motion between the different martensite variants yet formed and changed in their volumetric proportion;

These two mechanisms could act separately ($T > M_S$ or $T < M_F$) or in the same time ($M_F < T < M_S$). In this work it is considered that only the first mechanism could exist. First of all, a kinematic study of transformation plasticity determines the action of the different elementary mechanisms in the overall behaviour. Therefore, two kinds of Transformation Plasticity are distinguished. Pure Transformation Plasticity (P.T.P.), where the mechanism is intrinsic and Coupled Transformation Plasticity (C.T.P.) in which the microstructure of the transformation (habit plane...) depends on the parent phase plastic yielding. In this paper, only P.T.P. is studied. The single crystal flow rule is determined from the thermomechanical point of view based on Gibb's free energy. And finally, the polycrystal behaviour is described by two different approaches, a phenomenological one which extends the single crystal results, and a micro-macro transition scheme which takes into account the microstructure of the transformation in the aggregate behaviour. The results of these theoretical analyses have been compared with the experimental data obtained with Cu Zn Al pseudoelastic alloys tested in uniaxial tension.

2. Kinematics of transformation plasticity

In this part kinematic studies of transformation plasticity are developed in order to determine, in the overall behaviour, the strain induced by phase transformation or by other mechanisms (elasticity, plasticity, thermal effects). Afterwards, the transformation strain is analysed from the crystallographic point of view.

Let us consider a macrohomogeneous unit volume V of the parent phase. In the initial state, this unit volume is at the temperature T and unstressed. If an external stress or a variation of temperature is imposed, a part V_M of this volume can be transformed into martensite. This phenomenon produces the total local strain $\varepsilon_{ij}^T(r)$ composed with an elastic and inelastic part. The macroscopic strain E_{ij}^T may be obtained by using a standard relationship for averaging:

$$(2.1) \quad E_{ij}^T = \frac{1}{V} \int_V \varepsilon_{ij}^T(r) dV.$$

If V_A and V_M denote, respectively, the austenite and martensite volumes contained in the overall volume, the relation (2.1) may be expressed as:

$$(2.2) \quad E_{ij}^T = \frac{1}{V} \int_{V_A} \varepsilon_{ij}^T(r) dV + \frac{1}{V} \int_{V_M} \varepsilon_{ij}^T(r) dV.$$

If ε_{ij}^{TA} and ε_{ij}^{TM} denote the average total strain in austenite and martensite and if $f = V_M/V$ is the volumetric fraction of martensite, the relation (2.2) takes the following form:

$$(2.3) \quad E_{ij}^T = (1-f) \varepsilon_{ij}^{TA} + f \varepsilon_{ij}^{TM}.$$

This deformation is caused by both the deformation in the two phases and the deformation associated with phase transformation. The strain rate equation (2.3) becomes [8]

$$(2.4) \quad \dot{E}_{ij}^T = (1-f) \dot{\varepsilon}_{ij}^{TA} + f \dot{\varepsilon}_{ij}^{TM} + \varepsilon_{ij}^{AM} \dot{f},$$

where \dot{f} denotes the transformation rate, and ε_{ij}^{AM} is the transformation strain. The average strain rates in the two phases are composed with three terms of different physical meanings: the thermal strain rate $\dot{\varepsilon}_{ij}^{th}$; elastic strain rate $\dot{\varepsilon}_{ij}^e$, associated with local stress, and plastic strain rate $\dot{\varepsilon}_{ij}^p$, induced by both the applied and the internal stress caused by the transformation. $\varepsilon_{ij}^{AM} \dot{f}$ is the only term directly associated with the progress of the transformation. But this term is not independent because the mechanism of transformation needs another inelastic strain to accommodate Bain's strain. If the expansion coefficient and the elastic compliances are both considered as equal in the two phases, the thermal and the elastic strain rates are

$$(2.5) \quad \dot{\varepsilon}_{ij}^{th} = \alpha_{ij} \dot{\theta}, \quad \dot{\varepsilon}_{ij}^e = S_{ijkl} \dot{\sigma}_{kl}^A, \quad \dot{\varepsilon}_{ij}^{eM} = S_{ijkl} \dot{\sigma}_{kl}^M,$$

where α_{ij} denotes the thermal expansion tensor and S_{ijkl} the elastic compliance tensor. The total strain rate is now expressed by

$$(2.6) \quad \dot{E}_{ij}^T = \dot{E}_{ij}^{th} + \dot{E}_{ij}^e + \dot{E}_{ij}^{PT}$$

with the following expressions for \dot{E}_{ij}^{th} and \dot{E}_{ij}^e :

$$(2.7) \quad \begin{aligned} \dot{E}_{ij}^{th} &= \alpha_{ij} \dot{\theta}, \\ \dot{E}_{ij}^e &= S_{ijkl} [(1-f) \dot{\sigma}_{kl}^A + f \dot{\sigma}_{kl}^M] = S_{ijkl} \dot{\Sigma}_{kl}, \end{aligned}$$

where $\dot{\Sigma}_{kl}$ denotes the macroscopic stress rate. Using the relations (2.4) and (2.6), the total transformation strain rate is

$$(2.8) \quad \dot{E}_{ij}^{PT} = (1-f) \dot{\varepsilon}_{ij}^{PA} + f \dot{\varepsilon}_{ij}^{PM} + \varepsilon_{ij}^{AM} \dot{f}.$$

This relation takes into account both the plastic strain rates in the two phases ($\dot{\varepsilon}_{ij}^{PA}$ and $\dot{\varepsilon}_{ij}^{PM}$) and the transformation strain rate.

The dependence of the characteristics of ε_{ij}^{AM} on $\dot{\varepsilon}_{ij}^{PA}$ and $\dot{\varepsilon}_{ij}^{PM}$ is a function of the local stress level (internal and applied) with respect to the yield points of the two phases. Thus two classes of transformation plasticity may be distinguished:

- (i) In the first class the local stresses are too small to reach the yield point; consequently, the transformation strain is only provided by the transformation rate and by the strain ε_{ij}^{AM} that is now completely defined. Thermoelastic martensitic transformations belong to this class because the martensite growth produces no excessive internal stresses.

This class is called Pure Transformation Plasticity (P.T.P.). Phenomena like shape memory effects or pseudoelasticity belong to it.

