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Micromechanics-based modeling of plastic polycrystals: an affine formulation

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Abstract

Recent comparisons of predictions associated with Hill's original 'incremental' formulation for the self-consistent modelling of elastoplastic polycrystals with a newly available nonlinear upper bound for the moduli have brought to light the fact that this formulation leads to a frequent violation of this bound. This conclusion has motivated the conception of a new formulation, called the 'affine formulation', which is expected to yield softer predictions. The principle of this formulation is first reported for the simpler case of nonlinear elasticity (or viscosity) and compared with other approaches. It is then extended to cases for which the current responses depend on the loading path, with specification to the self-consistent scheme in order to model transient responses of polycrystals; though no variational approach exists in these cases, the obtained predictions can be considered as improved ones since they are shown to be, as expected, softer than those derived from other models. © 2000 Elsevier Science S.A. All rights reserved.

Keywords: Plastic polycrystals; Affine formulation; Moduli

1. Introduction

The first attempt to model the overall behaviour of elastoplastic polycrystals through a self-consistent micromechanical approach was proposed by Kröner [1] almost 40 years ago. It was proved to be based on an elastic analysis of the mechanical interactions between grains and then to yield too stiff predictions. An improved approach was then proposed by Hill [2] who used an 'incremental' formulation based on the (multi-branched) linearization of the local constitutive equations relating the strain and stress rates through instantaneous elastic-plastic moduli which were considered as uniform within every constituent phase. The same approach was used later by Hutchinson [3] for viscoplastic materials by simply changing the strain rate into its second order time-derivative; incidentally, when applied to power-law creep, this formulation was shown to be integrable into a 'secant' (total) one which makes use of secant creep compliances relating the creep rate to the stress, both locally and globally. More recently, a different approach was proposed by Moli-

nari et al. [4] for viscoplastic power-law polycrystals; it can be considered as a 'tangent' approach since it makes use of local tangent creep moduli while the treatment is no more incremental: at any stage, the actual local nonlinear constitutive equations for every phase are replaced by linearized ones using tangent moduli and a pre-stress variable; the overall linearized behaviour is determined through a self-consistent procedure which assumes a power-law relation for the overall quantities. Starting from a similar local linearization procedure, a different homogenization treatment was proposed by Rougier et al. [5] for rate-dependent elastoplastic polycrystals: if we omit here the specific complication which arises from the viscoelastic coupling and if we make an extrapolation to viscoplasticity, this treatment, which is not restricted to power-law relations, is of a thermo-viscoelastic type and can be considered as a prototype of the 'affine' formulation which is defined hereafter. In this respect, it has some common features with the 'second-order procedure' which has been proposed recently by Ponte Castañeda [6] within a potential approach.

Most of these current efforts for improved formulations in the field of nonlinear homogenization have been stimulated by recent comparisons [7] between

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several classical estimates and newly available nonlinear upper bounds for the moduli [8]: these comparisons have brought to light the fact that most of the classical estimates can violate these bounds, which indicates that the corresponding predictions of the overall behaviour are generally too stiff. This conclusion has motivated too the systematic development of the ‘affine formulation’ both for hereditary and non-hereditary constitutive behaviour since it was expected to yield softer predictions than the incremental and secant ones. This is the main matter of this paper: the principle of this formulation is first reported for the simpler case of nonlinear elasticity (or viscosity) and compared with similar, but different, other approaches. It is then extended to hereditary cases for which the current responses depend on the loading path, with specification to the self-consistent scheme in order to model transient responses of polycrystals; though no variational approach leading to bounds still exists in these cases, the obtained predictions can be considered as improved ones since they are shown to be, as expected, softer than those derived from other models.

2. The linear comparison heterogeneous medium

Most of the above mentioned methods for the derivation of nonlinear estimates of the overall behaviour of heterogeneous materials actually rely on the use of a linear ‘comparison’ heterogeneous medium (LCHM say): this fictitious body can be roughly defined as derived from the actual nonlinear one at some given stage by keeping the same microstructure but replacing at each point the nonlinear mechanical properties by linearized ones. The overall response of the actual body at this stage is then assimilated to the one of the associated linear comparison medium. Since the mechanical variables which have to be used for the definition of the linearized properties vary from one point to another, even within a given phase, the derivation of the effective behaviour of this LCHM would be untractable without additional assumptions: that is why the linearized properties are usually supposed to be uniform and defined at some reference state, e.g. the average strain or strain rate per phase.

