An "Affine" Micromechanical Approach for the Prediction of the Elastoplastic Behavior of Polycrystals at Finite Strain

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Abstract: The so-called "affine" formulation, already proposed at small strain, has been proved to improve significantly on former treatments such as Hill's incremental one. This paper reports on an extension of this treatment at finite strain. A linearization procedure, consistent with the one used for small strains, is proposed. This extension has to solve general problems related to the application of classical homogenization schemes to finite strain situations, as well as new ones which are specific to the affine formulation. Preliminary results concerning the tensile stress-strain response of FCC polycrystals are favorably compared with those derived from Hill's approach.

Keywords: Polycrystals, elastoplasticity, finite strain, homogenization.

1. Introduction

Until a very recent past, Hill's incremental method was unanimously considered the most appropriate micromechanical treatment to predict the elastoplastic behavior of polycrystals. Recently, Gilormini [2] proved that this approach, applied to viscoplastic two-phase materials, can lead to an upper bound violation. This shows that the incremental treatment must be somewhat "softened" in order to yield more realistic predictions. This conclusion has motivated the conception of a new approach, the so-called "affine formulation", proposed by Masson et al. [9]. Initially defined, in the context of infinitesimal strain, for nonlinear elasticity or viscosity, it has been extended to history-dependent constitutive behavior such as rate-independent or rate-dependent elastoplasticity.

This paper aims at extending the affine elastoplastic approach to finite strain. In the first section, we briefly recall the small strain affine formulation for nonlinear elasticity and elastoplasticity. The second section is devoted to the finite strain extension: we first focus on the choice of the appropriate (lagrangian, eulerian...) description framework; we then address the question of the single crystal constitutive equations and the specific problems of the affine approach when finite deformations are considered and when the self-consistent scheme is adopted. Preliminary predictions of the overall response of polycrystals, compared with those derived from Hill's approach, are reported in the last section. Here, a polycrystal is considered as an aggregate of perfectly bound and randomly distributed crystals which only differ by their lattice orientation: all the grains which have the same crystallographic orientation define a "phase" of this multiphase material. Plastic deformation is only due to glide on slip systems, the system α being defined by the unit normal to its slip plane $\boldsymbol{n}_\alpha$ and its unit slip direction $\boldsymbol{m}_\alpha$.

2. Affine formulation for small strains

2.1. NONLINEAR ELASTICITY OR VISCOPLASTICITY

In this section, the crystal constitutive behavior is derived from a convex stress energy function $u(\boldsymbol{\sigma})$ (a similar approach could be developed from a strain energy function). The strain response at any point $\boldsymbol{x}$ in the considered representative volume element V is independent of the loading path:

$$\boldsymbol{\varepsilon}(\boldsymbol{x}) = \frac{\partial u}{\partial \sigma}(\boldsymbol{x}, \boldsymbol{\sigma}(\boldsymbol{x})). \tag{1}$$

According to the affine approach and using the local tangent compliance $\boldsymbol{M}(\boldsymbol{x})$, the nonlinear constitutive equations (1) are linearized with respect to the current stress value at each point $\boldsymbol{x}$. The linearization takes place once and for all without any incremental process:

$$\begin{aligned} \boldsymbol{\varepsilon}(\boldsymbol{x}) &= \boldsymbol{M}(\boldsymbol{x}) : \boldsymbol{\sigma}(\boldsymbol{x}) + \boldsymbol{\eta}(\boldsymbol{x})\,, \\ \boldsymbol{M}(\boldsymbol{x}) &= \frac{\partial^2 u}{\partial \boldsymbol{\sigma}^2}(\boldsymbol{\sigma}(\boldsymbol{x}), \boldsymbol{x})\,, \\ \boldsymbol{\eta}(x) &= \frac{\partial^2 u}{\partial \boldsymbol{\sigma}^2}(\boldsymbol{\sigma}(\boldsymbol{x}), \boldsymbol{x}) - \boldsymbol{M}(\boldsymbol{x}) : \boldsymbol{\sigma}(\boldsymbol{x})\,. \end{aligned} \tag{2}$$