(ii) In the case of second class, the local stresses are greater than the yield point of one of the phases, then the total transformation strain rate depends on the three terms of the relation (2.8), and the characteristics of ε_{ij}^{AM} are modified by the level of plastic strain. This case is called Coupled Transformation Plasticity (C.T.P.).

This study is limited to P.T.P. associated with the thermoelastic martensitic transformation. The transformation strain rate is then expressed by

$$(2.9) \quad \dot{E}_{ij}^{PT} = \varepsilon_{ij}^{AM} \dot{f}.$$

In addition, the martensitic transformation is characterized by Bain's strain, an invariant lattice strain and a lattice rotation that is necessary to realize the existence of an invariant plane (the habit plane). The macroscopic strain ε_{ij}^{AM} produced by this mechanism is composed of a shear along the habit plane and of an extension normal to it. Geometric conditions [12, 14] allow to calculate the normal \mathbf{n} to the habit plane, the direction \mathbf{m} of the transformation and the magnitude g of the displacement in this direction. The symmetries of the phase lattices are responsible for the existence of numerous equivalent orientations called variants. The following section details the expression for the transformation strain rate, initially for a single crystal with one or several variants, and finally for a polycrystal with or without crystallographic texture.

2.1. Single-crystal kinematics in pure transformation plasticity

The transformation of a macrohomogeneous austenitic single-crystal unit volume by the formation of only one martensite variant is considered at first. In this case the displacement vector of a point P of this volume is a function of the variant habit plane normal \mathbf{n} , the direction of transformation \mathbf{m} and the magnitude g of the displacement in this direction. All these values are crystallographically defined [12]. Denoting by x_k the initial components of point P , the displacement vector components are

$$(2.10) \quad u_i = g x_k n_k m_i,$$

and the gradient of the displacement tensor is

$$(2.11) \quad \beta_{ij} = g m_i n_j.$$

This tensor is composed of a symmetric part which is the transformation strain ε_{ij}^{AM} and of an antisymmetrical one which is the transformation rotation ω_{ij}^{AM} .

$$(2.12) \quad \varepsilon_{ij}^{AM} = \frac{1}{2} (m_i n_j + m_j n_i) g = R_{ij} g,$$

$$(2.13) \quad \omega_{ij}^{AM} = \frac{1}{2} (m_i n_j - m_j n_i) g = P_{ij} g,$$

R_{ij} is called the orientation tensor of the variant. The strain rate and the rotation rate associated with the transformation rate \dot{f} are expressed by

$$(2.14) \quad \dot{E}_{ij}^{PT} = R_{ij} g \dot{f}, \quad \dot{\Omega}_{ij}^{PT} = P_{ij} g \dot{f}.$$

When several equivalent variants are activated, the relations (2.14) become

$$(2.15) \quad E_{ij}^{PT} = g \sum_n R_{ij}^n \dot{f}^n, \quad \dot{\Omega}_{ij}^{PT} = g \sum_n p_{ij}^n \dot{f}^n,$$

where R_{ij}^n and \dot{f}^n denote, respectively, the orientation tensor and the transformation rate of variant n , and where the summation is extended to all activated variants ($\dot{f}^n \neq 0$).

2.2. Polycrystal kinematics in pure transformation plasticity

In a polycrystal the macrohomogeneous volume V is described by the distribution function $F(\psi)$ of the crystal orientations where ψ denotes Euler's angles that described the orientation of an austenite grain in the aggregate. The macroscopic strain rate is now expressed by

$$(2.16) \quad \dot{E}_{ij}^{PT} = \frac{1}{V} \int_V \dot{\epsilon}_{ij}(r) dV = \int_{\psi} \dot{\epsilon}_{ij}(\psi) F(\psi) d\psi.$$

As $\dot{\epsilon}_{ij}(\psi)$ is considered to be homogeneous in each grain, it can be replaced by the expression (2.15) of the single crystal strain rate:

$$(2.17) \quad \dot{E}_{ij}^{PT} = \int_V \sum_n g R_{ij}^n(\psi) \dot{f}^n(\psi) F(\psi) d\psi,$$

And with a discrete description of the function $F(\psi)$ this relation becomes

$$(2.18) \quad \dot{E}_{ij}^{PT} = g \sum_N F^N \sum_n R_{ij}^{nN} \dot{f}^{nN},$$

where N is the number of grains considered and F^N is their volumetric fraction.

In the next section, a single crystal constitutive relation is proposed by a thermodynamic approach based on the study of Gibb's free energy. This makes it possible to relate the transformation rate with the macroscopic stress and changes of temperature.

3. Single-crystal thermomechanical behaviour in pure transformation plasticity

In this section a thermomechanical flow rule based on the study of the variation of Gibb's free energy is proposed. The martensite plates are considered to be stress-induced under isothermal conditions. This corresponds to the case of pseudoelasticity by transformation. Two states could be distinguished in the formation mechanism of the martensite. The first one is a nucleation process which is considered in this study as having no effect on the macroscopic behaviour, and the second is the plate growing. The thermodynamical analysis of the transformation could be limited to the study of a single component system because martensitic transformation is a displacive phase transformation which occurs without diffusion.

A thermomechanical approach based on Gibb's free energy enables to demonstrate the existence of a pseudoelastic potential and to define a transformation criterion. The importance of the volumetric fraction of martensite in the overall behaviour is underlined by the building of an "end of transformation" criterion.

3.1. Single crystal yield function in pure transformation plasticity

When in an austenitic matrix of volume V , n martensitic variants of volume V^n are formed, the variation of Gibb's free energy is expressed by [15, 17]

$$(3.1) \quad \Delta G = \Delta G^c \sum_n V^n + \Gamma S + E_{\text{ext}} + E_{\text{int}},$$

where ΔG^c denotes the variation of the chemical free energy. This variation is a linear function of the temperature and is equal to the difference of the free energies of the two phases. At the thermochemical equilibrium temperature T_0 , ΔG^c becomes equal to zero.