Whereas the explicit recourse to the LCHM concept was initially proposed by Ponte Castañeda [8] within a new variational approach, it can be checked that an implicit use of this notion was already made before. According to Kröner’s conception, the linear moduli at each point of the LCHM (i.e. for each phase) reduce to the elastic ones, which obviously leads to a strong overestimation of the overall moduli. According to Hill’s incremental formulation which aims at predicting an infinitesimal evolution from the current one, the instantaneous moduli, which are generally much lower

than the elastic ones, are used for the definition of the LCHM; these moduli, which are supposed to be uniform within each phase, are defined as the tangent moduli of the considered phase for a particular strain value, the average one. According to a secant formulation, a similar treatment (except for the fact that it is no more incremental) would be adopted by use of the ‘secant’ moduli (at some reference strain) instead of the ‘tangent’ ones.

Once again, we emphasize the fact that, except for Kröner’s treatment, the local linearized properties should have to vary from one point to another within a given phase whereas they are actually assumed to be uniform per phase. This approximation may have more or less important consequences on the resulting estimate according to the chosen formulation. For instance, on a typical nonlinear uniaxial stress-strain curve (e.g. $\sigma = k\varepsilon^m$), it is easy to check that the range of variation of the secant modulus E_s (e.g. $E_s = k\varepsilon^{m-2}$) associated to a given strain fluctuation $\Delta\varepsilon$ from a given strain ε_0 (e.g. $\Delta E_s = k(m-1)\varepsilon_0^{m-2}\Delta\varepsilon$) is larger than the one of the tangent modulus E_t (e.g. $\Delta E_t = km(m-1)\varepsilon_0^{m-2}\Delta\varepsilon = m\Delta E_s$, with $0 < m < 1$). Consequently, the assumption of uniform per phase secant moduli could be thought to be more approximate than the same one for tangent moduli. But an incremental ‘à la Hill’ procedure using tangent moduli would make the approximation errors cumulate by integration along the loading path so that it could practically be not better than a secant procedure (and it actually gives identical results in the case studied by Hutchinson [3]).

Note that this discussion is qualitative only: in actual 3 D situations, the definition of secant moduli is not even unique (see [9,10]). Nevertheless, for non-hereditary behaviours for which the response does not depend on the loading path, so that an incremental procedure is not necessary, it can suggest an intermediate approach which would borrow its ‘total’ character from the secant one and the use of ‘tangent’ (i.e. softer) properties from the incremental one. This has led to the so-called ‘affine’ formulation which is reported first for non linear elasticity or viscosity.

3. The affine formulation for nonlinear elasticity (or viscosity)

Let us focus on the case of elasticity: nonlinear viscosity would be treated in the same way by simply changing strains by strain rates and elastic moduli and compliances by creep quantities. According to the affine formulation, we approximate the actual behaviour of every constituent phase at any stage by its tangent compliance or modulus at some reference state (for instance the average strain or stress) and the associated uniform pre-stress or pre-strain. Due to this pre-stress

or pre-strain, which may be assimilated to an eigenstress or eigenstrain, the resultant LCHM can be considered as a ‘thermoelastic’ body whose overall behaviour can be derived by using the classical homogenization procedure for linear thermoelasticity.

Let the local constitutive equations at any point x of a given phase (r) be written in the form:

$$\sigma(x) = h_r(\varepsilon(x)) \quad \text{or} \quad \varepsilon(x) = g_r(\sigma(x)) \quad (1)$$

Their linearized ‘affine’ expression at some stress $\tilde{\sigma}$ or strain $\tilde{\varepsilon}$ reads:

$$\sigma(x) = l_r(x):\varepsilon(x) + \sigma^0(x) \quad \text{or} \quad \varepsilon(x) = m_r(x):\sigma + \varepsilon^0(x)$$

with

$$l_r = \frac{d h_r}{d \varepsilon}(\tilde{\varepsilon}) \quad \text{and} \quad m_r = \frac{d g_r}{d \sigma}(\tilde{\sigma}) \quad (2)$$

$$\sigma^0 = h_r(\tilde{\varepsilon}) - \frac{d h_r}{d \varepsilon}(\tilde{\varepsilon}):\tilde{\varepsilon} \quad \text{and} \quad \varepsilon^0 = l_r(\tilde{\sigma}) - \frac{d g_r}{d \sigma}(\tilde{\sigma}):\tilde{\sigma}$$