These linearized equations may be considered as associated to a linear thermoelastic composite constituted of an infinite number of phases (the notation $\boldsymbol{C} : \boldsymbol{D}$ means: $\boldsymbol{C}_{ijkl}\boldsymbol{D}_{kl}$, where summation is done over repeated indices). To deal with such a composite, one has, as usual, to adopt the simplification of piecewise constant compliances and prestrains per phase. Accordingly, for each phase,

we assign their value at some reference stress $\boldsymbol{\sigma}_s$ to the tangent compliances and prestrains. In this paper, the reference stresses are the mean value of the stresses over the concerned phase. By this way we obtain a thermo-elastic linear composite with a finite number of phases. This composite represents the linear comparison medium (LCM) as developed by Ponte Castañeda [12]. The homogenization problem related to this composite can be solved by classical linear homogenization techniques for thermoelastic media, such as the self-consistent scheme when one deals with polycrystals.

Various discussions and results (Masson et al. [9]) have proved the viscoplastic affine formulation to offer an improved alternative to previous treatments such as the Hill-Hutchinson secant treatment (Hutchinson [5]) or the "tangent" model (Molinari et al. [10], Lebensohn and Tomé [7]). It differs from the second-order procedure (SOP) (Ponte Castañeda [13]) by making use of the direct stress-strain relations (1) instead of deriving the stresses from the overall potential: consequently, on the one hand, the SOP takes better into account the local intraphase heterogeneity and then gives better predictions for nonlinear elasticity or viscosity; on the other hand, the affine method, unlike the SOP, does not lead to any duality gap and can be extended to any constitutive behavior which, such as rate-dependent or rate-independent elastoplasticity, does not derive from a single potential.

2.2. RATE-INDEPENDENT ELASTOPLASTICITY

In this section, rate-independent elastoplastic polycrystals are considered in the framework of small strains. The local strain rate is decomposed into its elastic and plastic parts:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^e + \dot{\boldsymbol{\varepsilon}}^p = \boldsymbol{K}^{-1} : \dot{\boldsymbol{\sigma}} + \sum_\alpha \dot{\gamma}^\alpha \boldsymbol{R}_\alpha \,, \tag{3}$$

with $\boldsymbol{K}$ the elastic moduli and $\dot{\gamma}^\alpha$ the non-negative plastic slip rate on system α with the orientation tensor $\boldsymbol{R}_\alpha = (\boldsymbol{n}_\alpha \otimes \boldsymbol{m}_\alpha)^S$ ($\boldsymbol{A}^S$ denotes the symmetric part of the second-order tensor $\boldsymbol{A}$). Associate plasticity theory is used with the Schmid law, with the critical resolved shear stress τ_c^α on a slip system α. Such a system is a potentially active system (P.A.S.) if $\boldsymbol{R}_\alpha : \boldsymbol{\sigma} = \tau_\alpha^c$. It is active (A.S.) if, in addition, $\boldsymbol{R}_\alpha : \dot{\boldsymbol{\sigma}} = \dot{\tau}_\alpha^c$. We adopt the following hardening law:

$$\dot{\tau}_\alpha^c = \sum_\beta H_{\alpha\beta} \dot{\gamma}^\beta \,, \tag{4}$$

where the hardening matrix $H_{\alpha\beta}$ is assumed to be constant (we could also deal with a non constant matrix through an appropriate linearization procedure, but the associated technical developments are not essential here). Thus, the local

elastoplastic constitutive equations read:

$$\dot{\boldsymbol{\sigma}} = \boldsymbol{L} : \dot{\boldsymbol{\varepsilon}}\,,$$
$$\boldsymbol{L} = \boldsymbol{K} : (\boldsymbol{I} - \sum_{\alpha,\beta} D^{\alpha\beta} \boldsymbol{R}_\alpha \otimes \boldsymbol{R}_\beta : \boldsymbol{K})\,, \tag{5}$$

where $D^{\alpha\beta} = (H_{\alpha\beta} + \boldsymbol{R}_\alpha : \boldsymbol{K} : \boldsymbol{R}_\beta)^{-1}$ and the summation on (α, β) is limited to active systems.