The second term of the relation (3.1), ΓS , is the free energy of the interface between the two phases. For thermoelastic transformation, this energy may be neglected. The third term, E_{ext} , denotes the interaction energy with the externally applied stress σ_{ij} . It will be obtained by using ESHELBY'S relation [15]

$$(3.2) \quad E_{\text{ext}} = - \int_V \sigma_{ij} E_{ij}^{\text{PT}} dV.$$

With respect to the relations (2.15), the relation (3.2) takes the following form:

$$(3.3) \quad E_{\text{ext}} = - \sigma_{ij} g \sum_n R_{ij}^n V^n.$$

The last term, E_{int} , is the elastic energy associated with the internal stresses caused by the incompatibilities of transformation. This energy depends on interactions existing between the different variants. Its accurate evaluation requires the knowledge of the microstructure (shapes and spatial positions of the variants). Indirect evaluations may be realised by using the solution of the problem of the plastic inclusion pair [18, 19] or by the calculation of the elastic energy associated to the interface between two incompatible or compatible variants [20, 21]. These two methods give the same expression for E_{int} :

$$(3.4) \quad E_{\text{int}} = V \left[\sum_n g^2 E^n f^n + \frac{1}{2} \sum_{n,m} g^2 H^{nm} f^n f^m \right],$$

E^n denotes the interaction energy between a martensite inclusion and the parent phase. This energy could be calculated with the solution of the plastic inclusion problem as given by ESHELBY [15]. E^n is equal to zero for an infinitely thin inclusion with a plate shape, this is the case of the martensite variants during the growth process for a thermoelastic transformation. Interactions between the different martensite variants are represented by the matrix H^{nm} . This matrix is composed with two kinds of term; a very low one that describes the interactions between the self-accommodating variants and a very significant one (about $\mu/30$) when variants are incompatible [22, 23]. This gives to matrix H^{nm} a great anisotropy. In the case of self-accommodating variants, a compatible common interface does exist between them: there is no accommodation elastic strain. For incompatible variants their common interface must take a position such that the associated elastic energy is minimized; this minimum is different from zero. Other mechanisms of accommodation could exist to lower these interactions. Finally, with regard to the relations (3.1), (3.3) and (3.4), the variation of Gibb's free energy associated with the creation of stress-induced martensite has the following form:

$$(3.5) \quad \Delta G = \Delta G^c \sum_n V^n - \sigma_{ij} g \sum_n R_{ij}^n V^n + g^2 V \left[\sum_n E^n f^n + \frac{1}{2} \sum_{n,m} H^{nm} f^n f^m \right]$$

and, for unit volume,

$$(3.6) \quad \frac{\Delta G}{V} = \Delta G^c \sum_n f^n - \sigma_{ij} g \sum_n R_{ij}^n f^n + g^2 \left[\sum_n E^n f^n + \frac{1}{2} \sum_{n,m} H^{nm} f^n f^m \right].$$

Relation (3.6) defines a pseudoelastic potential $\Delta G/V$. It describes the state of the austenite-martensite system from the temperature (T), the applied stress (σ_{ij}) and the internal variables gf^n . Thermodynamical forces t^n are associated with the internal variables gf^n ; they are obtained by the classical relation

$$(3.7) \quad \begin{aligned} t^n &= \frac{1}{g} \frac{\partial(\Delta G/V)}{\partial f^n}, \\ t^n &= \frac{\Delta G^c}{g} - \sigma_{ij} R_{ij}^n + gE^n + g \sum_m H^{nm} f^m. \end{aligned}$$

At the thermodynamical equilibrium, t^n is equal to zero and the relation (3.7) becomes

$$(3.8) \quad \sigma_{ij} R_{ij}^n = \frac{\Delta G^c}{g} + gE^n + g \sum_m H^{nm} f^m,$$

$\sigma_{ij} R_{ij}^n$ denotes the resolved stress on the variant n . This variant may be activated when the resolved stress reaches a critical value dependent on the temperature (because of the dependence of ΔG^c), on the volumic fraction of the other variants and on the nature of these variants (compatible or incompatible). At the beginning of the transformation, when no variant is yet formed, and if the energy E^n is considered as negligible, the equation of the yield surface of a variant n has the following expression:

$$(3.9) \quad \sigma_{ij} R_{ij}^n = \frac{\Delta G^c(T)}{g} = \frac{B^n}{g} (T - M_S).$$

The yield surface of the single crystal is formed by the intersection of all the hyperplanes that are defined for each variant by Eq. (3.9). This generalizes the well-known relation of PATEL and COHEN [24] that has a very good agreement with experiment. This criterion states that the first variant formed is the one that has the maximal resolved stress. Variation of the critical resolved stress with respect to the temperature is given by the relation (3.9). If there is no applied stress, the relation (3.9) indicates that all the variants must be formed simultaneously when the temperature reaches the thermodynamic equilibrium temperature. In fact, the interaction between them acts to favorize a self-accommodating group of variants.

3.2. Single crystal flow rule in pure transformation plasticity

When the relation (3.6) is verified, if the loading parameters change, the transformation may advance. In this case, for an activated variant, the variation of the thermodynamic forces dt^n , associated with the internal variables gf^n , must be equal to zero.

$$(3.10) \quad dt^n = \frac{\partial t^n}{\partial T} dT + \frac{\partial t^n}{\partial \sigma_{ij}} d\sigma_{ij} + \frac{\partial t^n}{\partial f^m} df^m = 0.$$

Now, if it is assumed that the only quantity that is temperature-dependent is the chemical free energy, the relation (3.10) becomes

$$(3.11) \quad \frac{1}{g} \frac{\partial \Delta G^c(T)}{\partial T} dT - R_{ij}^n d\sigma_{ij} + g \sum_m H^{nm} df^m = 0.$$

This relation enables to calculate df^m by using the loading parameters $d\sigma_{ij}$ and dT :

$$(3.12) \quad g \sum_m H^{nm} df^m = R_{ij}^n d\sigma_{ij} - \frac{1}{g} \frac{\partial \Delta G^c(T)}{\partial T} dT.$$

If the interaction matrix H is invertible and denoting by B^n/g the quantities $\frac{1}{g} \frac{\partial \Delta G^c(T)}{\partial T}$, the relation (3.12) may be transformed into

$$(3.13) \quad g df^m = \sum_n H_{nm}^{-1} \left\{ R_{ij}^n d\sigma_{ij} - \frac{B^n}{g} dT \right\}.$$

This relation states that the growth of a variant m depends on the increase of the resolved stress, on itself and on the growth of the other variants. If a variation dT occurs while the loading remains constant, the interactions between variants modify the forces df^m in order to favour the group of variants which has weak interaction. Now the single crystal behaviour could be completely described:

(i) If all the following conditions, derived from Eqs. (2.15) and (3.13) are satisfied, some active variant n could exist,

$$(3.14) \quad \begin{aligned} f < 1 \quad \left(\text{with } f = \sum_n f^n \right), \\ dT < 0, \quad df^m \geq 0, \\ \sigma_{ij} R_{ij}^n = \frac{B^n}{g} (T - M_s) + g \sum_m H_{nm} f^m, \\ R_{ij}^n d\sigma_{ij} = \frac{B^n}{g} dT + g \sum_m H_{nm} df^m \end{aligned}$$

in this case, dE_{ij}^{PT} is different from zero and the Pure Transformation Plasticity constitutive relation is obtained from Eqs. (2.15) and (3.13)

$$(3.15) \quad dE_{ij}^{PT} = \sum_n R_{ij}^n \sum_m H_{nm}^{-1} \left(R_{kl}^m d\sigma_{kl} - \frac{B^m}{g} dT \right).$$

(ii) If only one of the conditions (3.14) is not verified, no transformation could take place in the single crystal and dE_{ij}^{PT} is equal to zero.