Notice that, due to the existence of a stress or strain elastic potential, l_r and m_r exhibit the usual symmetry of elastic moduli and compliances. Let us assume for a while that we are able to deal with this continuous heterogeneity throughout the body by using some linear homogenization procedure which allows us to derive the strain or stress concentration tensor fields $A_r(x)$ and $B_r(x)$ for homogeneous strain or stress boundary conditions, respectively, when no pre-stress or pre-strain is present. If the strain or stress field was known, the overall behaviour would be easily derived from the classical equations:

$$\Sigma = L^{\text{eff}}:E + \Sigma^0 \quad \text{or} \quad E = M^{\text{eff}}:\Sigma + E^0$$

with

$$L^{\text{eff}} = \langle l:A \rangle \quad \text{or} \quad M^{\text{eff}} = \langle m:B \rangle \quad (3)$$

$$\Sigma^0 = \langle {}^t A:\sigma^0 \rangle \quad \text{or} \quad E^0 = \langle {}^t B:\varepsilon^0 \rangle$$

where ${}^t A$ denotes the transposed tensor of A and $\langle \cdot \rangle$ indicates a spatial average. In order to solve the problem completely, we have to combine these equations with the local strain or stress concentration relations associated with the chosen linear homogenization scheme, so that the whole problem is defined by a set of implicit nonlinear equations. This task is practically untractable and it has to be simplified.

We then adopt the essential approximation of uniformity per phase of the moduli and pre-stress (or the compliances and pre-strain) by defining the local l_r or m_r at some reference state, e.g. defined by the average strain $\bar{\varepsilon}_r$ or stress $\bar{\sigma}_r$. Eqs. (2) and (3) are unchanged, except for the fact that l_r and m_r , as well as σ^0 and ε^0 are now defined at $\bar{\varepsilon}_r$ and $\bar{\sigma}_r$, so that the phase averages \bar{A}_r , \bar{B}_r , ${}^t \bar{A}_r$ and ${}^t \bar{B}_r$ are only needed. The concentration equations also have to correlate only $\bar{\varepsilon}_r$ or $\bar{\sigma}_r$ with the macroscopic strain or stress and the local and

overall variables ε_r^0 and E^0 or σ_r^0 and Σ^0 . The resulting set of equations may be considered as a nonlinear system for the main unknown variables, namely $\bar{\varepsilon}_r$ or $\bar{\sigma}_r$.

As an example, if we apply this affine formulation to the particular case of the selfconsistent scheme, the corresponding equations are specified as follows:

$$\Sigma = L^{\text{SC}}:E + \Sigma^0 \quad \text{or} \quad E = M^{\text{SC}}:\Sigma + E^0$$

$$L^{\text{SC}} = \sum_r c_r l_r: A_r^{\text{SC}} \quad \text{or} \quad M^{\text{SC}} = \sum_r c_r m_r: B_r^{\text{SC}} \quad (4)$$

$$\Sigma^0 = \sum_r c_r {}^t A_r^{\text{SC}}:\sigma_r^0 \quad \text{or} \quad E^0 = \sum_r c_r {}^t B_r^{\text{SC}}:\varepsilon_r^0$$

with c_r the volume fractions; the concentration tensors are defined by:

$$A_r^{\text{SC}} = (I + P_r^{\text{SC}}:\delta l_r^{\text{SC}})^{-1}:\langle (I + P^{\text{SC}}:\delta l^{\text{SC}})^{-1} \rangle^{-1} \quad \text{with}$$

$$l_r^{\text{SC}} = l_r - L^{\text{SC}}$$

or

$$B_r^{\text{SC}} = (I + Q_r^{\text{SC}}:\delta m_r^{\text{SC}})^{-1}:\langle (I + Q^{\text{SC}}:\delta m^{\text{SC}})^{-1} \rangle^{-1}$$

$$\text{with} \quad m_r^{\text{SC}} = m_r - M^{\text{SC}} \quad (5)$$

and the concentration equations are given by:

$$\bar{\varepsilon}_r = (I + P_r^{\text{SC}}:\delta l_r^{\text{SC}})^{-1}:[E_0 + P_r^{\text{SC}}:(l_r:\varepsilon_r^0 - L^{\text{SC}}:E^0)] \quad \text{with}$$

