Incremental homogenization approach for ageing viscoelastic polycrystals

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ABSTRACT

An approximate self-consistent modelling is proposed to estimate the effective viscoelastic response of polycrystals presenting an ageing constitutive behaviour. This approach makes use of the equivalence between the Dirichlet series approximation of the viscoelastic functions and an internal variables formulation. An illustrative application is performed for model 2D polycrystals for which the exact expression of the continuous effective relaxation spectrum is given.

1. Introduction

In the context of effective mechanical properties of heterogeneous materials derived by scale transition, viscoelasticity has a special place and still represents a challenging problem. The specificity of this class of behaviours, as compared to elasticity, lies in the occurrence of "memory effects" due to the spatio-temporal interactions between the constituents [1]. This prevents from using directly standard homogenization techniques and the whole stress and strain histories must be taken into account to describe the response of the material at a given time [2]. For that goal, two routes have been explored: (i) the building of approximate solutions making use of a restricted set of internal variables which keep track of the stress (or strain) histories [3,4]; and (ii) the use of the correspondence principle [5] to solve the homogenization problem [6–9]. The latter approach, which relies on the Laplace–Carson (LC) transforms technique, allows to express the linear viscoelastic problem as a symbolic linear elastic problem in the LC space. Provided that the inversion of the symbolic effective properties can be performed accurately, it yields the exact solution (for a given homogenization scheme) of the viscoelastic homogenization problem. In more general situations, the LC inversion can be estimated by approximating the involved quantities by Dirichlet series. However, for ageing viscoelastic materials, the constitutive behaviour cannot be expressed anymore as a convolution product between a viscoelastic modulus (resp. compliance) and a strain (resp. stress) history. As a consequence, the classical correspondence principle does not apply directly [10]. In this framework, the aim of the present article is to propose an approximate treatment to describe the effective ageing behaviour of polycrystalline materials in a general context of anisotropy. For this purpose, we are making use of the recent work of Ricaud and Masson [11] which have shown that the classical formulation derived from the correspondence principle combined with the Dirichlet series approximation is equivalent to an internal variables formulation with a finite number of variables. This equivalence can be advantageously used to build an incremental self-consistent approach for the description of the viscoelastic response of ageing polycrystals. A similar formulation, making use of the localization relations, has been given in the context of hardening thermoviscoelastic polycrystals [12].

The outline of the article is as follows. To start with, the internal variables formulation of the self-consistent model for ageing viscoelasticity is presented. Then, this general framework is applied to a model 2D polycrystal deformed by antiplane shear. For this class of polycrystals, the exact expression of the effective relaxation modulus, which exhibits a continuous spectrum, is obtained and used to assess the approximation based on Dirichlet series.

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2. Effective behaviour of ageing viscoelastic polycrystals: an internal variables formulation

Let us consider a polycrystalline material with volume Ω containing grains with N different crystalline orientations (r). The set of all grains with the same orientation represents the constitutive phase (r) occupying the non-connex volume Ω_r described by the characteristic function $\chi_r(\mathbf{x})$ which is equal to 1 if $\mathbf{x} \in \Omega_r$ and 0 otherwise. The volumic fraction of phase (r) is thus $c_r = \langle \chi_r \rangle$. The phases are perfectly bonded and each phase obeys a non-ageing linear viscoelastic behaviour. In addition, the strain and stress fields throughout Ω are assumed to be zero for any time t lower than the initial loading time $t = 0$. For non-ageing material, the constitutive strain–stress relation is given by a Sieljes convolution product as follows:

$$\boldsymbol{\sigma}(\mathbf{x}, t) = \int_0^t \mathbf{L}(\mathbf{x}, t-u) : \dot{\boldsymbol{\varepsilon}}(\mathbf{x}, u)\,\mathrm{d}u, \quad \forall \mathbf{x} \in \Omega, \text{ with } \mathbf{L}(\mathbf{x}, t) = \sum_r \chi_r(\mathbf{x}) \mathbf{L}_r(t) \tag{1}$$

In this relation, possible discontinuities of the involved quantities, considered as generalized functions, have to be taken into account while $\mathbf{L}_r(t)$ denotes the relaxation function of phase (r). The overall behaviour of the considered material submitted to a known macroscopic history of strain $\bar{\boldsymbol{\varepsilon}}(t)$ reads

$$\bar{\boldsymbol{\sigma}}(t) = \int_0^t \tilde{\mathbf{L}}(t-u) : \dot{\bar{\boldsymbol{\varepsilon}}}(u)\,\mathrm{d}u \tag{2}$$

