Numerical homogenization of nonlinear viscoplastic two-dimensional polycrystals [⋆]

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Abstract

In this paper, we numerically determine the effective stress-strain relation of some two-dimensional polycrystals. These are aggregates of a few tens of perfectly bonded single-crystal (hexagonal atomic lattice) grains, with varying orientations. Each grain obeys a given nonlinear viscoplastic stress-strain relation, which depends on the orientation of the grain. Precise calculations performed with this microscopic model are compared with calculations done with a macroscopic approximate model (in which matter has no microstructure) in order to determine the macroscopic constitutive law. We find an effective behaviour for the stationary response which appears to be also consistent for the transient response. The influence of the number of the grains as well as that of the distribution of the grain orientations are investigated.

Key words: Numerical homogenization, Polycrystal, Effective constitutive law, Finite Element Method

1 Introduction

The theoretical prediction of the effective response of an heterogeneous material is still an essentially open question. In some few simple cases, an analytic closed form expression is known. For instance, this is the case for a linear elastic matrix with linear elastic inclusions, in the dilute limit (that is, inclusions are considered too far away from one another to have an interaction) [7].

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A more general case is that of an *hyperelastic* material [6,9]. Let us recall for consistency that, by definition, an hyperelastic material is a material for which there exists a differentiable real-valued function $U(x, \sigma)$ such that the constitutive law (also named the *stress-strain relation*) reads

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

The function U is the heterogeneous *elastic stress potential*, $\sigma(x, t)$ is the *stress tensor* (the first Piola-Kirchhoff tensor), and $\varepsilon(x, t)$ is the *strain tensor*, which is linked to the displacement field $u(x)$ by the linearized *compatibility equation*

$$\varepsilon = \frac{1}{2} \left(\nabla u + {}^t \nabla u \right). \tag{2}$$

In this setting, one can derive various bounds and estimates on the effective behaviour [4,8,10–12]. Let us note that, in general, no closed form expression for the effective elastic stress potential is available.

The situation is the same for nonlinear *viscoplastic* materials, for which the constitutive law reads

$$\dot{\varepsilon}(x, t) = \frac{\partial U}{\partial \sigma}(x, \sigma(x, t)). \tag{3}$$

In this case, U is the *viscoplastic stress potential*, $\sigma(x, t)$ is the stress tensor and the *strain rate tensor* $\dot{\varepsilon}(x, t)$ is the time derivative of the strain tensor.

However, there exist materials for which the constitutive relation cannot be written as in (1) nor (3). *Elasto-viscoplastic* materials are such ones. For some of these materials, the strain rate tensor $\dot{\varepsilon}$ depends both on the stress tensor σ and the stress rate tensor $\dot{\sigma}$ along

$$\dot{\varepsilon}(x, t) = \frac{\partial U^{vp}}{\partial \sigma}(x, \sigma(x, t)) + \frac{\partial U^e}{\partial \dot{\sigma}}(x, \dot{\sigma}(x, t)), \tag{4}$$

where U^{vp} is the *viscoplastic stress potential* and U^e is the *elastic stress potential*. In such a case, when the stress-strain relation cannot be written with a unique potential, there are no theoretical bounds known.

In this article, we numerically investigate the effective behaviour of a heterogeneous polycrystal obeying such an elasto-viscoplastic law [1]. With a view to studying a more realistic and complex model in the future, we want to check here whether an effective constitutive law of type (4) can be inferred from the examination of the material at lower scale.

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The article is organized as follows. The polycrystal model is presented in Section 2. Let us just mention in this Introduction that a *polycrystal* is an aggregate of perfectly bonded single-crystal grains, and that each grain is homogeneous and obeys a given nonlinear stress-strain relation. This relation depends on parameters which are not the same from one grain to another one, thus making the polycrystal heterogeneous. Section 3 is dedicated to the theoretical study of such an heterogeneous law. We first recall some definitions and classical results on the derivation of an effective law for heterogeneous materials, by an homogenization procedure. As above stated, the classical procedure does not apply for our model, since the microscopic law cannot be written by using a single potential. We however decide to make use of the classical procedure separately on the elastic potential and on the viscoplastic potential, thus obtaining an effective elastic potential and an effective viscoplastic potential, up to some unknown parameters. Collecting these two effective potentials, we are able to postulate some expression for the effective constitutive law (see (24) below).