The overall stress response at time t now depends on the whole previous loading path. Thus, a step by step procedure is needed (Masson et al. [9]). The steps can be defined as separating two consecutive "events": an event occurs at time t_n when some new system becomes active or inactive in any phase of the polycrystal. The step by step procedure (which does not lead to an incremental approach!) can be described as follows: from the stress values obtained at the end of the former step, we determine, at the beginning of the current step ($t = t_n$), which systems are potentially active. Among all these P.A.S., we select one branch, i.e., a given combination of A.S.. According to (5), this choice helps to compute the tangent moduli in each phase, up to the next event. Meanwhile, according to (5), these moduli, say $\boldsymbol{L}_s$, are constant. The local constitutive equations are then linearized in the usual affine manner:

$$\boldsymbol{\sigma}_s = \boldsymbol{L}_s : \boldsymbol{\varepsilon} + \boldsymbol{\theta}_s\,, \qquad \boldsymbol{\theta}_s = \boldsymbol{\sigma}_s - \boldsymbol{L}_s : \boldsymbol{\varepsilon}_s\,, \tag{6}$$

where $\boldsymbol{\varepsilon}_s$ and $\boldsymbol{\sigma}_s$ are the strain and stress averages in phase s obtained at the end of the previous step. From the known moduli and prestresses of the linear comparison composite, we derive the macroscopic elastoplastic tangent modulus $\tilde{\boldsymbol{L}}$ and the macroscopic prestress $\tilde{\boldsymbol{\theta}}$, which characterize the macroscopic behavior during the current step. We can also calculate the concentration tensors and then the local variables during the current step and especially at the end of the step which is defined by the occurrence of the next nearest event. From these values, the consistency of the chosen branch can be checked, i.e., the selected A.S. must be still active and the initially non active P.A.S. still inactive at the end of the step. If this consistency is verified, we go on to the next step. If not, we go back to the beginning of the step and we select another branch until consistency conditions are satisfied. Resuming the same procedure at each new increment up to t provides the expected macroscopic response of the polycrystal at time t.

3. The affine formulation at finite strain

3.1. Choice of the general description framework

In view of applications to metal forming, which involve very large deformations, an extension of the affine formulation at finite strain is needed. We have first to

specify the general description framework. For several reasons listed below, we have adopted a mixed description instead of the classical eulerian or lagrangian ones (Iwakuma and Nemat-Nasser [6], Lipinski et al. [8], Harren [3]). This description makes special use of the deformation gradient tensor defined both on the initial and the current configurations. The small strains constitutive equation $\dot{\boldsymbol{\sigma}} = \boldsymbol{L} : \dot{\boldsymbol{\varepsilon}}$ of the single crystal now reads $\dot{\boldsymbol{n}} = \boldsymbol{N} : \dot{\boldsymbol{F}}$ where $\boldsymbol{n}$ is Hill's nominal stress tensor, $\boldsymbol{F} = \partial \boldsymbol{x}/\partial \boldsymbol{X}$ is the deformation gradient tensor and $\boldsymbol{x}$ and $\boldsymbol{X}$ are the position vectors on the current and the reference configuration respectively. The main advantage of this formulation relies on the fact that the macroscopic values of the nominal stress tensor and of the deformation gradient are the average over the initial configuration, which is known unambiguously, of their microscopic counterparts. Moreover, unlike for the Cauchy or the Kirchhoff stress tensors, this property also holds for their time derivatives (Hill [4]):

$$\bar{\boldsymbol{n}} = \langle \boldsymbol{n} \rangle_{\Omega_0} , \quad \bar{\boldsymbol{F}} = \langle \boldsymbol{F} \rangle_{\Omega_0} , \quad \dot{\bar{\boldsymbol{n}}} = \langle \dot{\boldsymbol{n}} \rangle_{\Omega_0} , \quad \dot{\bar{\boldsymbol{F}}} = \langle \dot{\boldsymbol{F}} \rangle_{\Omega_0} . \tag{7}$$

In the affine approach, we have rather to keep the reference configuration constant all along the loading path because we do not know the current configuration at the beginning of a new step. The main implication of this choice concerns the implicit description of the microstructure evolution. Though the derivations are performed on a fixed geometry (e.g., the constraint tensor, considered in the following, is calculated on a fixed ellipsoid), the evolution of the phase distribution is taken into account through that of the local tangent moduli which depend on the per phase average of the total and the elastic deformation (see below).