2.1. Self-consistent estimates

To derive the overall behaviour of viscoelastic heterogeneous materials, the correspondence theorem [5] is customarily used. The Laplace–Carson (LC) transform[1] helps transforming the non-ageing linear viscoelastic behaviour into a symbolic elastic one. The LC transform of the constitutive relation (1) reads

$$\hat{\boldsymbol{\sigma}}(\mathbf{x}, p) = \hat{\mathbf{L}}(\mathbf{x}, p) : \hat{\boldsymbol{\varepsilon}}(\mathbf{x}, p), \quad \forall \mathbf{x} \in \Omega, \text{ with } \hat{\mathbf{L}}(\mathbf{x}, p) = \sum_r \chi_r(\mathbf{x}) \hat{\mathbf{L}}_r(p) \tag{3}$$

for which the classical homogenization techniques apply. In the sequel, the self-consistent (SC) scheme is considered since it is known to deliver accurate results for the effective behaviour and the statistics of local fields within elastic polycrystals, see for instance [13,14]. The SC estimate of the effective compliance $\hat{\tilde{\mathbf{M}}}_{SC}(p) = \hat{\tilde{\mathbf{L}}}_{SC}^{-1}(p)$ is given by [7]

$$\begin{cases} \hat{\tilde{\mathbf{M}}}_{SC}(p) = \sum_s c_s \hat{\mathbf{M}}^{(s)}(p) : \hat{\mathbf{B}}_{SC}^{(s)}(p) \\[2mm] \hat{\mathbf{B}}_{SC}^{(r)}(p) = \left(\hat{\mathbf{M}}^{(r)}(p) + \left[\hat{\mathbf{Q}}_{SC}(p)\right]^{-1}\right)^{-1} : \left(\hat{\tilde{\mathbf{M}}}_{SC}(p) + \left[\hat{\mathbf{Q}}_{SC}(p)\right]^{-1}\right) \\[2mm] \sum_s c_s \hat{\mathbf{B}}_{SC}^{(s)}(p) = \mathbf{I} \end{cases} \tag{4}$$

where $\mathbf{I}$ denotes the fourth-order unit tensor, $\hat{\mathbf{Q}}_{SC}(p)$ is the Hill constraint tensor and $\hat{\mathbf{B}}_{SC}^{(r)}$ is the average stress concentration tensor over phase (r). The Hill constraint tensor depends on the effective symbolic elastic moduli $\hat{\tilde{\mathbf{L}}}_{SC}(p)$ as well as the Eshelby tensor $\hat{\mathbf{S}}(p)$ through

$$\hat{\mathbf{Q}}_{SC}(p) = \hat{\tilde{\mathbf{L}}}_{SC}(p) : \left[\hat{\mathbf{S}}^{-1}(p) - \mathbf{I}\right] \tag{5}$$

Finally, at a given time t, the phase-averaged stresses $\boldsymbol{\sigma}^{(r)}(t)$ are solutions of the following system of linear integral equations:

$$\begin{cases} \boldsymbol{\sigma}^{(r)}(t) - \bar{\boldsymbol{\sigma}}(t) = -\int_0^t \mathbf{Q}_{SC}(t-u) : \left(\dot{\boldsymbol{\varepsilon}}^{(r)}(u) - \dot{\bar{\boldsymbol{\varepsilon}}}(u)\right)\,\mathrm{d}u \\[3mm] \boldsymbol{\sigma}^{(r)}(t) = \int_0^t \mathbf{L}_r(t-u) : \dot{\boldsymbol{\varepsilon}}^{(r)}(u)\,\mathrm{d}u \\[3mm] \bar{\boldsymbol{\varepsilon}}(t) = \sum_s c_s \boldsymbol{\varepsilon}^{(s)}(t) \quad \text{and} \quad \bar{\boldsymbol{\sigma}}(t) = \sum_s c_s \boldsymbol{\sigma}^{(s)}(t) \end{cases} \tag{6}$$

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[1] The Laplace–Carson transform of a function $f(t)$ reads $\hat{f}(p) = p \int_0^{+\infty} f(t) e^{-pt}\,\mathrm{d}t$.

2.2. Internal variables formulation

To solve the system (6), it is required to determine the time function $\mathbf{Q}_{SC}(t)$ by inversion of its LC transform defined by relation (5). Apart from some particular cases for which this inversion can be performed *exactly* (see [15,16] and Section 3 of the present paper) and the specific case of the "quasi-elastic" *approximation* [7,17,18], the inversion of the involved LC transforms is generally performed numerically thanks to the collocation method [19]. This method consists in approximating Hill's constraint tensor by the Dirichlet series expansion

$$\mathbf{Q}_{SC}(t) \approx \mathbf{Q}_{SC}^*(t) = \sum_{i=1}^{N_p} \mathbf{Q}_{SC(\tau_i)} e^{-\frac{t}{\tau_i}} \tag{7}$$

with the following constraint $\sum_{i=1}^{N_p} \mathbf{Q}_{SC(\tau_i)} = \mathbf{Q}_{SC}^e$ ($\mathbf{Q}_{SC}^e$ denotes the Hill constraint tensor corresponding to the purely elastic problem, that is $\hat{\mathbf{Q}}_{SC}(+\infty)$). It is worth noting that other asymptotic relations exist [20]. As remarked by Ricaud and Masson [11], this approximation is equivalent to an internal variables formulation. Indeed, the introduction of the approximation (7) in the integral relation (6) yields