Our aim is to use, in the future, the effective law in the following way. Computing the response of a structure (composed of a large number of grains) by using the microscopic law is very expensive. Recall that, if one uses a finite element method, the mesh size has to be smaller than the grain size. Using an effective homogeneous law is much cheaper, for it allows for larger mesh sizes. In this article, as a first step, we look for an effective constitutive law which is consistent with the microscopic law. This consistency is checked by comparing the numerical results that are obtained on the basis of the effective law with the numerical results that are obtained (through a costly calculation) with the microscopic law. For this purpose, we choose some test problems, and make two computations, one with the macroscopic model, one with the microscopic model (by using a very fine finite element mesh). Numerical results are given in Section 4.

In this study, we have worked in 2.5D, that is to say we just simulate a 2D layer of the polycrystal, and the displacement is a function from $\mathbb{R}^3$ to $\mathbb{R}^3$ but its dependence with respect to the third space variable is *a priori* specified up to a few number of parameters. Strain and stress tensors are 3×3 tensors, but on the top and bottom faces of the layer, we impose that the normal stress $\sigma \cdot n$ be zero (n is the normal vector to the layer). We can thus work with 3D tensors whereas the geometry is 2D.

2   The microscopic model

As mentioned above, a polycrystal is a set of a large number of perfectly-bonded single-crystal grains [1] (see Fig. 1), which occupies the region Ω.

We will only consider polycrystals made of grains of isotropic shape (there is no special direction in the grain shape). Each grain is characterized by its orientation, which will be detailed in the following. For the materials we deal with, the characteristic size of a grain is 5.10^{-6} m, which is much larger than the atomic scale (10^{-10} m). The stress-strain relation inside a grain just depends on its orientation, and the heterogeneity in the polycrystal comes from the fact that this orientation is not the same from one grain to another one.
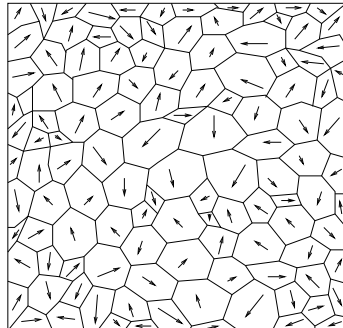

Fig. 1. Internal structure of a polycrystal (the arrow is a symbol for the orientation inside each grain).

The materials we deal with are metals which have an hexagonal atomic lattice (see Fig. 2). The orientation of the lattice is not uniform in the polycrystal. By definition, a *grain* is a domain of the polycrystal in which the orientation stays constant. The large size of a grain with respect to the atomic scale makes it possible to use a continuum model to describe the constitutive relation inside a grain. At this scale, the stress tensor is $\sigma_\mu(x,t)$, the displacement is $u_\mu(x,t)$ and the strain tensor $\varepsilon_\mu(x,t)$ is linked to the displacement by the linearized compatibility equation (2). We do not include in our model any grain interface properties, and we only suppose that the displacement and the normal stress are continuous at the grain interfaces (we recall that the normal stress is $\sigma(x) \cdot n(x)$, where σ is the stress tensor and n is the normal vector to the grain interface).

We suppose in the following that for all grains, the *basal plane* of the atomic lattice (see Fig. 2) is the same, namely the (e_x, e_y) plane. So, the orientation of the grain is defined by an angle between 0 and $\pi/6$. We also make the assumption that the orientations of the grains occur with equal probability (there are actually very few experimental data for the metals we deal with, so this assumption is the most sensible one). In Fig. 3, we draw the atomic lattice of two different grains, with two different orientations.