$$\sum_r c_r \bar{\varepsilon}_r = E_r$$

or

$$\bar{\sigma}_r = (I + Q_r^{\text{SC}}:\delta m_r^{\text{SC}})^{-1}:[\Sigma_0 + Q_r^{\text{SC}}:(m_r:\sigma_r^0 - M^{\text{SC}}:\Sigma^0)]$$

$$\text{with} \quad \sum_r c_r \bar{\sigma}_r = \Sigma. \quad (6)$$

Here, the polarization tensors P_r^{SC} and Q_r^{SC} refer to the classical integral over an ellipsoid Ω_r of the Green operator Γ^{SC} :

$$P_r^{\text{SC}} = \int_{\Omega_r} \Gamma^{\text{SC}}(x - x') d x'$$

$$x \in \Omega_r \quad Q_r^{\text{SC}} = L^{\text{SC}} - L^{\text{SC}}:Q_r^{\text{SC}}:L^{\text{SC}} \quad (7)$$

As classical, for identically shaped and oriented ellipsoids, these tensors do not differ from one phase to another and the concentration equations reduce to:

$$\bar{\varepsilon}_r = A_r^{\text{SC}}:[E + P^{\text{SC}}:(\Sigma^0 - \sigma_r^0)] \quad \text{or}$$

$$\bar{\sigma}_r = B_r^{\text{SC}}:[\Sigma + Q^{\text{SC}}:(E^0 - \varepsilon_r^0)] \quad (8)$$

Such an ‘affine self-consistent scheme’ can be numerically implemented according to the following iterative procedure, e.g. for prescribed macroscopic strain E conditions: we start with $\bar{\varepsilon}_r^{(1)} = E$ and we determine the corresponding tangent moduli $l_r^{(1)}$ and pre-stresses $\sigma_r^{(1)}$; we then solve Eq. (4), according to usual self-consistent iterative procedures, for a first estimate of the overall moduli and pre-stress $L^{\text{SC}(1)}$ and $\Sigma^{0(1)}$. At some further step (k), this is then used for updated estimates of the phase average strain tensors according to:

$$\bar{\varepsilon}_r^{(k+1)} = A_r^{\text{SC}(k)} \cdot [E + P^{\text{SC}(k)} \cdot (\Sigma^{0(k)} - \sigma_r^{0(k)})] \quad (9)$$

until some convergence criterion is reached.

4. Comparison with other formulations

This affine formulation uses the same linearization procedure at the microscale as the ‘tangent’ one which had already been proposed for finite strains by Molinari et al. [4] and developed by Lebensohn and Tome [11] but it definitely differs from it for the derivation of the overall behaviour. Instead of solving directly the linear thermoelastic problem defined by Eq. (3), the tangent formulation makes use of a presumed expression of the overall nonlinear constitutive equations so as to derive the overall moduli from the condition of being ‘tangent’ moduli for these equations. That is the reason why these authors have thought necessary to restrict themselves to power-law creep (with the same

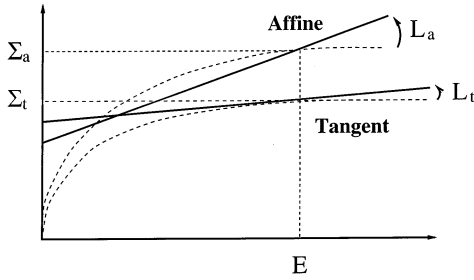


Fig. 1. Schematic illustration of the difference between the macroscopic responses as predicted by the affine (L_a, Σ_a) and tangent (L_t, Σ_t) formulations, respectively.

