Plasticity of metallic polycrystals at large strains by the self-consistent method

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1 INTRODUCTION

The determination of the effective properties of heterogeneous materials from those of each its constituents is a field of research closely related to the development of modern technologies. Linear problems such as elasticity, thermal conductivity or dielectric properties of materials were recently solved by Kröner (1980) and Dederichs and Zeller (1973) using the general statistical approach. Until very recently, studies on plastic or elastoplastic properties of heterogeneous materials, for example metallic polycrystals, have been limited to classical and very simplified models like those of Taylor (1938) or Sachs (1928). The self-consistent scheme proposed initially by Kröner (1958), (1961) was developed by Hill (1965), Berveiller and Zaoui (1979), Hutchinson (1970) within the framework of small strains.

It is obvious that forming processes generally lead to finite elastoplastic deformations which modify the internal structure and the mechanical state of the polycrystal. The internal structure is concerned essentially by the critical shear stress on the glide systems, the internal stresses associated with plastic incompatibilities, and the formation of crystallographic as well as morphologic textures. Thus, at large strains, it is necessary to take into account the evolution of these physical parameters in order to model the overall material behaviour in a correct manner. Behaviour of material and geometry of transformations being non-linear, the following related problems must be parallelly solved :

- The choice of a reference configuration and the transition operations from the microscopic scale to the macroscopic level.
- The concentration operators which link the local stress or strain fields to the corresponding fields at the macroscopic level.
- The description of the single crystal elastoplastic constitutive law. The model proposed by Hill and Rice (1972), Asaro (1979) and Nemat-Nasser (1979) is adopted in this study, and is not recalled here.

The first question is treated in paragraph 2 where Hill's (1972) solutions are largely used. In paragraph 3, an integral equation for the velocity gradient is proposed, and a new self-consistent solution of it is given. Finally, a few applications are discussed in the last part of the paper.

2 MICRO-MACRO TRANSITION OPERATIONS

The common starting point of all the micro-macro models is the averaging operation. It is interesting to choose such a description which preserves the simple form of the averaging operators used in the small strain approach. Let's consider the gradient of the relative deformation :

$$\underline{\underline{f}}_t = \overline{\text{grad}}\ \bar{x} \tag{1}$$

and its instantaneous derivative with respect to the time τ.

$$\underline{\underline{g}} = \dot{\underline{\underline{f}}}_t(t) = \partial_\tau \underline{\underline{f}}_t \,|\, \tau = t \tag{2}$$

Defining the strain rate tensor and the rate of rotation (spin) as the symmetric and antisymmetric parts of $\underline{\underline{g}}$ respectively :

$$\begin{aligned} \underline{\underline{d}} &= \frac{1}{2}(\underline{\underline{g}} + {}^t\underline{\underline{g}}) \\ \underline{\underline{w}} &= \frac{1}{2}(\underline{\underline{g}} - {}^t\underline{\underline{g}}) \end{aligned} \tag{3}$$

it is possible to demonstrate that $\underline{\underline{g}}$ is simultaneously the spatial gradient of the velocity vector $\bar{v} = \dot{\bar{x}}$

$$\underline{\underline{g}} = \overline{\text{grad}}\ \bar{v} \tag{4}$$

Expression (4) shows that $\underline{\underline{g}}$ is independent of the choice of a reference configuration. Hill (1972) demonstrated the fundamental relation which is the basis of all averaging theories at large strains. He showed that the average value of the product $\underline{\underline{g}} \cdot \dot{\underline{\underline{n}}}$ was equal to the product of the corresponding averages.

$$\frac{1}{V_t}\int_{V_t} \underline{\underline{g}}.\dot{\underline{\underline{n}}}\ dV_t = \left(\frac{1}{V_t}\int_{V_t} \underline{\underline{g}}\ dV_t\right).\left(\frac{1}{V_t}\int_{V_t} \dot{\underline{\underline{n}}}\ dV_t\right) \tag{5}$$

Noting the averages by capital letters, this last equation may be rewritten as :

$$\frac{1}{V_t}\int_{V_t} \underline{\underline{g}}.\dot{\underline{\underline{n}}}\ dV_t = \underline{\underline{G}}.\dot{\underline{\underline{N}}}$$