3.2. SINGLE CRYSTAL ELASTOPLASTIC CONSTITUTIVE EQUATIONS

From the elastic-plastic decomposition $\boldsymbol{F} = \boldsymbol{F}^e.\boldsymbol{F}^p$, the plastic kinematic relation $\dot{\boldsymbol{F}}^p.(\boldsymbol{F}^p)^{-1} = \dot{\gamma}^\alpha \boldsymbol{m}_\alpha \otimes \boldsymbol{n}_\alpha$ and Hooke's law $\dot{\boldsymbol{S}}^e = \boldsymbol{K} : \dot{\boldsymbol{E}}^e$, where $\boldsymbol{S}^e$ is the second Piola-Kirchhoff stress tensor based on the configuration obtained after plastic deformation and $\boldsymbol{E}^e$ the elastic Green-Lagrange strain tensor, the following equation can be derived (see Harren [3]):

$$\dot{\boldsymbol{n}} = \hat{\boldsymbol{N}} : \dot{\boldsymbol{F}} - \sum_\alpha \dot{\gamma}^\alpha \boldsymbol{Y}_\alpha \tag{8}$$

with

$$\begin{aligned} \hat{N}_{ijkl} &= F^{p-1}_{ia} F^e_{jb} K_{abcd} F^{p-1}_{kc} F^e_{ld} + \delta_{ik}\delta_{jl} , \\ \boldsymbol{A}_\alpha &= (\boldsymbol{F}^{eT}.\boldsymbol{F}^e.\boldsymbol{m}_\alpha \otimes \boldsymbol{n}_\alpha)^S , \qquad & \boldsymbol{B}_\alpha &= (\boldsymbol{m}_\alpha \otimes \boldsymbol{n}_\alpha.\boldsymbol{S}^e)^S , \\ \boldsymbol{Y}_\alpha &= \boldsymbol{F}^{-p}.(\boldsymbol{K} : \boldsymbol{A}_\alpha + 2\boldsymbol{B}_\alpha).\boldsymbol{F}^{eT} , \qquad & \boldsymbol{S}^e &= \boldsymbol{F}^{e-1}.\boldsymbol{F}.\boldsymbol{n}.\boldsymbol{F}^{e-T}. \end{aligned} \tag{9}$$

Note that $\hat{\boldsymbol{N}}$ in (8) exhibits diagonal symmetry (i.e., $\hat{N}_{ijlk} = \hat{N}_{klji}$).

The Schmid law reads at finite strain:

$$f_\alpha = \boldsymbol{m}^e_\alpha.\boldsymbol{\tau}.\boldsymbol{n}^e_\alpha - \tau^c_\alpha = 0\,, \quad \boldsymbol{m}^e_\alpha = \boldsymbol{F}^e.\boldsymbol{m}_\alpha\,, \quad \boldsymbol{n}^e_\alpha = \boldsymbol{n}_\alpha.(\boldsymbol{F}^e)^{-1}\,, \quad (10)$$

where $\boldsymbol{\tau} = det(\boldsymbol{F})\boldsymbol{\sigma}$ is the Kirchhoff stress. The resolved shear stress used in the Schmid law is the projection of the surface traction $\boldsymbol{\tau}.\boldsymbol{n}^e_\alpha$ not on the initial ($\boldsymbol{m}_\alpha$) but on the current slip direction $\boldsymbol{m}^e_\alpha$. This choice is physically questionable and has significant consequences on the symmetry of the tangent modulus for the single crystal. We still use the hardening law (4) for the critical resolved shear stress. The slip rate $\dot\gamma^\alpha$, which is a linear function of $\dot{\boldsymbol{F}}$, can be derived from the consistency condition and reintroduced into (8), so as to derive the expected constitutive equation for the single crystal:

$$\begin{aligned} &\dot{\boldsymbol{n}} = \boldsymbol{N} : \dot{\boldsymbol{F}}\,, \\ &\boldsymbol{N} = \hat{\boldsymbol{N}} + \sum_{\alpha,\beta}(H_{\alpha\beta} + 2\boldsymbol{B}_\alpha : \boldsymbol{A}_\beta + \boldsymbol{A}_\beta : \boldsymbol{K} : \boldsymbol{A}_\alpha)^{-1}\boldsymbol{Y}_\alpha \otimes \boldsymbol{Y}_\beta\,. \end{aligned} \quad (11)$$

Note that, even if $H_{\alpha\beta}$ is symmetric, the moduli $\boldsymbol{N}$ do not exhibit diagonal symmetry anymore. Since this fact can induce some difficulties for finite strain homogenization schemes which rely on the use of Green techniques, we decide arbitrarily to replace $H_{\alpha\beta}$ by $\hat H_{\alpha\beta}$ such that

$$\hat H_{\alpha\beta} = (H_{\alpha\beta})^S + \boldsymbol{B}_\beta : \boldsymbol{A}_\alpha - \boldsymbol{B}_\alpha : \boldsymbol{A}_\beta \quad (12)$$

in order to save the diagonal symmetry of $\boldsymbol{N}$.