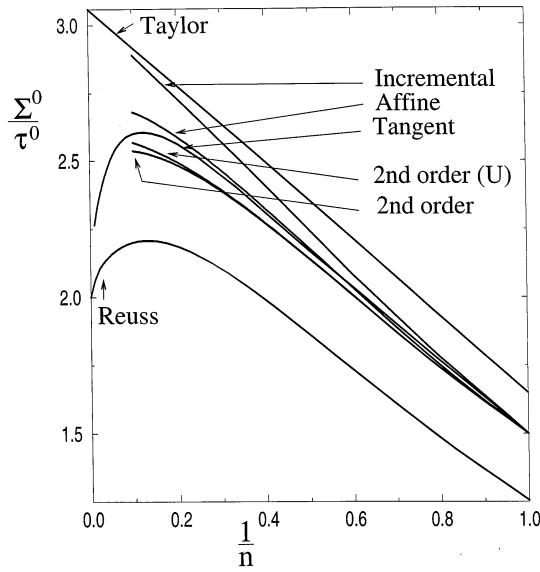


Fig. 2. Predicted normalized creep reference stress Σ^0/τ^0 for power-law untextured FCC polycrystals as a function of the rate sensitivity factor $1/n$: Taylor and Reuss bounds and incremental (or secant), affine, tangent and ‘second-order’ self-consistent estimates.

exponent for all the phases and for all the slip systems in case of polycrystals), a situation for which they supposed the overall creep to obey the same dependence: as shown hereabove, the affine formulation has obviously no need of such a restriction. On the contrary, it has been proved [12] that the ‘tangent condition’ for the overall moduli which is a basic assumption of the tangent formulation is actually inconsistent with the LCHM approach according to which the overall moduli as derived from Eq. (3) are not tangent moduli for the overall behaviour. For power-law creep, this property results from the following inequality

$$\langle {}^t A : I_r : \varepsilon \rangle_r \neq {}^t \bar{A}_r : I_r : \bar{\varepsilon}_r \quad (10)$$

whereas the tangent formulation implicitly considers the equality to hold, despite the nonuniformity of the strain and strain concentration fields within the phases. In addition, some confusion between secant and tangent moduli when deriving the concentration equations for the self-consistent scheme leads the tangent formulation to far too soft predictions, tending towards Reuss’s estimate, for an increasing nonlinearity. Fig. 1 shows a schematic illustration of the

More recently, Ponte Castañeda [6] has proposed a new formulation, the so-called ‘second-order procedure’, based on a second-order Taylor development of the local strain or stress potential, which has some common features with the affine formulation. Roughly speaking, this procedure, which is restricted to single potential behaviours, deals with the same linear thermoelastic problem as the affine formulation but the homogenized properties of this medium are derived from the effective either strain or stress potential. It can be shown [12] that, if the same homogenization model has been chosen for both formulations, the average strains (resp. stresses) per phase are the same when the strain (resp. stress) potentials are used but that the average stress (resp. strain) estimates are different. According to the affine formulation the following approximations are made for each phase:

$$\bar{\sigma}_r = h_r(\bar{\varepsilon}_r) \quad \text{or} \quad \bar{\varepsilon}_r = g_r(\bar{\sigma}_r) \quad (11)$$

whereas the second-order procedure can take better into account the strain or stress fluctuations within each phase. Consequently this procedure leads to predictions which are generally a little bit softer than those derived from the affine formulation, with an increasing discrepancy with increasing nonlinearity.

We can see on Fig. 2 an illustrative application of various formulations to the prediction of the creep resistance of power-law untextured FCC polycrystals as a function of the rate sensitivity factor $m = 1/n$. Whereas Hutchinson’s incremental (or secant) prediction tends to Taylor’s bound and the tangent one to Reuss’s bound for increasing n values, the affine and second-order (with ‘U’ for the stress formulation) pre-

dictions are rather similar but they are likely to deviate from one another for n going to infinity. Whereas one could credit the second-order procedure with a more accurate treatment of the ‘intrapphase’ heterogeneity, it can be stressed that the affine formulation has the definite advantage of permitting an extension to hereditary behaviours for which the current response depends on the loading history, so that they cannot be described by one single potential.

5. The affine formulation for hereditary constitutive behaviour

From the foregoing description of the affine formulation for nonlinear elasticity or viscosity, it has not to be concluded that it is inappropriate in case of a hereditary behaviour. Actually, its basic linearization assumption can easily be combined with a dependence of the current response on the loading path provided the macroscopic loading history is given.

Let us first deal with the case of nonlinear viscoelasticity: this typical case of hereditary constitutive behaviour is concerned with the crucial (linear or nonlinear) viscoelastic coupling and its associated ‘long range memory effect’ which is especially responsible for the fact that the overall behaviour of a blend of maxwellian constituents is no longer maxwellian, due to the delayed mechanical interactions between the phases. For linear viscoelasticity, as already shown by Laws and McLaughlin [13] for the self-consistent scheme, this difficulty may be overcome by use of the correspondence principle or of the Laplace–Carson transformation which permits the conversion of the linear viscoelastic problem into a classical linear elastic one. For nonlinear viscoelasticity, the LCHM approach could in principle have recourse to the same technique provided the local linear properties of this comparison medium are defined unambiguously.