The particular form of the flow rule (3.15), which is derived from the same relation as the criterion (2.9), indicates that the single crystal is a standard material for P.T.P. The experimental measurements which are described in Sect. 5 show a good agreement with this constitutive relation. In the following section, a more complex polycrystal behaviour is analysed from two different points of view.

4. Polycrystal behaviour in pure transformation plasticity

In a polycrystal, the individual grains deform heterogeneously and large internal stresses are generated by the incompatibilities between the grains. This leads to a more complex problem than in the single crystal case. The polycrystal behaviour may be analysed in two ways.

(i) One is to develop a phenomenological constitutive relation. This approach was presented in previous papers [25, 26] for pure transformation plasticity. In this way, the polycrystal is considered as a standard material and its flow rule is obtained by defining a transformation criterion analogous to the Von Mises one. This model shows good agreement with experimental measurements for a pseudoelastic alloy of Cu Zn Al tested in tension (Fig. 4) [26, 27]. But the predictive capabilities of this model are limited because no reference is made to the microstructural state.

(ii) The second approach [28] is based on a micro-macro modelling. The transformation is described from a microstructural point of view and an integral equation is established for the thermomechanical behaviour of the aggregate. This equation is solved by using the new self-consistent method developed by LIPINSKI and BERVEILLER [29, 31].

In this paper the second approach is developed but in a simpler way by using the a priori elasto-plastic self-consistent scheme. Each grain is successively regarded as an inclusion within an equivalent homogeneous matrix that is formed with all the other grains. The polycrystal behaviour is then calculated by using an averaging process that assumed an elasto-plastic accommodation. This model gives good predictions for monotonous loading in the classical plasticity case [32]. To apply this scheme for Pure Transformation Plasticity, two major differences with classical plasticity must be taken into account: the volume changes during transformation and the interaction law must be a thermomechanical one. The uniform stress in the inclusion is recalculated without neglecting the changing volume and assuming that the elasticity is isotropic and linear [15].

$$(4.1) \quad \sigma_{ij} = 2\mu \left(\varepsilon_{ij}^e + \frac{\nu}{1-2\nu} \varepsilon_{kk}^e \delta_{ij} \right),$$

μ denotes the elastic shear modulus and ν the Poisson's ratio. The elastic strain is obtained by using Eshelby's tensor:

$$(4.2) \quad \varepsilon_{ij}^e = S_{ijkl} \varepsilon_{kl}^{PT} - \varepsilon_{ij}^{PT}.$$

For a spherical inclusion Eshelby's tensor is simply expressed in a scalar form. Relation (4.1) becomes

$$(4.3) \quad \sigma_{ij} = 2\mu \left[(\beta - 1) \varepsilon_{ij}^{PT} + \frac{1}{2} (\beta - \gamma) \varepsilon_{kk}^{PT} \delta_{ij} \right]$$

with

$$(4.4) \quad \beta = \frac{2(4-5\nu)}{15(1-\nu)},$$

$$\gamma = \frac{2}{3(1-\nu)},$$

β and γ both depend only on Poisson's ratio and are, respectively, roughly equal to 0.5 and 1. Now, if the matrix is deformed with uniform macroscopic transformation strain E_{ij}^{PT} and if uniform macroscopic stress Σ_{ij} is superposed, the stress in the inclusion is

$$(4.5) \quad \sigma_{ij} = \Sigma_{ij} + 2\mu \left[(1-\beta)(E_{ij}^{PT} - \varepsilon_{ij}^{PT}) + \frac{1}{2}(\gamma-\beta)(E_{kk}^{PT} - \varepsilon_{kk}^{PT}) \delta_{ij} \right].$$

In this relation the internal stresses are accommodated only in an elastic way. As the volume changing for the thermoelastic martensitic transformation is low, in order to have an elasto-plastic accommodation, the elastic shear modulus μ may be replaced by the elasto-plastic shear modulus $\alpha\mu$. Relation (4.5) becomes with $\beta = 0.5$ and $\gamma = 1$.

$$(4.6) \quad \sigma_{ij} = \Sigma_{ij} + \alpha\mu(E_{ii}^{PT} - \varepsilon_{ij}^{PT}) + \frac{\alpha\mu}{2}(E_{kk}^{PT} - \varepsilon_{kk}^{PT}) \delta_{ij}.$$

This is the elasto-plastic interaction law between homogeneous matrix and an inclusion in Pure Transformation Plasticity. The thermomechanical behaviour of the inclusion must now be specified. In the polycrystal, the grains are supposed to be homogeneous inclusions and to have the single-crystal behaviour previously described by the relation (2.30).

$$(4.7) \quad d\varepsilon_{ij}^{PT} = \sum_n R_{ij}^n \sum_m H_{nm}^{-1} \left[R_{kl}^m d\sigma_{kl} - \frac{B^m}{g} dT \right].$$

In each grain, 24 variants may be activated. It is assumed that the initial critical shear stress is the same for all the 24 variants and that no changing occurs in the thermomechanical loading path. Thus, from a given state of loading, the increase of volumetric fraction, of a martensite variant, df^n is given by the following relations which are derived from Sect. 3:

(i) for an active variant which remains active

$$(4.8) \quad \begin{aligned} f^n &< 1, \\ \sigma_{ij} R_{ij}^n &= \frac{B^n}{g} (T - M_S + g) \sum_m H_{nm} f^m \end{aligned}$$

and

$$R_{ij}^n d\sigma_{ij} = \frac{B^n}{g} dT + g \sum_m H_{nm} df^m.$$

Thus the transformation rate of this variant is

$$(4.9) \quad df^n = \frac{1}{g} \sum_m H_{nm}^{-1} \left\{ R_{ij}^m d\sigma_{ij} - \frac{B^m}{g} dT \right\}$$

and the strain induced by its formation is given by

$$(4.10) \quad (d\varepsilon_{ij}^{PT})^n = g R_{ij}^n df^n.$$

(ii) for an active variant which becomes passive

$$(4.11) \quad \begin{aligned} f^n &< 1, \\ \sigma_{ij} R_{ij}^n &= \frac{B^n}{g} (T - M_S) + g \sum_m H_{nm} f^m \end{aligned}$$

and

$$R_{ij}^n d\sigma_{ij} < \frac{B^n}{g} dT + g \sum_m H_{nm} df^m, \\ f^n = 1.$$

(iii) for a passive variant

$$(4.12) \quad \sigma_{ij} R_{ij}^n < \frac{B^n}{g} (T - M_S) + g \sum_m H_{nm} f^m, \\ \text{or } f^n = 1.$$

(iiii) if $\Sigma f^m = 1$ all the variants must be passive, the grain is entirely transformed.

Using these conditions and the interaction law (4.6), the following relations are determined for each active variant n of grain I.

$$(4.13) \quad R_{ij}^n d\sigma_{ij}^I = R_{ij}^n d\Sigma_{ij} + \alpha\mu (dE_{ij}^{PT} - (d\varepsilon_{ij}^{PT})^I) + \frac{\alpha\mu}{2} (dE_{kk}^{PT} - (d\varepsilon_{kk}^{PT})^I) \delta_{ij} \\ = \frac{B^n}{g} dT + \sum_m H_{nm} g df^{mI}.$$

Now, if the transformation strain for both polycrystal and grain are related to the microstructural description established by the kinematic study (relations (2.15) and (2.18)), the relation (4.13) turns into a linear equation system where the volumetric fraction of each variant in each grain are the parameters). Thus the basic equation for an active variant may now be expressed as

$$(4.14) \quad \alpha\mu g \left[\sum_m R_{ij}^{mI} df^{mI} + \frac{\delta_{ij}}{2} \sum_m R_{kk}^{mI} df^{mI} - \left(\sum_N F^N \sum_m R_{ij}^{mN} df^{mN} \right. \right. \\ \left. \left. + \frac{\delta_{ij}}{2} \sum_N F^N \sum_m R_{kk}^{mN} df^{mN} \right) \right] + \sum_m H_{nm} g df^{mI} = R_{ij}^n d\Sigma_{ij} - \frac{B^n}{g} dT.$$

5. Application to uniaxial tensile test for pseudoelastic alloys

The relations derived in this paper are now used to describe the uniaxial tensile test of Cu Zn Al pseudoelastic alloys. In these alloys the volume change induced by transformation is small and will be neglected. In the single crystal uniaxial tensile test, the stress-induced martensite is formed with only one variant [33].

5.1. Single crystal experimental results

In this case, when the loading is radial, the only variant formed is the one that has the greatest resolved shear stress. The orientation factor of this variant was determined by using a Laue diagram. The composition of the alloy was Cu - 16 at % Zn - 15 at % Al for

$M_s = -60^\circ\text{C}$. The single crystal was grown by the Bridgman method and was water-quenched. A sheet tensile specimen ($2.1 \times 2.05 \times 18$ mm, gauge length 10 mm) was cut from the single crystal. Tensile tests were carried out in a Zwick machine with a strain rate of $1.7 \cdot 10^{-3} \text{ s}^{-1}$. In order to test at different temperatures, the specimen was kept in a chamber in which the temperature was held constant during the test (between -54°C and 24°C). The measurement of elongation was made with a LVDT extensometer. To make obvious the thermomechanical behaviour of the single crystal in pure transformation plasticity, the tensile test with constant load was performed while changing temperature (with constant stress ranging from 65 MPa to 210 MPa). To describe the uniaxial tensile test of this alloy, the relations established in Sect. 3 of this paper must be applied to this particular loading, taking into account the fact that there is no volume change and only one variant formed. The transformation criterion (3.9) is now expressed by

$$(5.1) \quad \tau^0 = R\sigma^0 = \frac{B}{g}(T - M_s)$$

and the flow rule becomes

$$(5.2) \quad dE^{PT} = \frac{R}{H} \left(R d\sigma - \frac{B}{g} dT \right)$$

with H denoting the transformation slope $\frac{d\tau}{gdf}$ during an uniaxial tensile test at constant temperature, $R (= R_{33})$ is the Schmid factor for the active variant at constant temperature. Figures 1 and 2 give typical uniaxial tensile test curves for a single crystal of a pseudoelastic

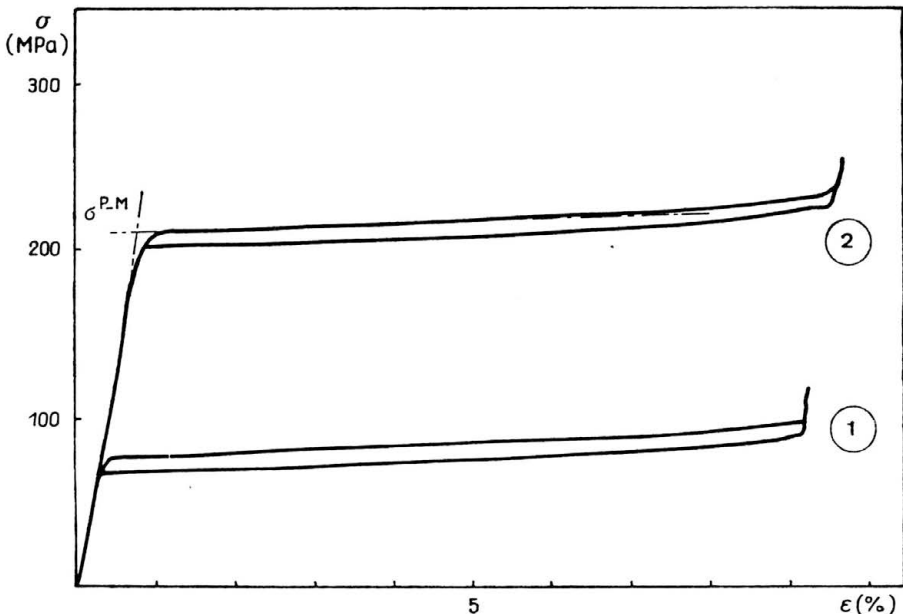


FIG. 1. Single-crystal uniaxial tensile test curves of a pseudoelastic Cu - 16 at % Zn - 15 at % Al alloy for different test temperature (test σ_T); 1) $T = -34^\circ\text{C}$, 2) $T = 18^\circ\text{C}$.