3.3. Specific features of the affine approach at finite strain

Linearization of the constitutive stress-strain relations. The tangent moduli $\boldsymbol{N}$ are no more constant between two consecutive events because they depend on $\boldsymbol{F}(t,\boldsymbol{x})$, $\boldsymbol{F}^e(t,\boldsymbol{x})$, $\boldsymbol{n}(t,\boldsymbol{x})$. In view of an explicit prediction, we choose to linearize the constitutive equations at the beginning of the current step at time $t = t_n$:

$$\begin{aligned} \boldsymbol{n}(t,\boldsymbol{x}) &= \boldsymbol{N}(t_n,\boldsymbol{x}) : \boldsymbol{F}(t,\boldsymbol{x}) + \boldsymbol{p}(t_n,\boldsymbol{x})\,, \\ \boldsymbol{N}(t_n,\boldsymbol{x}) &= \boldsymbol{N}(\boldsymbol{F}(t_n,\boldsymbol{x}), \boldsymbol{F}^e(t_n,\boldsymbol{x}), \boldsymbol{n}(t_n,\boldsymbol{x}))\,, \\ \boldsymbol{p}(t_n,\boldsymbol{x}) &= \boldsymbol{n}(t_n,\boldsymbol{x}) - \boldsymbol{N}(t_n,\boldsymbol{x}) : \boldsymbol{F}(t_n,\boldsymbol{x})\,. \end{aligned} \quad (13)$$

These are the constitutive equations of a continuously heterogeneous linear thermoelastic composite under finite strain.

Approximation of piecewise uniformity. Once again, the problem is simplified through the approximation of piecewise uniformity of the moduli$\boldsymbol{N}(t_n,\boldsymbol{x})$ and the prestresses $\boldsymbol{p}(t_n,\boldsymbol{x})$, which depend on $\boldsymbol{x}$ through $\boldsymbol{F}(t_n,\boldsymbol{x})$, $\boldsymbol{F}^e(t_n,\boldsymbol{x})$ and $\boldsymbol{n}(t_n,\boldsymbol{x})$: in phase s, they are ascribed to take their value at $\boldsymbol{F}_s(t_n) =$

$\langle \boldsymbol{F}(t_n, \boldsymbol{x})\rangle_{\Omega_s}, F^e_s(t_n) = \langle F^e(t_n, x)\rangle_{\Omega_s}$ and $n_s(t_n) = \langle n(t_n, x)\rangle_{\Omega_s}$ (with $\langle A\rangle_{\Omega_s}$ the average of A in phase s). This approximation results at step n in the following constitutive equations of the linear thermoelastic multiphase comparison material:

$$\begin{aligned} \boldsymbol{n}(t, \boldsymbol{x}) &= \boldsymbol{N}_s(t_n) : \boldsymbol{F}(t, \boldsymbol{x}) + \boldsymbol{p}(t_n)\,, \\ \boldsymbol{N}_s(t_n) &= \boldsymbol{N}(\boldsymbol{F}_s(t_n), \boldsymbol{F}^e_s(t_n), \boldsymbol{n}_s(t_n))\,, \\ \boldsymbol{p}_s(t_n) &= \boldsymbol{n}_s(t_n) - \boldsymbol{N}_s(t_n) : \boldsymbol{F}_s(t_n)\,. \end{aligned} \tag{14}$$