$$\begin{cases} \boldsymbol{\sigma}^{(r)}(t) - \overline{\boldsymbol{\sigma}}(t) = -\mathbf{Q}_{SC}^e : \left(\boldsymbol{\varepsilon}^{(r)}(t) - \overline{\boldsymbol{\varepsilon}}(t) - \sum_{i=1}^{N_p} \boldsymbol{q}_{\tau_i}^{(r)}(t) \right) \\[2ex] \dot{\boldsymbol{q}}_{\tau_i}^{(r)}(t) + \frac{1}{\tau_i} \boldsymbol{q}_{\tau_i}^{(r)}(t) = \frac{1}{\tau_i} \left[\mathbf{Q}_{SC}^e \right]^{-1} : \mathbf{Q}_{SC(\tau_i)} : \left(\boldsymbol{\varepsilon}^{(r)}(t) - \overline{\boldsymbol{\varepsilon}}(t) \right) \quad \text{with } \boldsymbol{q}_{\tau_i}^{(r)}(0) = 0 \end{cases} \tag{8}$$

where $\boldsymbol{q}_{\tau_i}^{(r)}(t)$ is a second-order tensorial internal variable relative to phase (r) and collocation time τ_i. Hence, a set of $N * N_p$ internal variables is defined. This rewriting of the viscoelastic homogenization problem making use of Dirichlet series approximation does not provide a new framework for non-ageing behaviours. However, we can take advantage of this equivalence between the hereditary approach and an internal variables formulation to build an approximate incremental model for ageing viscoelastic materials.

2.3. Extension to ageing behaviours

It is now assumed that the constitutive phases of the polycrystal display an ageing viscoelastic behaviour

$$\boldsymbol{\sigma}(\mathbf{x}, t) = \int_0^t \mathbf{L}(\mathbf{x}, t, u) : \dot{\boldsymbol{\varepsilon}}(\mathbf{x}, u) \, \mathrm{d}u, \quad \forall \mathbf{x} \in \Omega, \text{ with } \mathbf{L}(\mathbf{x}, t, u) = \sum_r \chi_r(\mathbf{x}) \mathbf{L}_r(t, u) \tag{9}$$

where $L_{(ijkl)r}(t, u)$ denotes the (ij) component of the stress state at time t caused by a unit strain with component (kl) applied at time u. As a result, the effective behaviour reads [10]

$$\overline{\boldsymbol{\sigma}}(t) = \int_0^t \tilde{\mathbf{L}}(t, u) : \dot{\overline{\boldsymbol{\varepsilon}}}(u) \, \mathrm{d}u \tag{10}$$

It is pointed out that the effective relaxation function depends separately on times t and u by contrast with a non-ageing behaviour for which it depends only on the time difference $(t - u)$. As a result, the correspondence theorem does not apply to this situation. To circumvent this difficulty, it is proposed to apply incrementally the internal variables formulation derived in the previous section by imposing the continuity of the internal variables.

We consider a strain loading path on the time interval $[0; t - \delta t]$, with δt a small time increment, and we aim at deriving the overall stress response at time t. On the time interval $[t - \delta t; t]$, we define a non-ageing viscoelastic material constituted with phases whose relaxation functions read

$$\mathbf{L}_r(u) = \mathbf{L}_r(t + (\xi - 1)\delta t, u), \quad \forall r \in [1; N]$$

with ξ a numerical parameter ranging from 0 to 1. By denoting $\mathbf{Q}_{SC}(t, u)$ the Hill constraint tensor corresponding to the SC estimate of this non-ageing viscoelastic problem, defined on the time interval $[t - \delta t, t]$, the following Dirichlet series approximation can still be adopted:

$$\mathbf{Q}_{SC}(t, u) \approx \sum_{i=1}^{N_p} \mathbf{Q}_{SC(\tau_i)}(t) e^{-\frac{u}{\tau_i}} \tag{11}$$

with the following constraint $\sum_{i=1}^{N_p} \mathbf{Q}_{SC(\tau_i)}(t) = \mathbf{Q}_{SC}(t, 0)$. $\mathbf{Q}_{SC}(t, 0)$ denotes the Hill constraint tensor corresponding to the purely elastic problem. If the elastic properties are ageing, this fourth-order tensor may be different from $\mathbf{Q}_{SC}^e = \mathbf{Q}_{SC}(t = 0,$

$u = 0$) and is denoted hereafter by $\mathbf{Q}^e_{SC}(t)$. It is also remarked that the number (N_p) and the values of the collocation times $(\tau_1, \ldots, \tau_{N_p})$ do not depend on time t, by opposition to the fourth-order tensors $(\mathbf{Q}_{SC(\tau_1)}(t), \ldots, \mathbf{Q}_{SC(\tau_{N_p})}(t))$. This approximation is physically meaningful if the number and the range of the collocation times are chosen large enough to cover the whole range of time variations of the constraint tensor (see Section 3.4). As a result, the unknown phase-averaged stresses at time t ($\boldsymbol{\sigma}^{(r)}(t)$) are solutions of the following system of differential equations