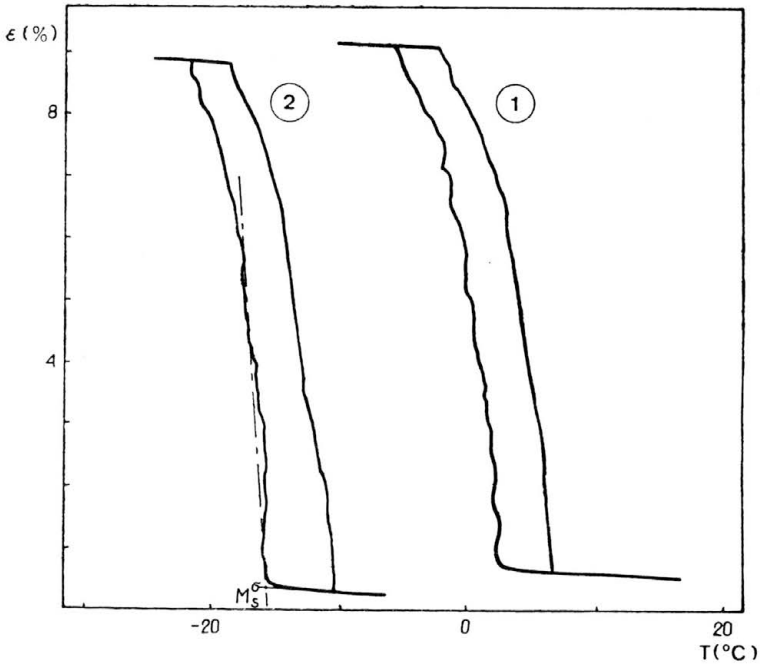


FIG. 2. Single-crystal tensile test at different constant load for a pseudoelastic Cu -16 at % Zn -15 at % Al alloy (test T_σ); 1) $\sigma_a = 174$ MPa, 2) $\sigma_a = 128$ MPa.

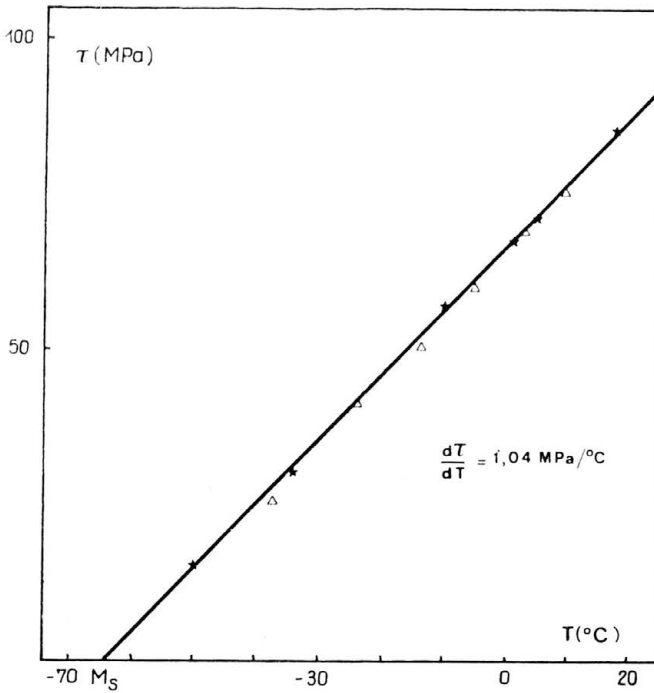


FIG. 3. Dependence of the single-crystal transformation yield point on the applied shear stress or on the test temperature for a pseudoelastic Cu -16 at % Zn -15 at % Al alloy; * — tensile test at constant temperature (test σ_T), Δ — tensile test at constant shear stress (test T_σ).

alloy. The shear magnitude g may be deduced from the measurement of the total transformation strain using the relation (2.9). The calculated value $g = 0.22$ is in good agreement with WECHSLER, LIEBERMAN and READ'S phenomenological theory [12]. The H parameter may be considered as constant during a tensile test. The variation of the transformation yield point τ^0 with the applied stress or the test temperature is represented in Fig. 3. This variation is a linear one, well described by the relation (5.1). The M_S temperature measured on this curve is equal to 209 K, that is nearly the theoretical value ($M_S = 213^\circ\text{K}$), and for this alloy $B/g = 1.04 \text{ MPa} \cdot \text{K}^{-1}$, that is in agreement with other authors [34, 36].

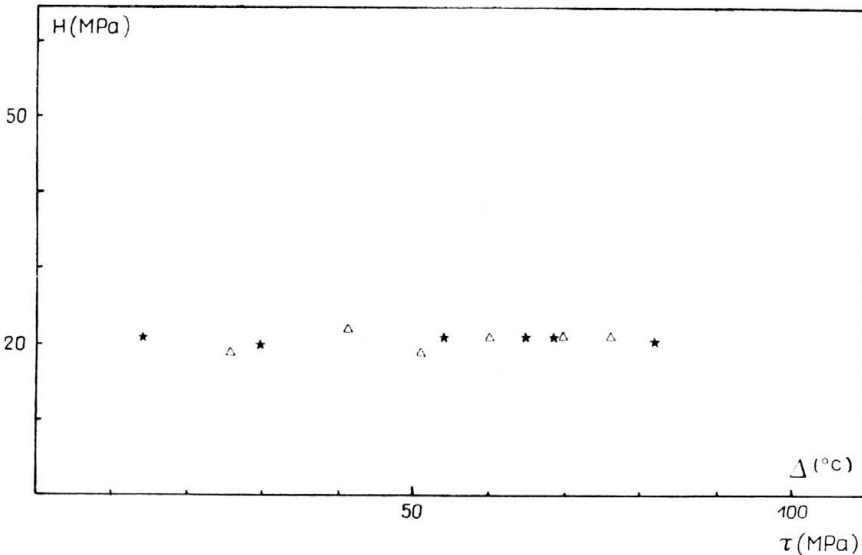


FIG. 4. Single crystal parameter H as a function of the tensile test temperature (test σ_T) or of the applied shear stress in the tensile test with constant loading (test T_σ); * — tensile test at constant temperature (test σ_T), Δ — tensile test at constant shear stress (test T_σ).

