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▶ To cite this version:

Pierre Navidi, Yves Rougier, André Zaoui. Self-consistent modelling of elastic-viscoplastic multiphase materials. IUTAM Symposium on Micromechanics of Plasticity and Damage of Multiphase Materials, Aug 1995, Sèvres, France. pp.123-130, 10.1007/978-94-009-1756-9_16. hal-00116414

HAL Id: hal-00116414 https://hal.science/hal-00116414v1

Submitted on 15 Nov 2022

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SELF-CONSISTENT MODELLING OF ELASTIC-VISCOPLASTIC MULTIPHASE MATERIALS

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Abstract

This paper is devoted to a self-consistent derivation of the overall behaviour of multiphase materials from those of the constituent phases when these phases obey ratedependent elastic-plastic constitutive equations. We have already proposed a solution to this still unsolved problem in the case of quite simple constitutive equations. In this paper, the formulation is extended to more general ones, including internal parameters: such a description can be specified for the case of rate-dependent elastic-plastic polycrystals and the classically associated constitutive equations. It is shown that the merits of the proposed formulation are saved at the expense of limited complication. A simple application is given as an illustration of the tractability of the method.

1. Introduction

The problem of deriving, through a self-consistent procedure, the overall behaviour of multiphase materials from those of the constituent phases when they obey rate-dependent elastic-plastic constitutive equations was still open until quite recently. However the first extension of the self-consistent scheme from elasticity to elastoplasticity was proposed more than thirty years ago by Kröner [1] by dealing with the plastic strain as with an eigenstrain, and by using directly Eshelby's well-known solution of the inclusion problem [2]. Consequently, the corresponding scheme considered only elastic interactions between the phases instead of the actual elastic-plastic ones. A few years later, this treatment was improved by Hill [3] who used a linearization procedure allowing a far better approximation of these interactions by considering, at each step, each phase as an ellipsoidal inhomogeneity, defined by its instantaneous (elastic-plastic) moduli, embedded in an infinite matrix with uniform instantaneous moduli: these moduli were those of the effective medium under investigation at the same step. A quite similar treatment was applied later to viscoplasticity [4], by simply replacing first by second order time derivatives of the strain tensors. Nevertheless, the method could not be extended to elastic-viscoplastic multiphase materials, due to the difficulty of dealing with the coupling between elasticity and viscosity.

On the other hand, this coupling was easily dealt with in the case of linear (non ageing) viscoelasticity [5] through the use of the correspondence principle and of the

Laplace transform technique, which allows one to convert the problem into a (symbolically) elastic one; unfortunately such an artifice cannot work for nonlinear viscoelastic (or rate-dependent elastic-plastic) materials. Apart from preliminary approximate treatments [6], the first attempts to solve this problem [7, 8, 9, 10] reiterated Kröner's misrepresentation of nonlinearity by considering now the viscoplastic strain as an eigenstrain. Now again, the corresponding scheme dealt with elastic interactions between the phases instead of the actual elastic-viscoplastic ones.

By combining Hill's linearization procedure and the use, at each step, of the Laplace transform technique, we have already shown [11, 12] that a new formulation can be defined which, in contrast with the existing ones, correctly accounts for the elastic-viscoplastic nature of the interphase interactions. This method is based on the fact that some auxiliary strain variable -which is not the viscoplastic one, but which expresses the nonlinear behaviour and its delayed effects on the response- can actually be considered as an eigenstrain: this property allows one to convert the elastic-viscoplastic problem into an incrementally linear viscoelastic one with eigenstrains (and then, through the Laplace technique, into a symbolically elastic one with eigenstrains).

However, this formulation was applied to constitutive equations which were too much simple (section 2) to allow one to deal with polycrystals. In this paper, the method is extended to more general constitutive equations, including internal parameters: such a description can be specified for rate-dependent elastoplastic polycrystals. It is shown (section 3) that the merits of the already proposed formulation are saved at the expense of limited complication. A simple application is given (section 4) as an illustration of the tractability of the method.