This definition is not as straightforward as it was in the case of nonlinear elasticity or viscosity due to the simultaneous occurrence of derivatives of different orders (e.g. $\dot{\varepsilon}$, $\ddot{\sigma}$ and σ) in the local constitutive equations, so that tangent or secant moduli cannot be easily determined. As already done by Kröner for elastoplasticity, one could of course adopt the convenient short cut of using the elastic moduli of the different phases as the local moduli of the LCHM: this was first proposed by Weng [14] for infinitesimal transformations and extended later by other authors ([15,16]) for finite strains but the corresponding schemes can in advance be considered as much too stiff and as neglecting the essential long range memory effect. On the contrary, one can define, according to the affine formulation, a ‘thermoviscoelastic’ LCHM which makes possible the recourse to the correspondence principle or the

Laplace–Carson transformation technique. Without reporting here this treatment completely (see e.g. [5,12,17] for further details), we can stress its main specific features for the simple case of local constitutive equations in the form:

$$\dot{\varepsilon} = s:\dot{\sigma} + g(\sigma) \quad (12)$$

with s the elastic compliance and g some nonlinear function of σ . Suppose the macroscopic stress path $\Sigma(u)$, $0 \leq u \leq \tau$ to be known; we are looking for the macroscopic strain tensor $E(\tau)$ at any prescribed time τ . For $t \geq \tau$, we could use the linearized expression:

$$\begin{aligned} t \geq \tau: \dot{\varepsilon}(t) &= s:\dot{\sigma}(t) + g(\sigma(\tau)) + m(\tau):[\sigma(t) - \sigma(\tau)] m(\tau) \\ &= \frac{d}{d\sigma} g(\sigma(\tau)) \end{aligned} \quad (13)$$

but what we really need is rather such a linearized expression for $t < \tau$ in order to predict the local and overall responses at time t . This means that we actually need the whole set of local variables for $0 \leq t < \tau$. Let them be considered for a while as already determined. Referring to the state of the LCHM at time τ , we could express its (linearized) local constitutive equations as:

$$\begin{aligned} \forall t: \dot{\varepsilon}(t) &= s:\dot{\sigma}(t) + m(\tau):\sigma(t) + \dot{\varepsilon}^0(\tau, t) \\ \dot{\varepsilon}^0(\tau, t) &= g(\tau) - m(\tau):\sigma(\tau) \\ &\quad + [g(t) - g(\tau)] \\ &\quad - m(\tau):(\sigma(\tau) - \sigma(t)).[1 - H(t - \tau)] \end{aligned} \quad (14)$$

with

$$g(\tau) = g(\sigma(\tau)) \quad \text{and} \quad g(t) = g(\sigma(t))$$

where $H(t)$ stands for the unit step function at $t = 0$. This expression, which fits with the nonlinear constitutive Eq. (12) for $t \leq \tau$ if $\sigma(t)$ has been determined on $[0, \tau]$, may be considered as defining a linear viscoelastic behaviour with the eigenstrain rate $\dot{\varepsilon}^0(\tau, t)$, i.e. a linear thermoviscoelastic behaviour. It could be put in the more familiar form:

$$\forall t: \varepsilon(t) = [m_\tau \otimes \sigma](\tau, t) + \varepsilon^0(\tau, t)$$

with

$$m_\tau(\tau, t) = s + m(\tau).t$$

$$\varepsilon^0(\tau, t) = \varepsilon(0_+) - s:\sigma(0_+) + \int_0^t \dot{\varepsilon}^0(\tau, u) du \quad (15)$$

$$[m_\tau \otimes \sigma](\tau, t) = \frac{d}{dt} \left[\int_0^t m_\tau(\tau, t-u):\sigma(u) du \right]$$

which assures the overall (linearized) constitutive equations to read:

$$\forall t: E(t) = [M_\tau \otimes \Sigma](\tau, t) + E^0(\tau, t) \quad (16)$$

where the overall viscoelastic compliance $M_\tau(\tau, t)$ has no longer a maxwellian expression. This effective com-