The H parameter value is then compared for different test temperatures and different types of loading. It is found that this value may be considered as a constant (Fig. 4). To conclude it is possible to say that the single crystal behaviour is well described by this modelization.

5.2. Polycrystal experimental results

The alloy used in this experimental part was elaborated by Trefimétaux (Cu–25 at % Zn–9 at % Zn), for a M_S temperature equal to 240 K. In this alloy tensile samples were annealed for 10 mn inside a furnace at 850°C and then water-quenched. Their grain size was about 0.3 mm. Tensile tests were carried out as previously described for the single crystal. Due to the existence of induced internal stress, the transition between elasticity and transformation plasticity was more difficult to be distinguished in the strain-stress curves obtained. Nevertheless, a transformation steady state with a constant slope, independent of the temperature, was observed. The transformation point was determined by using the intersection with a straight line defined by the elastic modulus. Transformation

points corresponding to different test temperatures or different applied stresses are not perfectly aligned as in the single crystal case, but a linear approximation gives $d\sigma_s/dT = 2.00 \text{ MPa}^\circ\text{K}^{-1}$ (Fig. 5). This experimental result is consistent with the phenomenological constitutive relation $\left(d\sigma_s/dT = \sqrt{3} \frac{B}{g} = 1.80 \text{ MPa K}^{-1}\right)$. This phenomenological modell-

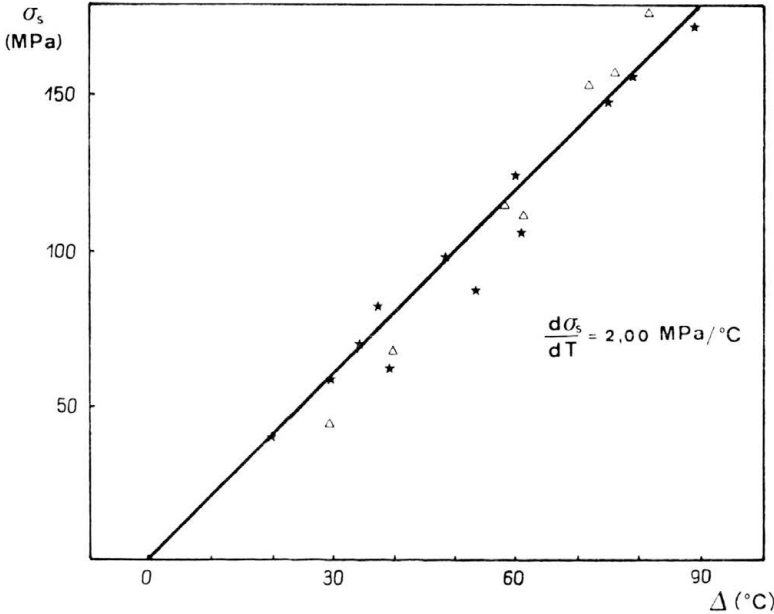


FIG. 5. Dependence of the polycrystal transformation yield point on the applied shear stress or on the test temperature. Experiment performed with a pseudoelastic Cu -25 at % Zn -9 at % Al alloy; * — tensile test at constant temperature (test σ_T), Δ — tensile test at constant shear stress (test T_σ).

ing may be compared with experimental results by using the following relation derived from a previous paper [26]:

$$(5.3) \quad \left(\frac{d\sigma}{dE^{PT}} \times \frac{dE^{PT}}{dT}\right)_{\text{polycrystal}} = \sqrt{3} \left(\frac{g df}{dT} \times \frac{d\tau}{g df}\right)_{\text{single crystal}}$$

This relation which related the steady state of transformation for both single crystal and polycrystal was experimentally verified as shown by Fig. 6. In conclusion, this phenomenological modelling may be considered as a good first approximation of polycrystal behaviour. Now, to take into account phenomena like the transient state between elasticity and transformation plasticity, or like the anisotropic behaviour, the micro-macro scheme previously defined must be applied. In the case of the Cu Zn Al alloys, the volume change induced by the transformation may be neglected, thus the interaction law (4.6) becomes

$$(5.4) \quad \sigma_{ij} = \Sigma_{ij} + \alpha\mu(E_{ij}^{PT} - \epsilon_{ij}^{PT})$$

and each active variant of each grain verified the following relation (from the relation (4.10)):

$$(5.5) \quad R_{ij}^n g \alpha \mu \left[\sum_m R_{ij}^{m1} df^{m1} - \sum_N F^N \left(\sum_m R_{ij}^{mN} df^{mN} \right) \right] + \sum_m H_{nm} g df^{m1} = R_{ij}^n d\Sigma_{ij} - \frac{B^n}{g} dT.$$

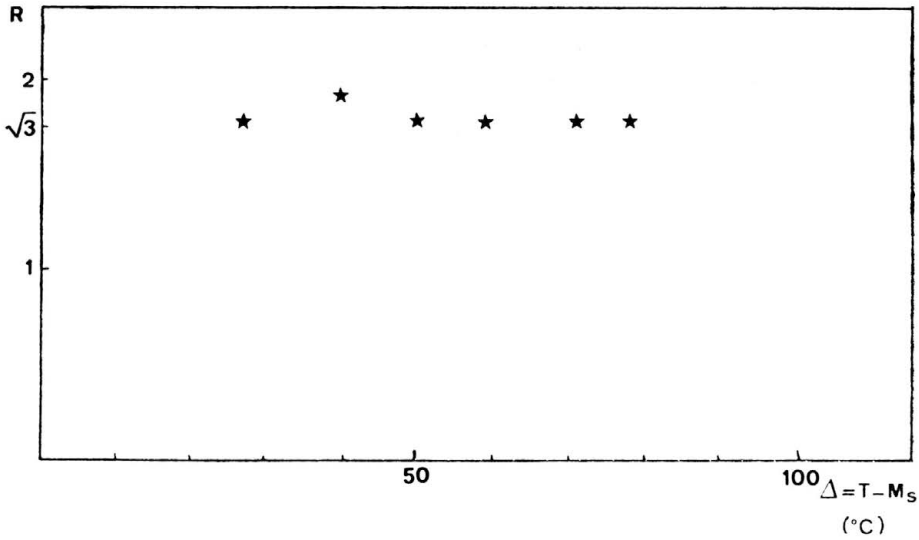


FIG. 6. Ratio R vs. Δ , the difference between the test temperature and the M_s value of the pseudoleastic alloy;

$$R = \frac{\left(\frac{d\sigma}{dE^{PT}} \times \frac{dE^{PT}}{dT} \right)_{\text{polycrystal}}}{\left(\frac{gdf}{dT} \times \frac{d\tau}{gdf} \right)_{\text{single crystal}}}$$