Tensors $\dot{\underline{\underline{n}}}$ and $\dot{\underline{\underline{N}}}$ are the unsymmetric local and overall nominal stress rates respectively. As it has been emphasized by Hill (1972), the equilibrium equation takes a particularly simple form when expressed in terms of this stress rate :

$$\text{div}\ \dot{\underline{\underline{n}}} = o \tag{6}$$

Moreover, the conjugated strain rate measure, defined by equation (5), exhibits a very convenient additive decomposition in elastic and plastic parts :

$$\underline{\underline{g}} = \underline{\underline{d}} + \underline{\underline{w}} = (\underline{\underline{d}}^e + \underline{\underline{d}}^p) + (\underline{\underline{w}}^e + \underline{\underline{w}}^p) \tag{7}$$

It can be shown that, the constitutive relation for the single crystal may be expressed with the help of these two measures, see for instance Hill and Rice (1972), Asaro (1979), Nemat-Nasser (1979) :

$$\dot{\underline{\underline{n}}}(x) = \underset{\sim}{\ell}(\bar{x}) : \underline{\underline{g}}(x) \tag{8}$$

where $\underset{\sim}{\ell}(\bar{x})$ is the local instantaneous moduli tensor. It depends on the material's elastic properties, active glide systems, Cauchy stress

tensor and a hardening matrix defining the interactions between dislocations in various glide systems.

As it will be shown in the following sections, the choice of the reference configuration and the stress and strain measures presented here preserves the form of nearly all the expressions elaborated in the small strain theory of the polycrystals plasticity. This feature constitutes the principal advantage of the chosen formulation.

3 INTEGRAL EQUATION FOR THE LOCAL VELOCITY GRADIENT

In this section, the systematic method of calculation of the effective macroscopic behaviour of polycrystals, in the case of large strains is presented. The infinite solid with a homogeneous velocity gradient $\underline{\underline{G}}$ imposed on its external surface S is supposed to verify the equilibrium equation (6) :

$$\operatorname{div} \underline{\underline{\dot{\pi}}} = o$$

The plastic events (activation and disactivation of the slip systems) are supposed to be known everywhere during the loading process so that critical and resolved shear stresses as well as their evolutions may be given. Therefore, the instantaneous local tensor of elasto-plastic moduli $\underset{\sim}{\ell}(\bar{x})$ can be determined. The system of equations to be solved contains the boundary conditions and the equilibrium equations for the material whose properties change from point to point. To solve this problem the decomposition of $\underset{\sim}{\ell}(\bar{x})$ into a spatially constant part $\underset{\sim}{L}^{\circ}$ and a deviation $\delta \underset{\sim}{\ell}(\bar{x})$, depending on the current position of the material point, is proposed

$$\underset{\sim}{\ell}(\bar{x}) = \underset{\sim}{L}^{\circ} + \delta \underset{\sim}{\ell}(\bar{x}) \qquad (9)$$

Moreover, the moduli tensor $\underset{\sim}{L}^{\circ}$ of the homogeneous fictitious medium must possess certain symmetries, see Lipinski and Berveiller (to be published).

Introducing (8) and (9) into (6) one has :

$$\operatorname{div}(\underset{\sim}{L}^{\circ} : \underline{\underline{g}}(\bar{x})) = -\bar{f}^{\circ}(\bar{x}) \qquad (10)$$

where $\bar{f}^{\circ}(\bar{x}) = \operatorname{div}(\delta \underset{\sim}{\ell}(\bar{x}) : g(\bar{x}))$ is a certain fictitious body force.