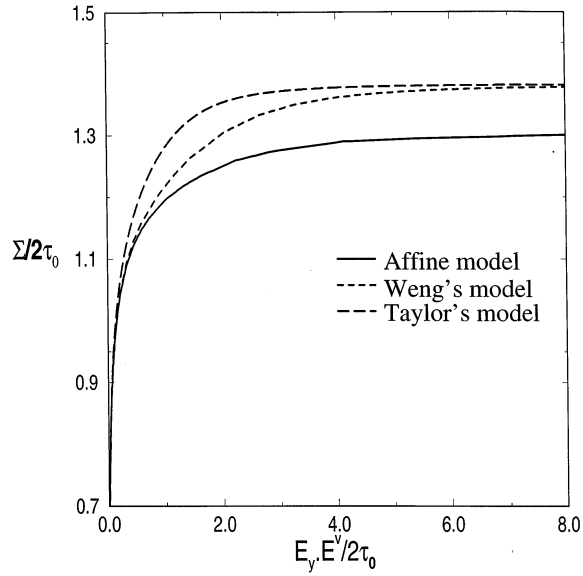


Fig. 3. Predicted normalized tensile stress-viscous strain E^v curves for an untextured FCC polycrystal: our model (solid line); Taylor's and Weng's models (dotted lines); ($\tau^0/E_y = 10^{-3}$, prescribed axial strain $\dot{E} = \dot{\gamma}^0$, $n = 5$).

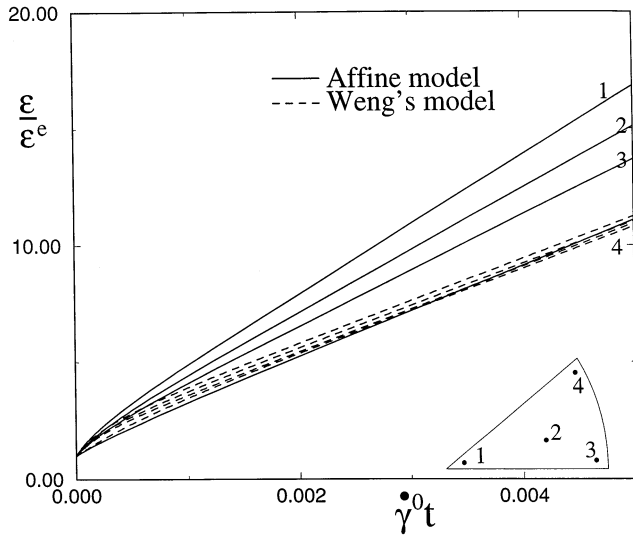


Fig. 4. Predicted intragranular equivalent strain during a tensile creep test for some crystals of an untextured FCC polycrystal: our model (solid lines) and Weng's model (dotted lines); ($n = 5$, $\tau^0/E_y = 10^{-3}$, $\Sigma/\tau^0 = 4$, ϵ^e is the equivalent elastic initial strain).

pliance as well as the macroscopic pre-strain $E^0(\tau, t)$ can now be determined, after choosing an appropriate linear homogenization scheme, by use of the correspondence principle and the transposition to viscoelasticity (e.g. through the Laplace–Carson transformation) of the classical thermoelastic relationships Eq. (3). Once again, the use of an affine formulation at $t = \tau$ makes this determination, which needs the one of the local variables, to result from the resolution of a set of nonlinear implicit equations (through an adequate iter-

ative numerical procedure).

These equations are actually doubly implicit, since we have still to determine the local variables $\sigma(u)$, $0 \leq u < \tau$ which have provisionally been considered as already known though they are not: this needs to discretize the time interval $[0, \tau]$ with a sufficient number of intermediate times θ_i , $i = 1$ to N in order to apply the affine procedure to the determination of the LCHM's behaviour at each time θ_i . This operation is performed better by making use of the causal nature of the involved constitutive equations, i.e. by proceeding through increasing times θ_i so as to use at each step the results obtained at the former ones.