$$
\begin{cases}
\boldsymbol{\sigma}^{(r)}(t) - \overline{\boldsymbol{\sigma}}(t) = -\mathbf{Q}^e_{SC}(t) : \left(\boldsymbol{\varepsilon}^{(r)}(t) - \overline{\boldsymbol{\varepsilon}}(t) - \sum_{i=1}^{N_p} \boldsymbol{q}^{(r)}_{\tau_i}(t) \right) \\[4mm]
\dot{\boldsymbol{q}}^{(r)}_{\tau_i}(t) + \dfrac{1}{\tau_i} \boldsymbol{q}^{(r)}_{\tau_i}(t) = \dfrac{1}{\tau_i} \left[\mathbf{Q}^e_{SC}(t) \right]^{-1} : \mathbf{Q}_{SC(\tau_i)}(t) : \left[\boldsymbol{\varepsilon}^{(r)}(t) - \overline{\boldsymbol{\varepsilon}}(t) \right] \\[4mm]
\boldsymbol{\sigma}^{(r)}(t) = \displaystyle\int_0^t \mathbf{L}_r(t, u) \dot{\boldsymbol{\varepsilon}}^{(r)}(u) \, \mathrm{d}u \\[4mm]
\overline{\boldsymbol{\varepsilon}}(t) = \displaystyle\sum_s c_s \boldsymbol{\varepsilon}^{(s)}(t) \quad \text{and} \quad \overline{\boldsymbol{\sigma}}(t) = \sum_s c_s \boldsymbol{\sigma}^{(s)}(t)
\end{cases}
\tag{12}
$$

with the initial conditions $\boldsymbol{q}^{(r)}_{\tau_i}(0) = 0$. Here, we assume continuity of the phase-average stresses $\boldsymbol{\sigma}^{(r)}$ (for a continuous overall loading) and internal variables $\boldsymbol{q}^{(r)}_{\tau_i}$ to solve for (12), when stepping from one time interval to the next time step. The internal variables being solutions of first-order differential equations, their time evolutions on the time interval $[t - \delta t; t]$ are entirely determined by these continuity conditions. It is worth emphasizing that these continuity conditions remain a simplification closely related to the fact that the collocations times do not depend on the considered time interval. However, this approximation remains consistent with the non-ageing situation, the system (12) with the initial and continuity conditions defined above being equivalent to the system (8) when the coefficients of the Dirichlet series expansion (11) do not depend on time.

3. Application to columnar 2D viscoelastic polycrystals

A 2D viscoelastic polycrystal, consisting of columnar orthorhombic grains with symmetry axes aligned with the $\mathbf{e}_{III}$ macroscopic direction, is considered. Each grain presents two slip systems (a) and (b) with common slip direction $\mathbf{e}_3$ and orthogonal slip planes of normal $\mathbf{e}_1$ and $\mathbf{e}_2$ in the crystalline reference frame. The corresponding Schmid tensors are

$$
\mathbf{R}^{(a)} = \frac{1}{2}(\mathbf{e}_1 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1) \quad \text{and} \quad \mathbf{R}^{(b)} = \frac{1}{2}(\mathbf{e}_2 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_2)
\tag{13}
$$

Such a polycrystal can only deform by antiplane shear. By assuming that the behaviour is Maxwellian on each slip system, the constitutive behaviour of the crystals is Maxwellian anisotropic. The LC transform of the viscoelastic compliance of phase (r) reads

$$
\hat{\mathbf{M}}^{(r)}(p) = \sum_k \frac{1}{\hat{\mu}^{(k)}(p)} \mathbf{R}^{(k)} \otimes \mathbf{R}^{(k)}, \quad k = a, b
\tag{14}
$$

with $\hat{\mu}^{(k)}$ the symbolic relaxation modulus of each slip system

$$
\hat{\mu}^{(k)}(p) = \mu_e^{(k)} \frac{p}{p + \frac{1}{\tau^k}}, \quad k = a, b
\tag{15}
$$

where $\mu_e^{(k)}$ and τ^k are respectively the elastic shear modulus and the characteristic relaxation time of slip system (k) ($\tau^k = \mu_v^{(k)}/\mu_e^{(k)}$). For the sake of simplicity, we consider the case of a polycrystal with a checkerboard microstructure[2] (Fig. 1) whose crystalline orientations are defined by the angle β between the crystal frame ($\mathbf{e}_1$, $\mathbf{e}_2$) and the reference frame ($\mathbf{e}_I$, $\mathbf{e}_{II}$): $\beta = 0°$ for phase (1) and $\beta = 90°$ for phase (2). Consequently, the overall response of the polycrystal is isotropic. The symbolic relaxation tensors of the two crystalline phases read, in the reference frame ($\mathbf{e}_I$, $\mathbf{e}_{II}$),

$$
\hat{\mathbf{L}}^{(1)}(p) = 2 \begin{pmatrix} \hat{\mu}^{(a)}(p) & 0 \\ 0 & \hat{\mu}^{(b)}(p) \end{pmatrix}, \qquad \hat{\mathbf{L}}^{(2)}(p) = 2 \begin{pmatrix} \hat{\mu}^{(b)}(p) & 0 \\ 0 & \hat{\mu}^{(a)}(p) \end{pmatrix}
\tag{16}
$$