2. Principle of the proposed formulation

To begin with, let us consider the following simple local nonlinear viscoelastic (or elastic-viscoplastic) equations:

$$\dot{\varepsilon} = \mathbf{s} \cdot \dot{\sigma} + \mathbf{g}(\sigma),$$
 (1)

where s stands for the elastic compliances. We are supposed to have determined the local and overall responses to some given loading path from time t = 0 up to $t = t_n$ and we aim at deriving the response on the next infinitesimal time interval $[t_n, t_n + dt]$. The constitutive equations are linearized in the following form:

$$\dot{\varepsilon}(t) = \mathbf{s} : \dot{\sigma}(t) + \mathbf{m}_{(n)} : \sigma(t) + \dot{\varepsilon}_{(n)}^{0}(t, t_{n})$$

$$\dot{\varepsilon}_{(n)}^{0}(t, t_{n}) = \mathbf{g}[\sigma(t_{n})] - \mathbf{m}_{(n)} : \sigma(t_{n}) + \dots$$

$$\dots + \{\mathbf{g}[\sigma(t)] - \mathbf{g}[\sigma(t_{n})] - \mathbf{m}_{(n)} : [\sigma(t) - \sigma(t_{n})]\} [1 - \mathbf{H}(t - t_{n})]$$

$$\mathbf{m}_{(n)} = \frac{\mathbf{dg}}{\mathbf{d\sigma}} [\sigma(t_{n})],$$
(2)

where H(t) is the unit step function. Note that $\dot{\epsilon}_{(n)}^0(t, t_n)$ includes a term which vanishes for $t \ge t_n$ but which does not do so before, so as to allow us to take the actual constitutive equations (1) for $t \le t_n$: it is essential to do so in order to keep, from the initial stage up to t_n , the memory of the actual nonlinear behaviour for the prediction of the response after t_n , since it influences the subsequent response at any time. Despite this complication, the resulting linearized behaviour is quite simple: as a matter of fact, it reduces to a Maxwellian one, with the *eigenstrain* $\varepsilon_{(n)}^0(t, t_n)$. The crucial point is this: such a strain is actually an eigenstrain because its variation is completely known *a priori* and does not depend on the external loading applied beyond t_n ; its time derivative is constant for $t \ge t_n$ and variable *but known* on $[0, t_n]$. Such an auxiliary strain generalizes Eshelby's definition of a "stress-free strain" and can be dealt with in the following as a (variable but known) eigenstrain. On the contrary, the viscous strain ε^v is not an eigenstrain since the viscous strain rate $g(\sigma)$ is stress history-dependent: considering ε^v as an eigenstrain [7, 8, 9, 10] would lead to an elastic interphase strain accommodation treatment which conflicts with the viscoelastic nature of these interactions [13].

This analysis allows us to perform the homogenization procedure straightforwardly, by extending in a classical way the known treatment of linear viscoelasticity [5] to the case where eigenstrains are present: the use of the Laplace-Carson transform defined by

$$f^*(p) = p \int_0^{\infty} f(t) \exp(-pt) dt$$
(3)

which can apply to $\varepsilon_{(n)}^{0}(t, t_n)$ as well, allows us to convert the problem into a (symbolically) elastic one with eigenstrains. If A (B resp.) denotes the strain (stress resp.) elastic concentration tensor and, according to the correspondence principle, $A^{*}(p)$ (B*(p) resp.) the transformed viscoelastic (when no eigenstrains are present) equivalent, the whole set of equations reads classically:

$$\epsilon^{*} = s^{*}: \sigma^{*} + \epsilon_{(n)}^{0} * \quad \text{or} \quad \sigma^{*} = c^{*}: (\epsilon^{*} - \epsilon_{(n)}^{0}^{*}),$$

$$s^{*}(p) = s + \frac{\mathbf{m}_{(n)}}{p}, \quad c^{*}(p) = s^{*-1}(p),$$

$$\mathbf{E}^{*} = \mathbf{S}^{\text{hom}} *: \Sigma^{*} + \mathbf{E}_{(n)}^{0} * \quad \text{or} \quad \Sigma^{*} = \mathbf{C}^{\text{hom}} *: (\mathbf{E}^{*} - \mathbf{E}_{(n)}^{0}^{*}), \quad (4)$$

$$\mathbf{C}^{\text{hom}} *(p) = < \mathbf{c}^{*}(p): \mathbf{A}^{*}(p) > \text{ or } \quad \mathbf{S}^{\text{hom}} *(p) = < \mathbf{s}^{*}(p): \mathbf{B}^{*}(p) >,$$

$$\mathbf{B}^{*}(p) = \mathbf{c}^{*}(p): \mathbf{A}^{*}(p): < \mathbf{c}^{*}(p): \mathbf{A}^{*}(p) >^{-1},$$

$$\mathbf{E}_{(n)}^{0} *(p) = < \mathbf{B}^{*T}(p): \epsilon_{(n)}^{0} *(p) >.$$
(4)