This method has been applied to a number of typical situations (polymer blends, CFC and HCP polycrystals...) and models (classical and generalized self-consistent schemes). An illustrative example is given in Figs. 3 and 4 for an untextured FCC polycrystal with octahedric slip systems (s) obeying the flow equation $\dot{\gamma}_s = \dot{\gamma}^0 \left(\frac{\tau_s}{\tau^0} \right)^n .sg(\tau_s)$ where τ_s is the resolved shear stress on (s). It can be checked that, as expected, the overall response predicted from an affine self-consistent scheme is much softer than the ones deriving from Taylor's or Kröner–Weng's models. On Fig. 4, we can check that our formulation predicts much larger grain to grain strain variations than Weng's one: as already illustrated by Harren's simulations compared to Taylor's predictions [16], the assimilation of the linear moduli of the LCHM to the elastic moduli of the constituent phases hardly departs from Taylor's uniform strain assumption.

Another application of the affine formulation to hereditary behaviours can be performed by considering elastoplastic heterogeneous materials whose phases have to satisfy some plastic criterion so that their response depends on the loading path. This was the case originally considered by Hill [2] for elastoplastic polycrystals with crystals obeying the Schmid law. For such a problem, which does not need, of course, the use of the Laplace transformation, we have nevertheless still to adopt a step-by-step treatment; when combined with a (multibranch) linear self-consistent model, the affine formulation [18] then offers an alternative treatment to Hill's elastoplastic self-consistent scheme and to other simplified versions [9], with the advantage of yielding softer predictions (see Fig. 5).

6. Conclusion

The affine formulation has been shown to offer a consistent alternative to Hill's classical incremental treatment. When combined to any appropriate linear homogenization scheme, it is able to yield softer overall responses than Hill's one, whatever the considered con-

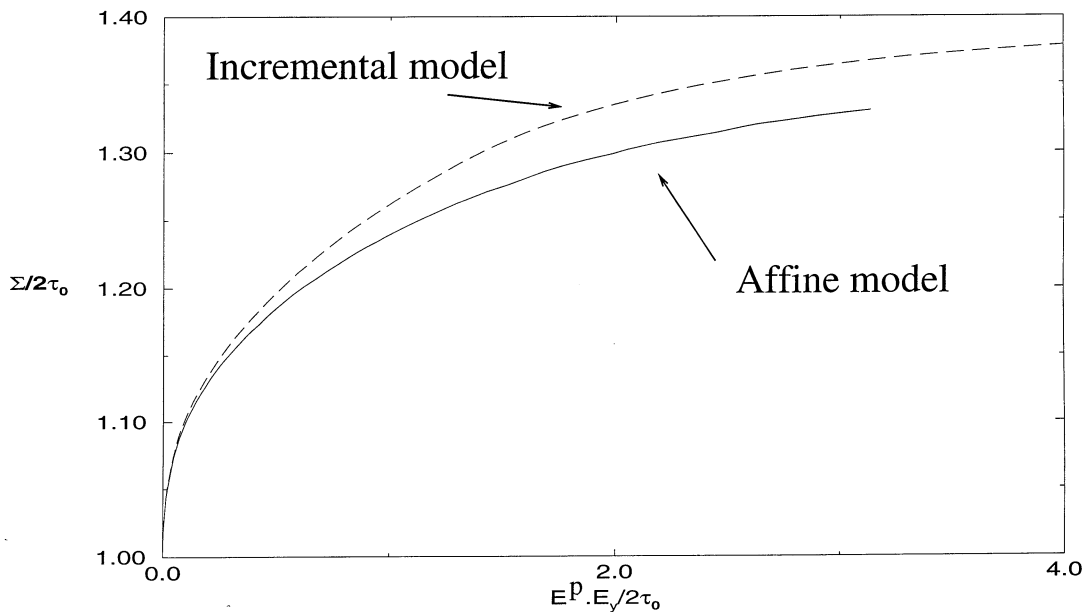


Fig. 5. Predicted normalized tensile stress-strain curves for an untextured FCC polycrystal (no hardening octahedric slip systems) according to the affine (solid line) and Hill's incremental (dotted line) self-consistent schemes.

stitutive behaviour. Whereas this property can be appreciated as attractive in the sense of a more favourable behaviour with respect to potential bounds violation, the affine formulation cannot be thought as immune to such a violation. Considerable improvements with respect to the above reported simplified version are likely to be performed by referring the local linearized properties to refined average quantities: for instance, instead of the plain strain average per phase, one could think of second order moments as proposed by Suquet [19] or of any appropriate averages which could make possible some definite connection with variational approaches.

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