The solution to equation (10) is given by the classical Green tensor $\underset{\sim}{\mathcal{G}}^{\circ}$ associated with the homogeneous fictitious medium $\underset{\sim}{L}^{\circ}$:

$$\underline{\underline{g}}(\bar{x}) = \underline{\underline{g}}^{\circ} + \int_{V_t} \underset{\sim}{\Gamma}(\bar{x}-\bar{x}') : \delta \underset{\sim}{\ell}(\bar{x}') : \underline{\underline{g}}(\bar{x}') dV'_t \qquad (11)$$

where

$$\underset{\sim}{\Gamma}(\bar{x}-\bar{x}') = \partial_{\bar{x}'} \partial_{\bar{x}'} \underset{\sim}{\mathcal{G}}^{\circ}(\bar{x}-\bar{x}') \qquad (12)$$

and $\underline{\underline{g}}^{\circ}$ is the solution of the homogeneous problem associated with (10). Knowing the solution of (11) one may determine all the evolution rules of the internal structure of the polycrystal discussed in the introduction.

In the next paragraph, the self-consistent solution of integral equation (11) is proposed which enables us to obtain the overall elasto-plastic moduli.

4 SELF CONSISTENT SCHEME OF THE INTEGRAL EQUATION SOLUTION

The self-consistent scheme is based on a particular choice of $\underset{\sim}{L}^{\circ}$ tensor which up to now has been considered as arbitrary. In order to use the Green's technique to solve the integral equation (16), this tensor must

possess the following symmetries $L^{\circ}_{ijk\ell} = L^{\circ}_{ikj\ell}$.

A "pseudo" self-consistent model is obtained introducing the following assumption :

$$L^{\circ}_{ijk\ell} = \frac{1}{2}(L^{eff}_{ijk\ell} + L^{eff}_{ikj\ell}) \tag{13}$$

To determine the effective moduli tensor $\underset{\sim}{L}^{eff}$, a supplementary approximation concerning the microstructure organization has to be made. It is supposed that the polycrystal may be represented by a set of inclusions, which model grains, embedded within a homogeneous medium with the elastoplastic moduli $\underset{\sim}{L}^{\circ}$. If $H^I(\bar{x})$ is the characteristic function for an inclusion V^I such that :

$$H^I(\bar{x}) = \begin{cases} 1 & \text{if } \bar{x} \in V^I \\ 0 & \text{if } \bar{x} \notin V^I \end{cases} \tag{14}$$

one has

$$\delta \underset{\sim}{\ell}(\bar{x}) = \Delta\underset{\sim}{\ell}^I(\bar{x})\ H^I(\bar{x}) \tag{15}$$

Neglecting heterogeneous deformations at the intracrystalline level, the approximation holds :

$$\begin{aligned} \Delta\underset{\sim}{\ell}^I(\bar{x}) &= \Delta\underset{\sim}{\ell}^I \\ \underset{=}{g}^I(\bar{x}) &= \underset{=}{g}^I \end{aligned} \tag{16}$$

This approximation is physically justified for rather small plastic deformations. It is well known that the large plastic strains lead to the creation of dislocation's cells, subgrains etc.

Substituting (15) and (16) into (11) and taking into account the properties of Eshelby's solution (1961) of the ellipsoïdal inclusion, one obtains :

$$\underset{=}{g}(\bar{x}) = \underset{=}{g}^{\circ} + \left(\int_{V^I} \underset{\sim}{\Gamma}(x-x')dV^I\right) : \Delta\underset{\sim}{\ell}^I : \underset{=}{g}^I \tag{17}$$

The mean value of $\underset{=}{g}$ over the grain volume may now be calculated. Denoting this value by $\underset{=}{g}^I$, a new relation is found :

$$\underset{=}{g}^I = \frac{1}{V^I}\int_{V^I} \underset{=}{g}(\bar{x})dV = \underset{=}{g}^{\circ} + \frac{1}{V_I}\left(\int_{V^I}\int_{V^I} \underset{\sim}{\Gamma}(\bar{x}-\bar{x}')dV'dV\right) : \Delta\underset{\sim}{\ell}^I : \underset{=}{g}^I \tag{18}$$