Here, B^T denotes the transposed tensor of B, <f> the average of f over all the phases and C^{hom} or S^{hom} are the homogenized (effective) moduli and compliances.

The last step consists in the Laplace-Carson inversion; in general, it has to be performed numerically according to adequate techniques such as collocation. Note that, due to the nonlinearity of the constitutive behaviour, an additional relation is needed between the local and global variables in order to determine the mechanical state of each phase at every step: of course, this concentration equation (when eigenstrains are present) is model-dependent.

When the (classical) self-consistent scheme is used, $A^*(p)$ in (4) - say $A^{SC*}(p)$ is derived from the Laplace-transform $\Gamma^{SC*}(p)$ of the viscoelastic Green operator associated to the elastic one by the correspondence principle:

$$\mathbf{A}_{r}^{SC} * (p) = [\mathbf{I} + \mathbf{P}_{r}^{SC} * (p): \delta \mathbf{c}_{r}^{SC} * (p)]^{-1} :< [\mathbf{I} + \mathbf{P}^{SC} * (p): \delta \mathbf{c}^{SC} * (p)]^{-1} >^{-1}, \delta \mathbf{c}_{r}^{SC} * (p) = \mathbf{c}_{r} * (p) - \mathbf{C}^{SC} * (p), \mathbf{P}_{r}^{SC} * (p) = \int \Gamma^{SC} * (p, \underline{\mathbf{x}}_{r}, \underline{\mathbf{x}}'_{r}) d\omega'_{r},$$
(5)

where Ω_r is the ellipsoidal inclusion which represents the phase (r).

The additional concentration equation mentioned herabove reads as classical:

$$\varepsilon_{r}^{*}(p) = [\mathbf{I} + \mathbf{P}_{r}^{SC}^{*}(p):\delta\varepsilon_{r}^{SC}^{*}(p)]^{-1}: \{\varepsilon_{0}^{*}(p)+... + \mathbf{P}_{r}^{SC}^{*}(p):[\varepsilon_{r}^{*}(p):\varepsilon_{(n)r}^{0}^{*}(p)-\mathbf{C}^{SC}^{*}(p):\mathbf{E}_{(n)}^{0}^{*}(p)]\},$$
(6)

where the auxiliary variable $\varepsilon_0^*(p)$ is identified through the condition that the average strain equals the macroscopic one ($\langle \varepsilon^*(p) \rangle = E^*(p)$). If all the ellipsoids have the same aspect ratios and orientation, P^{SC} is the same for all the phases so that the term $\langle [I + P^{SC}^*(p): \delta c^{SC}^*(p)]^{-1} \rangle$ reduces to unity and $\varepsilon_0^*(p)$ equals $E^*(p)$.

The tractability of this method has been checked on the quite simple case [14] of a shear relaxation test performed on an isotropic incompressible two-phase material (note that on the three curves of Figure 2(a) in [14], the E_0 values have to be inverted). Now we examine more general equations than (1) in order to see whether we can apply the proposed method to rate-dependent elastoplastic polycrystals.