For the uniaxial tensile test, a major assumption could be made in order to simplify the system of equations (5.5): only one variant is activated in each grain. With this assumption, the system of equations (5.5) turns into a linear system

$$(5.6) \quad \left(H + \frac{\alpha\mu}{2} \right) gdf^I - \frac{3}{2} \alpha\mu R^I \sum_N R^N F^N gdf^N = Rd\Sigma - \frac{B}{g} dT.$$

This system has as many equations as there are transforming grains. Transformation takes place in a grain if the conditions (4.8), are satisfied. These conditions are now expressed by

$$(5.7) \quad \begin{aligned} f^I &< 1, \\ \sigma^I R^I &= \frac{B}{g} (T - M_s), \\ R^I d\sigma &= \frac{B}{g} dT + gHdf^I. \end{aligned}$$

By using the condition (5.7) and the linear system (5.6), it is possible to determine for each grain the evolution df^I of the transformation corresponding to a variation of thermo-mechanical loading ($d\Sigma, dT$). Finally, the macroscopic behaviour is obtained by using the averaging relation (2.18) that is now expressed by

$$(5.8) \quad dE^{PT} = \sum_N F^N R^N gdf^N.$$

This scheme was used with the experimental data obtained for the single crystal ($\mu = 42\ 308\ \text{MPa}$, $H = 20\ \text{MPa}$, $g = 0.22$). The polycrystal macroscopic behaviour calculated was consistent with experimental measurements for the uniaxial tensile test (Fig. 7 and 8). The slope of transformation was well described and the relation between the two kinds

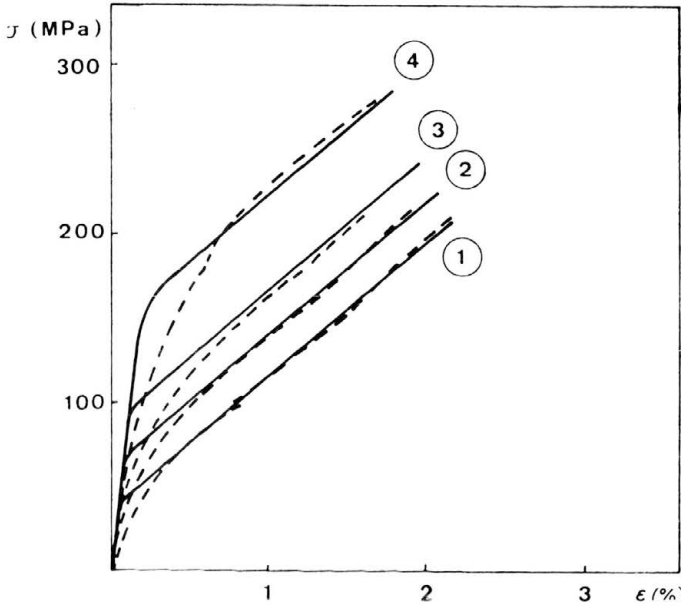


FIG. 7. Uniaxial tensile test curves of a pseudoelastic Cu -25 at % Zn -9 at % Al polycrystal alloy for different temperatures. Comparison between experimental results and theoretical predictions which are obtained by using a self-consistent scheme;
 ----- experimental results, ————— simulated behaviour,
 1) $T = 5^\circ\text{C}$, 2) $T = 19^\circ\text{C}$, 3) $T = 43^\circ\text{C}$, 4) $T = 68^\circ\text{C}$.

of experiments used in this study was respected. A transient behaviour between elasticity and transformation plasticity is obtained. When taking the single crystal experiment value of $B/g = 1.04\ \text{MPa K}^{-1}$, the calculated linear relation between the applied stress and the transformation temperature ($d\sigma_s/dT = 2.4\ \text{MPa K}^{-1}$) was slightly higher than the experimental one ($d\sigma_s/dT = 2.00\ \text{MPa K}^{-1}$). With a B/g value equal $0.87\ \text{MPa K}^{-1}$, which is still in agreement with the published results [35], the calculated and experimental value for the polycrystal was equal. This indicates that the origin of this difference may be the difference of composition between the single-crystal alloy and the polycrystal one used in this work. To conclude, it can be said that this micro-macro approach gives good results in a simpler manner and in spite of a strong assumption. A better result could be obtained using the new self-consistent scheme developed by LIPINSKI and BERVEILLER [29, 31].

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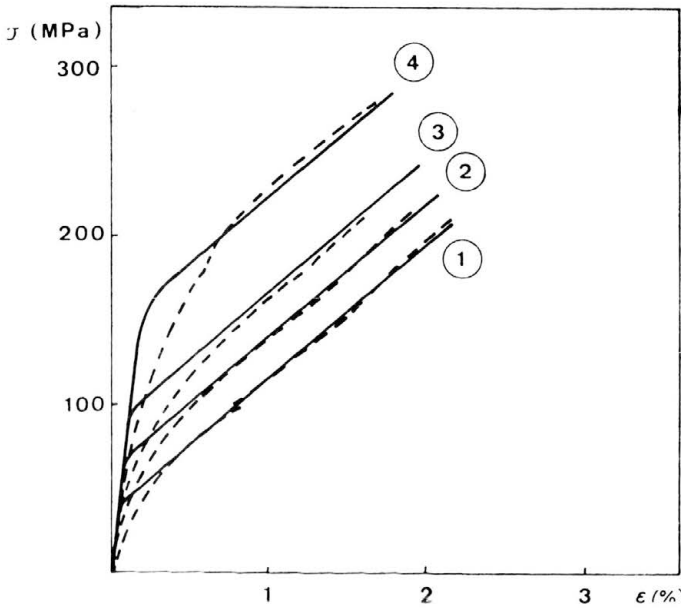


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Received March 24, 1988.