Introducing the tensor $\underset{\sim}{T}^{II}$ defined by :

$$\underset{\sim}{T}^{II} = \frac{1}{V^I}\int_{V^I}\int_{V^I} \underset{\sim}{\Gamma}(\bar{x}-\bar{x}')dV'\ dV \tag{19}$$

which is related to the Eshelby tensor $\underset{\sim}{S}^{\circ}$ by :

$$\underset{\sim}{T}^{II} = \underset{\sim}{S}^{\circ} : \underset{\sim}{L}^{\circ} \tag{20}$$

the solution of (17) may be presented as :

$$\underset{=}{g}^I = \underset{=}{g}^{\circ} + \underset{\sim}{T}^{II} : \Delta\underset{\sim}{\ell}^I : \underset{=}{g}^I \tag{21}$$

The mean value of the local velocity gradient $\underset{=}{g}^I$ may be calculated from (21)

$$\underset{=}{g}^I = (\underset{\sim}{I} - \underset{\sim}{T}^{II} : \Delta\underset{\sim}{\ell}^I)^{-1} : \underset{=}{g}^{\circ} = \underset{\sim}{B}^I : \underset{=}{g}^{\circ} \tag{22}$$

where the identity tensor $\underset{\sim}{I}$ has been introduced. $\underset{\sim}{B}^I = (\underset{\sim}{I} - T^{II} : \Delta\underset{\sim}{\ell})^{-1}$ is called the "pseudo"- concentration tensor.

The next step of the solution procedure consists in the determination of the overall tangent moduli $\underset{\sim}{L}^{eff}$. Using averaging operations which in the case of granular media become :

$$\underline{\underline{G}} = \langle \underline{\underline{g}}^I \rangle = \langle \underset{\sim}{B}^I \rangle : \underline{\underline{g}}^\circ \tag{23}$$

$$\dot{\underline{\underline{N}}} = \langle \dot{\underline{\underline{n}}}^I \rangle \tag{24}$$

From (23), one obtains the following expression for $\underline{\underline{g}}^\circ$:

$$\underline{\underline{g}}^\circ = \langle \underset{\sim}{B}^I \rangle^{-1} : \underline{\underline{G}}$$

and from (22), $\underline{\underline{g}}^I$ is

$$\underline{\underline{g}}^I = \underset{\sim}{B}^I : \langle \underset{\sim}{B}^I \rangle^{-1} : \underline{\underline{G}} \tag{25}$$

On the other hand, the local constitutive law and relation (25) allow to write :

$$\dot{\underline{\underline{n}}}^I = \underset{\sim}{\ell}^I : \underline{\underline{g}}^I = \underset{\sim}{\ell}^I : \underset{\sim}{B}^I : \langle \underset{\sim}{B}^I \rangle^{-1} : \underline{\underline{G}}$$

Therefore, according to (24), the overall stress rate is equal to :

$$\dot{\underline{\underline{N}}} = \langle \dot{\underline{\underline{n}}}^I \rangle = \langle \underset{\sim}{\ell}^I : \underline{\underline{B}}^I \rangle \ast \langle \underline{\underline{B}}^I \rangle^{-1} : \underline{\underline{G}}$$

This relation defines the effective moduli tensor $\underset{\sim}{L}^{eff}$ which finally can be written as :

$$\underset{\sim}{L}^{eff} = \langle \underset{\sim}{\ell}^I : \underline{\underline{B}}^I \rangle \ast \langle \underline{\underline{B}}^I \rangle^{-1} \tag{26}$$

Apparently simple, the solution of the above equations is very compli cated. This complexity is closely related to an implicit and nonlinear character of the problem.

5 APPLICATIONS AND CONCLUSIONS

All numerical calculations presented here simulate an FCC polycrystal. Ninety nine grain families have been chosen to model the polycrystal. The elastic behaviour of the polycrystal is supposed to be isotropic and defined by Poisson's ratio $\nu = 0.3$ and Lame's modulus $\mu = 10\,000$ daN/mm^2. The plastic slip on 24 easy glide systems of <111> (110) type is governed by the Schmid's law with the initial critical shear stress $\tau^\circ = 5$ daN/mm^2 and the hardening rule described by the constant matrix H composed on two types of terms. The first term, modelling the weak interactions, is equal to $\mu/250$ and the second term 1.5 times greater, reflects the strong interactions between dislocations.