3. Extension to polycrystal-type constitutive behaviour

Due to the disordered morphology of polycrystals and to the statistical meaning of the self-consistent scheme [15], this model is known to be especially adapted to the scale change from the single crystal to the polycrystal. The crystallography-based (small strain) constitutive equations of rate-dependent elastoplastic polycrystals are usually put in the following form:

$$\dot{\varepsilon} = \mathbf{s} : \dot{\sigma} + \sum_{s} \dot{\gamma}_{s} \mathbf{R}^{s}$$

$$\mathbf{R}^{s} = \frac{1}{2} (\underline{\mathbf{n}}_{s} \otimes \underline{\mathbf{m}}_{s} + \underline{\mathbf{m}}_{s} \otimes \underline{\mathbf{n}}_{s})$$

$$\dot{\gamma}_{s} = \dot{\gamma}_{s}^{0} (\frac{\tau_{s}}{\tau_{s}^{0}})^{\mathbf{v}_{s}}$$

$$\tau_{s} = \mathbf{R}^{s} : \sigma$$

$$\dot{\tau}_{s}^{0} = \sum_{t} \mathbf{H}^{st} \dot{\gamma}_{t},$$
(7)

where \underline{n}_s and \underline{m}_s are the unit normal and the unit vector of the slip system (s), $\dot{\gamma}_s$ is the shear rate on this system and Hst is the so-called "hardening matrix" which may depend on stress and strain. Such constitutive equations cannot reduce to the form (1) but they can be put in the following more general form:

$$\dot{\varepsilon} = \mathbf{s} : \dot{\sigma} + \mathbf{g}(\sigma, \alpha)$$

$$\dot{\alpha} = \mathbf{h}(\sigma, \alpha),$$
(8)

where α are some tensorial internal parameters. For the sake of simplicity, we consider in the following a vector $\underline{\alpha}$, whose components could be the N reference shear stresses τ_s^0 of (7), say $\underline{\alpha} = (\alpha_I)$ with I = 1 to N.

The principle of the linearization procedure leading from (1) to (2) can now be applied both to $\dot{\epsilon}$ and $\dot{\alpha}$:

$$\dot{\varepsilon}(t) = \mathbf{s} \cdot \dot{\sigma}(t) + \mathbf{g}(t_n) + \mathbf{m}_{(n)} \cdot [\sigma(t) - \sigma(t_n)] + \mathbf{n}_{(n)} \cdot [\underline{\alpha}(t) - \underline{\alpha}(t_n)] + \dots$$
$$\dots + \{\mathbf{g}(t) - \mathbf{g}(t_n) - \mathbf{m}_{(n)} \cdot [\sigma(t) - \sigma(t_n)] - \mathbf{n}_{(n)} \cdot [\underline{\alpha}(t) - \underline{\alpha}(t_n)] \} [1 - \mathbf{H}(t - t_n)]$$

$$\underline{\dot{\alpha}}(t) = \underline{h}(t_n) + p_{(n)}:[\sigma(t) - \sigma(t_n)] + q_{(n)}.[\underline{\alpha}(t) - \underline{\alpha}(t_n)] + \dots$$

$$\dots + \{\underline{h}(t) - \underline{h}(t_n) - p_{(n)}:[\sigma(t) - \sigma(t_n)] - q_{(n)}.[\underline{\alpha}(t) - \underline{\alpha}(t_n)]\}[1 - H(t - t_n)]$$
(9)

with:
$$\boldsymbol{m}_{(n)} = \frac{\partial \mathbf{g}}{\partial \sigma} [\sigma(t_n), \underline{\alpha}(t_n)], \quad \boldsymbol{n}_{(n)} = \frac{\partial \mathbf{g}}{\partial \underline{\alpha}} [\sigma(t_n), \underline{\alpha}(t_n)],$$

 $\boldsymbol{p}_{(n)} = \frac{\partial \underline{h}}{\partial \sigma} [\sigma(t_n), \underline{\alpha}(t_n)], \quad \boldsymbol{q}_{(n)} = \frac{\partial \underline{h}}{\partial \underline{\alpha}} [\sigma(t_n), \underline{\alpha}(t_n)].$

The Laplace-transforms of these equations are:

$$\varepsilon^*(p) = \mathbf{s}: \sigma^*(p) + \frac{1}{p} \mathbf{m}_{(n)}: \sigma^*(p) + \frac{1}{p} \mathbf{n}_{(n)} \cdot \underline{\alpha}^*(p) + \tilde{\varepsilon}_{(n)}^*(p)$$
$$\underline{\alpha}^*(p) = \frac{1}{p} \mathbf{p}_{(n)}: \sigma^*(p) + \frac{1}{p} \mathbf{q}_{(n)} \cdot \underline{\alpha}^*(p) + \underline{\tilde{\alpha}}_{(n)}^*(p)$$