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[2] It is stressed out that the results on the effective response derived hereafter do apply to any isotropic 2D polycrystalline microstructure.
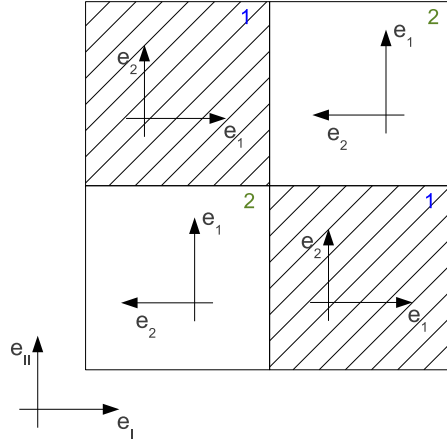
Fig. 1. Definition of the unit-cell of the checkerboard.

3.1. Effective behaviour

As noted by Ponte Castañeda and Nebozhyn [21], the SC estimate for the (symbolic) relaxation modulus $\hat{\tilde{\mu}}_{SC}(p)$ of the 2D polycrystal can be computed exactly when the compliances $\hat{\mathbf{M}}^{(r)}(p)$ are identical, except for a rotation. In this case, the SC estimate of the LC transform of the effective relaxation modulus reads

$$\hat{\tilde{\mu}}_{SC}(p) = \sqrt{\hat{\mu}^{(a)}(p)\hat{\mu}^{(b)}(p)} = \tilde{\mu}_e \frac{p}{\sqrt{(p + \frac{1}{\tau^a})(p + \frac{1}{\tau^b})}} \quad \text{with } \tilde{\mu}_e = \sqrt{\mu_e^{(a)}\mu_e^{(b)}} \tag{17}$$

which agrees with the analytical result of Dykhne [22] for the analogous conductivity problem. For this specific class of polycrystals, the SC scheme is thus exact and the overall relaxation function $\tilde{\mu}_{SC}(t)$ is straightforwardly obtained (see [23]). It reads, for $\tau^a < \tau^b$,

$$\tilde{\mu}_{SC}(t) = \tilde{\mu}^e e^{-\frac{t}{2\tau^a}} e^{-\frac{t}{2\tau^b}} J_0\left(\frac{\frac{1}{\tau^a} - \frac{1}{\tau^b}}{2} t\iota\right) \tag{18}$$

with J_0 the Bessel function of the first kind and $\iota^2 = -1$. Alternatively, starting from Sommersfeld's integral representation of $J_0(x)$, which can be expressed as [24]

$$J_0(x) = \frac{1}{2\pi} \int\limits_{-\pi}^{\pi} e^{-\iota x \sin(\tau)} \, d\tau$$

the relaxation function takes the form

$$\tilde{\mu}_{SC}(t) = \int\limits_{\tau^a}^{\tau^b} g(\tau) e^{-\frac{t}{\tau}} \, d\tau \tag{19}$$

where $g(\tau)$ denotes the relaxation spectrum[3]

$$g(\tau) = \frac{1}{\pi} \tilde{\mu}^e \frac{2\tau^a \tau^b}{(\tau^b - \tau^a)\tau^2} \frac{1}{\sqrt{1 - \left(\frac{\frac{2}{\tau} - \frac{1}{\tau^a} - \frac{1}{\tau^b}}{\frac{1}{\tau^a} - \frac{1}{\tau^b}}\right)^2}} \tag{20}$$

As former results derived with the SC scheme for a two-phase isotropic material [15], it is worth emphasizing that a continuous bounded spectrum $g(\tau)$ is obtained for this specific class of 2D polycrystals. This property is expected to hold for more general polycrystalline materials.

It is also remarked that the effective relaxation function is solution of a differential equation since $J_0(x)$ is, by definition, solution of the following differential equation

$$x^2 y''(x) + x y'(x) - x^2 y(x) = 0$$

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[3] The integrand $g(\tau)$ becomes unbounded when τ tends to τ^a or τ^b. However, the improper integral (19) is convergent.

Hence, it turns out to be solution of a second-order differential equation with nonconstant coefficients, namely[4]

$$t\ddot{\tilde{\mu}}(t) + \dot{\tilde{\mu}}(t)\left(\frac{t(\tau^a + \tau^b)}{\tau^a\tau^b} + 1\right) + \tilde{\mu}(t)\left(\frac{(\tau^a + \tau^b)}{2\tau^a\tau^b}\left[1 + \frac{(\tau^a + \tau^b)t}{2\tau^a\tau^b}\right] - t\left[\frac{1}{2}\frac{\tau^a - \tau^b}{\tau^a\tau^b}\right]^2\right) = 0 \tag{21}$$