Figure 1a presents the three tension curves obtained by simulation of loadings in three orthogonal directions. The crystallographic orientations of the 99 spherical grains have been generated randomly in order to approximate an isotropic polycrystal. The corresponding <111> pole figure is presented on figure 2a. These two figures confirm the good approximation of isotropy. The curves on figure 1a may be characterized by two stages. First, parabolic and second linear with the tangent modulus about $\mu/80$. The cited properties are in good agreement with the experimental observations by Jaoul (1957).

Figure 1b presents three others tension curves for the material defined by the stereographic projection shown in figure 2b. The differences are visible between these curves which manifest the presence of a crystallographic texture.

Next, the influence of a morphologic texture on the tension curves has been tested. The ellipsoïdal form of grains ($b = c = a/2$) has been

superimposed on the isotropic crystallographic texture. The important sensitivity of the model on the morphological texture is observed via the three corresponding tension curves presented on figure 3.

Finally, the response of the model on proportional biaxial loadings is presented. The equivalent stress evolution in function of the equivalent strain for two different loading paths is drawn on figure 4. Morphologically and crystallographically isotropic material has been tested. Figure 5 presents the initial yield surfaces for the various offset definitions respectively in the case of spherical and ellipsoïdal grains.

The same isotropic crystallographic texture has been chosen. Once again, the important influence of the grain form on the obtained results is visible.

Some others simulations have been developed, for instance non-proportional loadings, in order to model the evolution of subsequent yield surfaces.

The obtained results manifest the performance of the presented approach for modelling the elasto-plastic behaviour of polycrystals.

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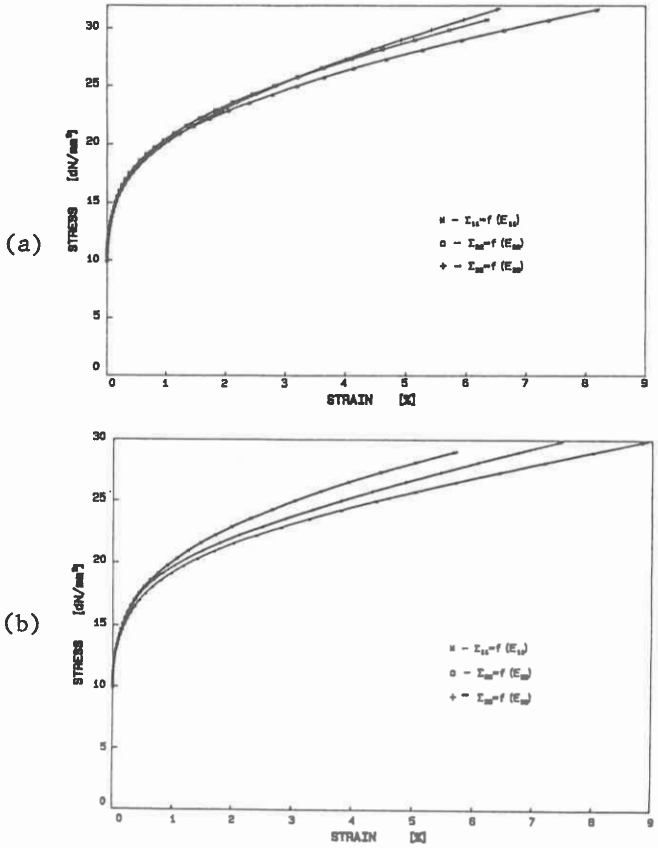
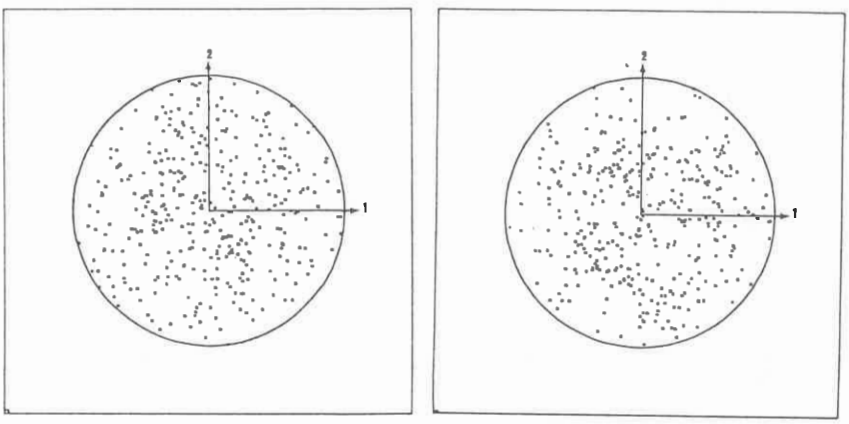