with:
$$\tilde{\varepsilon}_{(n)}^{*}(p) = \frac{1}{p} [\mathbf{g}(\mathbf{t}_{n}) - \mathbf{m}_{(n)}: \sigma(\mathbf{t}_{n}) - \mathbf{n}_{(n)}.\underline{\alpha}(\mathbf{t}_{n})] + \dots$$

$$\dots + \int_{0}^{\mathbf{t}_{n}} \{\mathbf{g}(\mathbf{t}) - \mathbf{g}(\mathbf{t}_{n}) - \mathbf{m}_{(n)}: [\sigma(\mathbf{t}) - \sigma(\mathbf{t}_{n})] - \mathbf{n}_{(n)}.[\underline{\alpha}(\mathbf{t}) - \underline{\alpha}(\mathbf{t}_{n})]\} \exp(-p\mathbf{t}) d\mathbf{t}$$
(10)

$$\underline{\tilde{\alpha}}_{(n)} * (p) = \frac{1}{p} [\underline{h}(t_n) - p_{(n)}: \sigma(t_n) - q_{(n)}.\underline{\alpha}(t_n)] + \dots$$

$$\dots + \int_{0}^{t_n} {\{\underline{h}(t) - \underline{h}(t_n) - p_{(n)}: [\sigma(t) - \sigma(t_n)] - q_{(n)}.[\underline{\alpha}(t) - \underline{\alpha}(t_n)]\}} \exp(-pt) dt.$$

From (9) and (10), $\underline{\alpha}^{*}(\mathbf{p})$ can be eliminated through the relation:

$$\underline{\alpha}^{*}(p) = [\mathbf{I} - \frac{1}{p} \boldsymbol{q}_{(n)}]^{-1} \cdot [\frac{1}{p} \boldsymbol{p}_{(n)}: \boldsymbol{\sigma}^{*}(p) + \underline{\tilde{\alpha}}_{(n)}^{*}(p)], \qquad (11)$$

where I is the second order unit tensor in a NxN space. This leads to the final relation:

$$\varepsilon^{*}(p) = [\mathbf{s} + \frac{1}{p} \mathbf{m}_{(n)} + \frac{1}{p} \mathbf{n}_{(n)} \cdot (p\mathbf{I} - \mathbf{q}_{(n)})^{-1} \cdot \mathbf{p}_{(n)}]; \sigma^{*}(p) + \dots$$

$$\dots + \mathbf{n}_{(n)} \cdot (p\mathbf{I} - \mathbf{q}_{(n)})^{-1} \cdot \underline{\tilde{\alpha}}_{(n)}^{*}(p) + \tilde{\varepsilon}_{(n)}^{*}(p),$$
(12)

which could be written as well:

$$\varepsilon^{*}(p) = s^{*}(p):\sigma^{*}(p) + \varepsilon^{0}_{(n)} * (p)$$

with: $s^{*}(p) = s + \frac{1}{p} m_{(n)} + \frac{1}{p} n_{(n)} \cdot (p\mathbf{I} - q_{(n)})^{-1} \cdot p_{(n)}$ (13)
 $\varepsilon^{0}_{(n)} * (p) = n_{(n)} \cdot (p\mathbf{I} - q_{(n)})^{-1} \cdot \underline{\tilde{\alpha}}_{(n)} * (p) + \tilde{\varepsilon}_{(n)} * (p).$

This means that, through a new definition of $s^*(p)$ and $\varepsilon_{(n)}^0^*(p)$, the structure of the local constitutive equations is basically the same as the one considered before (section 2, eqns 4): the auxiliary strain function $\varepsilon_{(n)}^0(t)$ can still be considered as a true eigenstrain and the homogenization treatment is unchanged (eqns 4 to 6 are still valid). Note that the fully developed form of (12) reads as follows:

$$\epsilon_{ij} * (p) = (s_{ijkl} + \frac{1}{p} m_{(n)ijkl} + \frac{1}{p} n_{(n)ijl} \omega_{IJ} p_{(n)Jkl}) \sigma_{kl} * (p) + \dots$$

...+ $n_{(n)ijl} \omega_{IJ} \cdot \tilde{\alpha}_{(n)J} * (p) + \tilde{\epsilon}_{(n)ij} * (p)$ (14)
with: $\omega_{(n)} = (p\mathbf{I} - q_{(n)})^{-1}$,

where i, j, k, l = 1 to 3 and I, J = 1 to N.