Homogenization. At finite strain, no minimum potential energy principle is available. Ball [1] showed the existence of a solution to the problem of energy potential minimization for a polyconvex potential. However, uniqueness is not ensured. Thus, only variational principles (see Ogden [11]) exist and estimates only can be derived. Here, we restrict ourselves to Hashin-Shtrikman-type estimates, including the self-consistent scheme for specific application to polycrystals. They are based on the use of Green techniques which can be discussed in the context of finite strains through the 9-dimensional Eshelby inclusion problem. In terms of variables $\boldsymbol{n}$ and $\boldsymbol{F}$, this problem is defined as follows:

$$\begin{aligned} &\boldsymbol{n}(\boldsymbol{X})_{ij,i} = 0 \quad \forall \boldsymbol{X}\,, \\ &\boldsymbol{n} = \boldsymbol{N}^0 : \boldsymbol{F} + \chi_I(\boldsymbol{X})\boldsymbol{n}^I\,, \qquad \boldsymbol{F} = \frac{\partial \boldsymbol{x}(\boldsymbol{X},t)}{\partial \boldsymbol{X}}\,, \\ &\lim_{\boldsymbol{X}\to\infty} \boldsymbol{F}(\boldsymbol{X}, t) = \bar{\boldsymbol{F}}\,, \end{aligned} \tag{15}$$

where $\chi_I(\boldsymbol{X})$ is the characteristic function of the ellipsoidal inclusion I and $\boldsymbol{n}^I$ is constant. The solution for $\boldsymbol{F}(\boldsymbol{X})$ is known to be uniform in I (Iwakuma and Nemat-Nasser [6]) and given by

$$\begin{aligned} &\boldsymbol{F}^T(\boldsymbol{X}_0) = \boldsymbol{P}^0 : \boldsymbol{n}^I + \bar{F} \quad \forall \boldsymbol{X}_0 \in I\,, \\ &P^0_{ijkl}(\boldsymbol{X}_0) = \int_I u_{lj,ik}(\boldsymbol{X} - \boldsymbol{X}_0)\, dV_X = \int_I \Gamma^0_{ijkl}(\boldsymbol{X} - \boldsymbol{X}_0)\, dV_X\,, \end{aligned} \tag{16}$$

where $\boldsymbol{u}(\boldsymbol{X} - \boldsymbol{X}_0)$ is the Green function for an infinite elastic medium with the moduli $\boldsymbol{N}^0$ and $\boldsymbol{\Gamma}^0$ is the associated strain-Green operator.

Opposite to the case of small strains, the skew-symmetric parts of $u_{lj,ik}$ with respect to (j,k) and (l,i) are taken into account in $\boldsymbol{\Gamma}^0$ which does not exhibit anymore minor symmetries. As mentioned above, some difficulties, related to the use of Green techniques at finite strain, arise when $\boldsymbol{N}^0$ does not exhibit anymore the diagonal symmetry. Although the uniqueness of the Green function is ensured, its existence is no more established, so that the derivation of $\boldsymbol{P}^0$ becomes problematic. That is why such a situation has been excluded in (3.2). Therefore, the solution (16) of the inclusion problem may be used to establish estimates for elastic or thermoelastic linear composites in terms of $\boldsymbol{n}$ and $\boldsymbol{F}$ in a way strictly similar to the one used for small strains. For the elasto-plastic affine

treatment, associated to the linear self-consistent scheme, the concentration equations at the current step n can be, according to (14), approximated by

$$\begin{aligned}
\boldsymbol{F}_s(t) &= \boldsymbol{A}_s(t_n) : \bar{\boldsymbol{F}} + \boldsymbol{a}_s(t_n) \qquad \forall t \in]t_n, t_{n+1}] \,, \\
\boldsymbol{A}_s(t_n) &= (\boldsymbol{I} + \boldsymbol{P}_{SC} : (\boldsymbol{N}_s(t_n) - \tilde{\boldsymbol{N}}_{SC}))^{-1} \,, \\
\boldsymbol{a}_s(t_n) &= ({\boldsymbol{P}_{SC}}^{-1} + \boldsymbol{N}_s(t_n) - \tilde{\boldsymbol{N}}_{SC})^{-1} : (\tilde{\boldsymbol{p}} - \boldsymbol{p}_s(t_n)) \,, \\
\boldsymbol{P}_{SC} &= \textstyle\int_I \boldsymbol{\Gamma}_{SC}(\boldsymbol{X} - \boldsymbol{X}_0)\, dV_X \,, \quad \tilde{\boldsymbol{p}} = \langle \boldsymbol{p}(t_n) : \boldsymbol{A}(t_n) \rangle \,,
\end{aligned} \tag{17}$$

where $\boldsymbol{\Gamma}_{SC}$ is attached to the infinite medium with moduli $\boldsymbol{N}_{SC}$.