Fig. 1 : Tension curves for (a) isotropic crystallographic texture and (b) polycrystal with small crystallographic texture.



(a) (b)

Fig. 2 : <111> pole figures for the two polycrystals

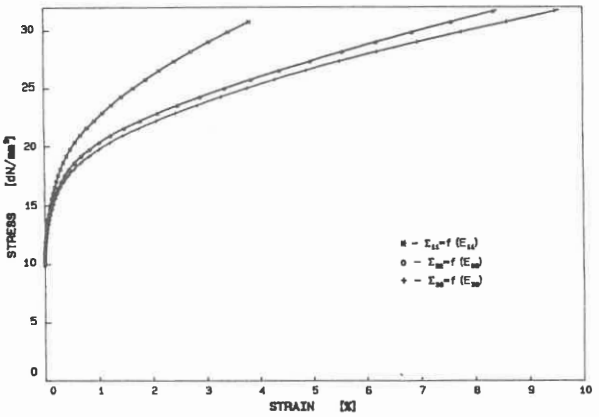


Fig. 3 : Influence of the morphological texture on tension curves for the polycrystal without crystallographical texture.

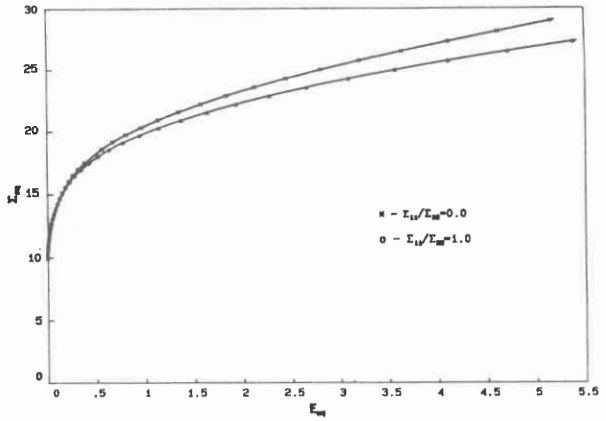


Fig. 4 : Equivalent stress as a function of the equivalent strain for two tensile directions.

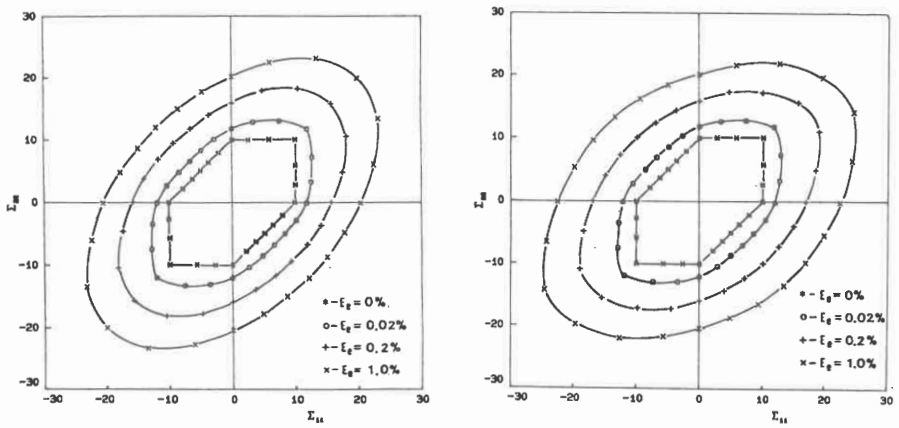


Fig. 5 : Initial yield surfaces for the polycrystal with (a) spherical and (b) ellipsoïdal grains form.