3.2. Effective behaviour: exact versus approximate results

By noting that for the 2D incompressible isotropic case, the Hill constraint tensor is equal to the properties tensor of the reference medium (which coincides with the effective medium for the SC model), that is $\tilde{\mathbf{Q}}_{SC}(t) = \tilde{\mathbf{L}}_{SC}(t)$, the LC transform of the constraint tensor reads

$$\hat{\mathbf{Q}}_{SC}(p) = 2\hat{\tilde{\mu}}_{SC}(p)\mathbf{K}$$

with $\mathbf{K}$ the isotropic deviatoric projection tensor. Consequently, the interaction equation (6) reduces to

$$\mathbf{s}^{(r)}(t) - \bar{\mathbf{s}}(t) = -2\int_0^t \tilde{\mu}_{SC}(t-u) : \left(\dot{\mathbf{e}}^{(r)}(u) - \dot{\bar{\mathbf{e}}}(u)\right) \mathrm{d}u \tag{22}$$

where $\mathbf{e}, \mathbf{s}$ denote the deviatoric parts of the strain and the stress fields, respectively. It is remarked that this relation is equivalent to

$$\mathbf{s}^{(r)}(t) - \bar{\mathbf{s}}(t) = -2\tilde{\mu}^e\left(\mathbf{e}^{(r)}(t) - \bar{\mathbf{e}}(t) - \int_{\tau^a}^{\tau^b} \boldsymbol{\alpha}_\tau^d(t)\,\mathrm{d}\tau\right) \tag{23}$$

where the internal variables associated to the continuous distribution of relaxation times $\tau \in [\tau^a; \tau^b]$ satisfy

$$\dot{\boldsymbol{\alpha}}_\tau^d(t) + \frac{1}{\tau}\boldsymbol{\alpha}_\tau^d(t) = \frac{1}{\tau}\frac{g(\tau)}{2\tilde{\mu}^e}\left(\mathbf{e}^{(r)}(t) - \bar{\mathbf{e}}(t)\right) \quad \text{with } \boldsymbol{\alpha}(0) = 0 \tag{24}$$

Relations (23) and (24), together with the expression (20) of the continuous relaxation spectrum $g(\tau)$, provide an exact description of the response of the model 2D polycrystal. It can be pointed out that the approximation (7) leads to a similar form. However, it presents the distinctive feature of a Dirac distribution of internal variables since the relaxation spectrum is approximated by $g(\tau) \approx g^*(\tau) = \sum_{i=1}^{N_p} g_{\tau_i}\delta(\tau - \tau_i)$, the constants τ_i and g_{τ_i} being related to the Dirichlet series expansion of the effective shear modulus, that is

$$\tilde{\mu}_{SC}(t) \approx \tilde{\mu}_{SC}^*(t) = \sum_{i=1}^{N_p} g_{\tau_i} e^{-\frac{t}{\tau_i}} \quad \text{with the constraint } \sum_{i=1}^{N_p} g_{\tau_i} = \tilde{\mu}^e$$

Fig. 2 shows the good agreement of the approximate model with the exact solution for the overall shear behaviour of a polycrystal subjected to a disrupted relaxation loading (see the overall strain loading on Fig. 3). The polycrystal exhibits a homogeneous elasticity and the contrast on the relaxation times is $\tau^b/\tau^a = 6$ ($\tau^a = 1s$). For the approximate estimate, five collocation points have been used between τ^a and τ^b.

3.3. Phase-averaged influence tensors

In a strictly equivalent manner to relations (23) and (24), the phase-averaged deviatoric stress and strain fields can be obtained by using the influence tensors which relate them to the macroscopic fields through the localization relations. The mechanical fields averaged over phase (r) can be expressed as

$$\mathbf{e}^{(r)}(t) = \int_0^t \mathbf{A}^{(r)}(t-u) : \dot{\bar{\mathbf{e}}}(u)\,\mathrm{d}u \quad \text{and} \quad \mathbf{s}^{(r)}(t) = \int_0^t \mathbf{B}^{(r)}(t-u) : \dot{\bar{\mathbf{s}}}(u)\,\mathrm{d}u \tag{25}$$

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[4] Two initial conditions have to be given to solve this (nonlinear) second-order differential equation. For a relaxation test starting at $t = 0$, the first condition is $\tilde{\mu}(0) = \tilde{\mu}^e$. Given that

$$\mathrm{LC}[\dot{\tilde{\mu}}](p) = p\left[\hat{\tilde{\mu}}(p) - \mu^e\right] \quad \text{and} \quad \lim_{p\to\infty} \mathrm{LC}[\dot{\tilde{\mu}}] = \lim_{t\to 0} \dot{\tilde{\mu}}(t)$$