Variables updating. Specializing equation (17) to the linear composite of the former step at time $t = t_n$ and proceeding similarly for the linear comparison composite of the current step at time$t = t_{n+1}$ lead to

$$\Delta \boldsymbol{F}_s = \boldsymbol{A}_s(t_n)\Delta \bar{\boldsymbol{F}} + (\boldsymbol{A}_s(t_n) - \boldsymbol{A}_s(t_{n-1}))\bar{\boldsymbol{F}}(t_n) + \boldsymbol{a}_s(t_n) - \boldsymbol{a}_s(t_{n-1}), \tag{18}$$

where $\Delta \boldsymbol{F}_s = \boldsymbol{F}_s(t_{n+1}) - \boldsymbol{F}_s(t_n)$ and $\Delta \bar{\boldsymbol{F}} = \bar{\boldsymbol{F}}(t_{n+1}) - \bar{\boldsymbol{F}}(t_n)$. The expression (18) of the deformation gradient increment clearly distinguishes the affine treatment from Hill's incremental one: according to Hill's method, this expression would reduce to $\Delta \boldsymbol{F}_s = \boldsymbol{A}_s(t_n)\Delta \bar{\boldsymbol{F}}$. The macroscopic stress increment $\Delta \bar{\boldsymbol{n}}$ and then the local stress increment $\Delta \boldsymbol{n}_s$ can be derived from (18), (11) as a function of the macroscopic deformation. The lattice rotation is obtained as usual by subtracting the plastic deformation gradient increment from the total one.

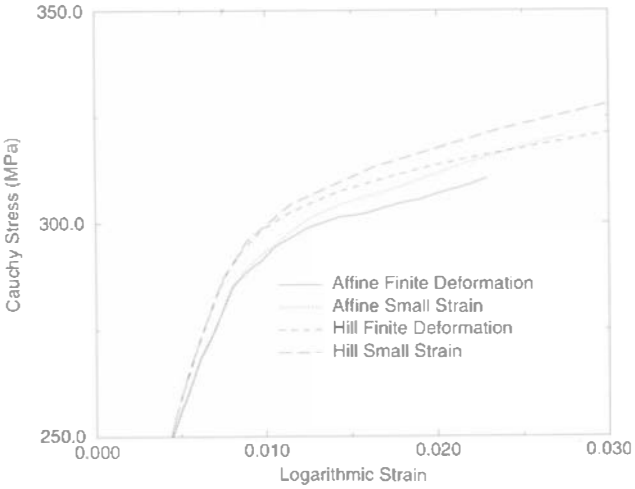

Figure 1. Tensile stress-strain curves of an untextured fcc polycrystal according to the incremental and affine models at small and finite strains.

4. Preliminary results and conclusion

Both the affine and the incremental approaches have been applied to derive the tensile stress-strain response of an untextured elastoplastic face-centred cubic polycrystal. Hill's method has been implemented by using a true mixed formulation as explained in section (3.1). The elastic behavior is assumed to be isotropic ($K = 44400$ MPA and $\mu = 30750$ MPA). The twelve octahedral slip systems are considered with the same critical resolved shear stress $\tau_\alpha^c = 100$ MPA $\forall\ \alpha$. Self and latent hardening are taken into account ($H_{\alpha\beta} = (1-q)\ h\delta_{\alpha\beta} + qh$) with $h = 200$ and $q = 0.3$. An initial quasi-isotropic texture (with ten orientations in the standard triangle) is considered.

Figure 1 provides the stress-strain tensile curves for both these approaches, for small as well as for large strains. We can see that the affine approach still yields softer predictions than Hill's one at finite strain. Moreover, both finite strain formulations yield softer predictions than their small strain counterparts. This result stems from the softening effect of the lattice rotations which are taken into account at finite strain.

According to these preliminary results, the affine approach can be thought to be able to improve significantly on Hill's incremental treatment for both small and large deformations. Nevertheless, future work is necessary to validate the affine finite strain formulation and especially to extend it to more general anisotropic initial textures.

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