4. An illustrative application

As an illustration of the tractability of the proposed treatment, we consider the problem of an isotropic multiphase material under radial loading. Each phase is incompressible and obeys the local isotropic constitutive equations:

$$\dot{\mathbf{e}} = \mathbf{a}\dot{\mathbf{s}} + \mathbf{b}(\frac{\sigma_{\text{equ}}}{\alpha})^{m-1}\mathbf{s}$$

$$\dot{\alpha} = \mathbf{h}(\frac{\sigma_{\text{equ}}}{\alpha})^{\mathbf{v}},$$
(15)

where σ_{equ} is the Von Mises equivalent stress, e and s are the strain and stress deviators and a, b, h, m and v are material constants which may differ from phase to phase. The number of phases is arbitrary. In this particular case, the problem reduces to a scalar one: we want to derive the macroscopic stress response S(t) from a known macroscopic strain path E(t) (or the reverse) through some macroscopic stress relaxation function $\mu^{SC}(t, t_n)$ and macroscopic eigenstrain $E_{(n)}^0(t, t_n)$ to be defined at each step t_n .

From (13), at time t_n , each phase (r) obeys linearized equations with the form:

$$\dot{e}_{r}(t) = a_{r}\dot{s} + b_{r}s + \dot{e}_{(n)r}^{0}$$

or:
$$e_{r} * (p) = \frac{s_{r} * (p)}{2\mu_{r} * (p)} + e_{(n)r}^{0} * (p)$$
(16)
with:
$$2\mu_{r} * (p) = \frac{p}{a_{r}(p+1/T_{r})}, \quad T_{r} = \frac{a_{r}}{b_{r}}.$$

Isotropy and incompressibility allow us to consider spherical inclusions for the selfconsistent procedure with the stress concentration function:

$$B_{r}^{*} = \frac{5\mu_{r}^{*}}{3\mu^{SC} * + 2\mu_{r}^{*}}.$$
 (17)

The overall stress relaxation function μ^{SC} at time t_n can be derived by an iterative scheme [11], previously proposed by Kröner [16] in the case of elasticity, through the recursive formula:

$$\mu_{(i+1)}^{SC} * = \left[\sum_{r} \frac{c_{r} \mu_{r} *}{3\mu_{(i)}^{SC} * + 2\mu_{r} *} \right] \left[\sum_{r} \frac{c_{r}}{3\mu_{(i)}^{SC} * + 2\mu_{r} *} \right]^{-1}$$
(18)



Figure 1: normalized stress evolution at constant strain rate "edot" (time unit arbitrary) (2 phases; $m_r = v_r = 2$; $a_r = \alpha_r(0) = 1$; $c_r = .5$, r = 1, 2; $b_1 = h_1 = 1$; $b_2 = h_2 = 5$).

with c, the phase volume fractions. Finally, the concentration equations which relate the local and the overall stresses and eigenstrains read:

$$s_{r}^{*} = \frac{5\mu_{r}^{*}}{3\mu^{SC} * + 2\mu_{r}^{*}} S^{*} + \frac{6\mu_{r}^{*} + \mu^{SC}^{*}}{3\mu^{SC} * + 2\mu_{r}^{*}} (E_{(n)}^{0} * - e_{(n)r}^{0} *)$$
with:
$$E_{(n)}^{0} * = \sum_{r} c_{r} B_{r}^{*} e_{(n)r}^{0} *.$$
(19)

Typical results are given on Figure 1 for a shear test with a prescribed constant shear strain rate \dot{E}_0 . The normalized stress response S/ \dot{E}_0 depends clearly on the strain rate amplitude, in agreement with the nonlinear local behaviour.

Similar computations applied to rate-dependent elastoplastic polycrystals are now in progress. Note that, according to the proposed treatment, no instantaneous plasticity is permitted.

Acknowledgements

Part of this work (section 2) was funded by EdF-SEPTEN for nuclear applications. We are grateful to Dr A. Pouya (LMS/G3S) for helpful discussions.

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