the second initial condition is given by $\dot{\tilde{\mu}}(0) = -\frac{1}{2}\tilde{\mu}^e\frac{\tau^a+\tau^b}{\tau^a\tau^b}$.
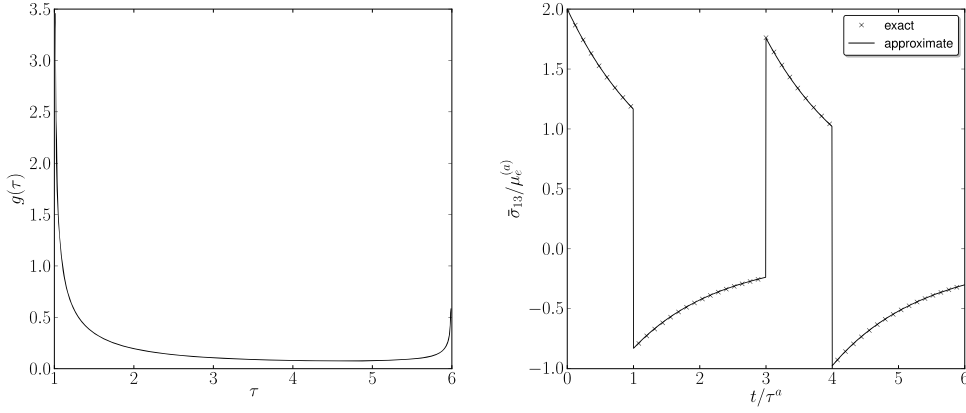
Fig. 2. Exact continuous relaxation spectrum of the 2D polycrystal (relation (20)) (left) and comparison of the overall shear stress evolution during a disrupted relaxation loading as predicted by the approximate model versus the exact solution (right).
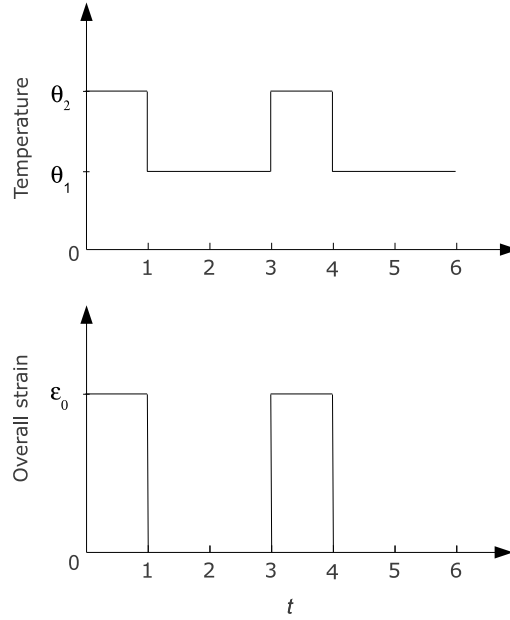
Fig. 3. Definition of the thermomechanical loading for the disrupted relaxation test.

with $\mathbf{A}^{(r)}(t)$ and $\mathbf{B}^{(r)}(t)$ the phase-averaged influence tensors. In the general case, their LC transforms are related to the Hill constraint tensor by relation (4). However, for the specific case of a two-phase polycrystal, the LC transform of the strain localization tensors, for instance, is simply given by

$$\hat{\mathbf{A}}^{(r)} = \frac{1}{c_r}\left(\hat{\mathbf{L}}^{(r)} - \hat{\mathbf{L}}^{(s)}\right)^{-1} : \left(\hat{\bar{\mathbf{L}}} - \hat{\mathbf{L}}^{(s)}\right), \quad (r, s) = (1, 2) \tag{26}$$

Moreover, for the considered polycrystal whose phases present a misorientation of 90° (Fig. 1), the influence tensors obey $\hat{\mathbf{A}}^{(r)} = \hat{\mathbf{B}}^{(s)}$ with $(r, s) = (1, 2)$ which is due to the fact that a 2D divergence-free field has the property of transforming into a curl-free field when rotated by 90° [22]. The LC transforms of the average strain localization tensors read, in the reference frame,

$$\hat{\mathbf{A}}^{(1)}(p) = 2\begin{pmatrix} 1 - \hat{\eta}(p) & 0 \\ 0 & \hat{\eta}(p) \end{pmatrix}, \qquad \hat{\mathbf{A}}^{(2)}(p) = 2\begin{pmatrix} \hat{\eta}(p) & 0 \\ 0 & 1 - \hat{\eta}(p) \end{pmatrix} \quad \text{with } \hat{\eta}(p) = \frac{1}{1 + \sqrt{\frac{\hat{\mu}^{(b)}(p)}{\hat{\mu}^{(a)}(p)}}} \tag{27}$$

The exact influence tensors of the viscoelastic homogenization problem can thus be obtained with the inverse LC transform of $\hat{\eta}(p)$. By noting that its Laplace transform $\eta^{\star} = \hat{\eta}/p$ can be written as

$$\eta^*(p) = \frac{\tau^a \tau^b}{\tau^a - \tau^b}\left[1 + \frac{1}{p\tau^b} - \frac{1}{p}\sqrt{\left(p + \frac{1}{\tau^a}\right)\left(p + \frac{1}{\tau^b}\right)} \right]$$

we eventually obtain

$$\eta(t) = \frac{\tau^a \tau^b}{\tau^a - \tau^b}\left[\frac{1}{\tau^b} - \sqrt{\frac{1}{\tau^a \tau^b}} - \frac{1}{\pi}\int_{\tau^a}^{\tau^b} \sqrt{\left(\frac{1}{\tau^a} - \frac{1}{\tau}\right)\left(\frac{1}{\tau} - \frac{1}{\tau^b}\right)}\frac{1}{\tau}e^{-\frac{t}{\tau}}\mathrm{d}\tau \right]$$

3.4. Ageing viscoelastic behaviour

The incremental homogenization approach proposed in Section 2 is now applied to describe the ageing viscoelastic response of the 2D polycrystal. For illustrative purpose, it is assumed that the viscous shear moduli $\mu_v^{(k)}$ depend on the temperature $\theta(t)$. This can be for example related to the temperature dependence of the critical shear stress necessary to activate dislocation glide on crystallographic planes. By approximating the effective shear moduli by a Dirichlet series expansion, the effective constitutive relation can be expressed as

$$\begin{cases} \dot{\bar{\boldsymbol{s}}}(t) = 2\left(\tilde{\mu}^e : \dot{\bar{\boldsymbol{e}}}(t) - \sum_i \tilde{\mu}_{SC(\tau_i)}(t)\dot{\boldsymbol{\alpha}}_{\tau_i}(t) \right) \\ \tau_i \dot{\boldsymbol{\alpha}}_{\tau_i}(t) + \boldsymbol{\alpha}_{\tau_i}(t) = \bar{\boldsymbol{e}}(t), \qquad \boldsymbol{\alpha}_{\tau_i}(0) = 0, \quad \forall i \in [1; N_p] \end{cases} \tag{28}$$

which is an alternative writing of the overall behaviour defined by system (12) for non-ageing elasticity. It is emphasized that $\tilde{\mu}_{SC(\tau_i)}(t)$ represent the collocation coefficients for the *non-ageing* shear viscoelastic effective behaviour defined at each time step $[t - \delta t; t]$. The overall stress increment $\Delta\bar{\boldsymbol{s}}(t)$ reads

$$\Delta\bar{\boldsymbol{s}}(t) = 2\left(\tilde{\mu}^e : \Delta\bar{\boldsymbol{e}}(t) - \sum_i \tilde{\mu}_{SC(\tau_i)}(t)\Delta\boldsymbol{\alpha}_{\tau_i}(t) \right) \tag{29}$$

where $\Delta\bar{\boldsymbol{e}}(t)$ includes possible strain discontinuities in the loading path. It is recalled that internal variables $\boldsymbol{\alpha}_{\tau_i}$ are supposed to be continuous between successive time steps.

We consider the relaxation response of the polycrystal subjected to simultaneous jumps of temperature and overall strain (see the overall disrupted thermomechanical loading on Fig. 3). The polycrystal is elastically homogeneous and the viscous shear moduli of each slip system vary with the temperature. For the present application, the relaxation times at temperature θ_2 are $\tau^a = 1$ s and $\tau^b = 6$ s while at temperature θ_1 we assume that $\tau^a = 2$ s and $\tau^b = 10^2$ s. Consequently, both slip systems "harden" when the temperature decreases and the viscous glide on slip system (*b*) is almost prevented when the polycrystal is at temperature θ_1. To estimate the effective response of this ageing polycrystal, five collocation points have been chosen between 1 s and 10^2 s to span the whole range of variations of the relaxation times during the considered thermomechanical loading. The accuracy of this approximation was evaluated by comparing the shear relaxation functions at both temperatures θ_1 and θ_2 as predicted by this approximation and the exact results (18). It yields an excellent agreement. On Fig. 4, the effective stress response for the ageing situation is compared to the non-ageing behaviour corresponding to temperature θ_2. As expected, the temperature ageing implies a reduced relaxation rate. However, it can be noted that this relaxation is non-vanishing since viscous glide can still occur on slip system (*a*).[5]

4. Concluding remarks

The equivalence between the collocation-like methods and an internal variables approach has been advantageously used to build an incremental self-consistent modelling of the ageing viscoelastic behaviour of polycrystals. This incremental formulation, which assumes continuity of the internal variables, has been applied to a model 2D polycrystal with a checkerboard microstructure. Interestingly, it has also been shown that the exact relaxation spectrum of such polycrystals is continuous and the analytical expression of the phase-averaged localization (concentration) tensors has been obtained. For further prospects, it is our contention that the proposed approach offers an attractive framework to tackle nonlinear viscoelastic behaviours.

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[5] In the limit $\tau^k \to +\infty$, $\forall k$, the polycrystal would become elastic and the stress would remain constant.
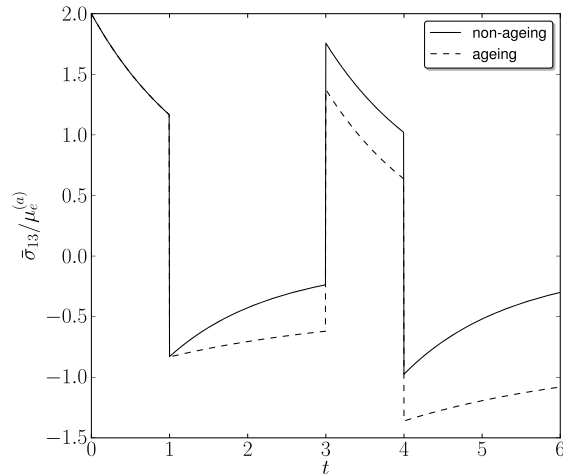
Fig. 4. Overall shear stress evolution during a disrupted relaxation test for non-ageing and ageing constitutive behaviours.

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