Let us now write the stress-strain relation inside a grain. In the metal we study, there are 12 preferred *slipping systems* that one knows as soon as the lattice orientation is known. These systems are defined by the plane in which the slip takes place (the normal direction to this plane is denoted by n_s), and
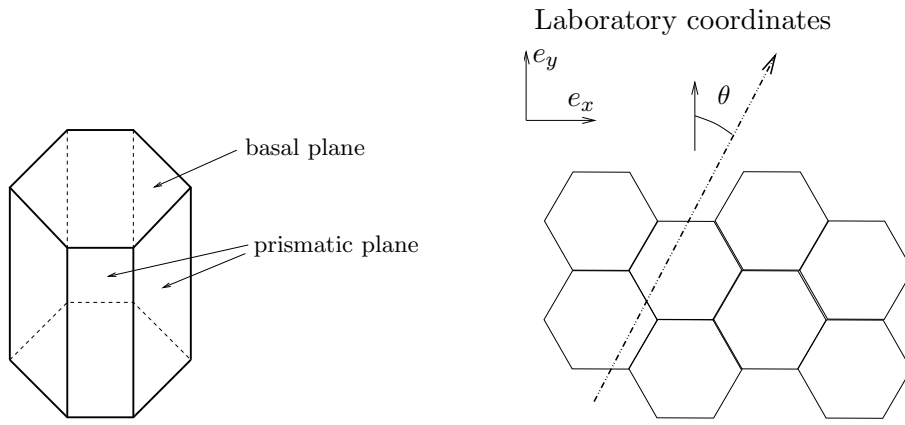
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Fig. 2. Atomic lattice inside a grain: 3D unit cell (left), 2D section along the basal plane inside a grain (right).
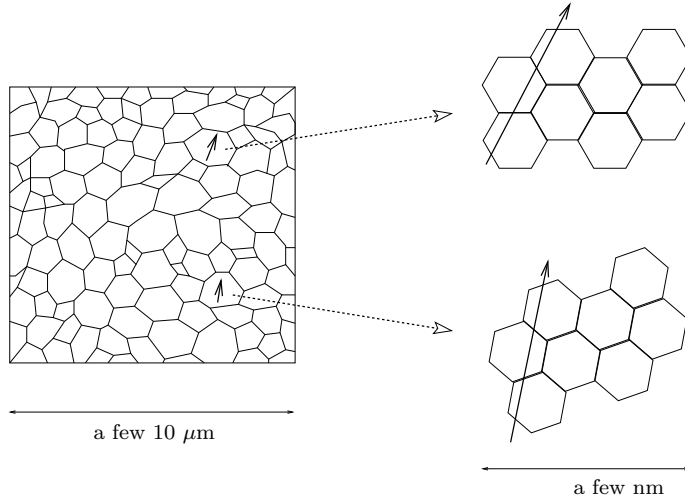

Fig. 3. Two grains with different orientations inside the polycrystal.

by the slipping direction l_s. Here, the vectors $n_s(x)$ and $l_s(x)$ depend on the space variable x, as they change from one grain to another one. In this article, we want to work in a 2D geometry in the (e_x, e_y) plane, so we only take into account the 3 systems for which the vectors $n_s(x)$ and $l_s(x)$ belong to the (e_x, e_y) plane (see Fig. 4).
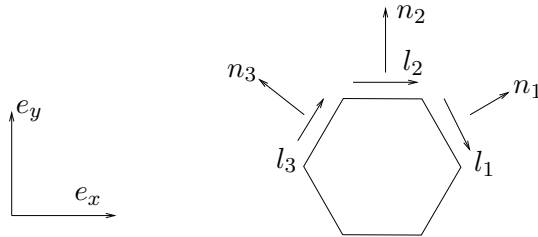

Fig. 4. The 3 slipping systems we take into account in a grain.

Knowing the slipping systems, one can compute the *orientation tensors $m_s(x)$*,

which are defined by

$$m_s(x) = \frac{1}{2} \left(n_s(x) \otimes l_s(x) + l_s(x) \otimes n_s(x) \right). \tag{5}$$

The intensity of the stress in the slipping direction is the so-called "resolved shear stress", which is given by $\sigma_\mu : m_s$.

The strain rate tensor $\dot{\varepsilon}_\mu$ is the sum of two terms, the *elastic strain rate tensor* $\dot{\varepsilon}_\mu^e$ and the *viscoplastic strain rate tensor* $\dot{\varepsilon}_\mu^{vp}$. The elastic term is given by the linear Hooke law

$$\varepsilon_\mu^e(x,t) = \Lambda : \sigma_\mu(x,t).$$

We do not include in our model any nonlinear elastic effects, for they are small in comparison to the efforts we account for. We suppose that the elastic characteristics are homogeneous in the polycrystal, so the fourth order tensor Λ does not depend on x. We also suppose that this elastic term is isotropic. Using the Young modulus E and the Poisson ratio ν, the elastic term reads

$$\varepsilon_\mu^e(x,t) = \frac{1+\nu}{E} \, \sigma_\mu(x,t) - \left(\frac{\nu}{E} \operatorname{tr} \sigma_\mu(x,t) \right) \, I, \tag{6}$$

where I is the identity 3×3 tensor. On the other hand, we assume the viscoplastic term to be of a power-law type

$$\dot{\varepsilon}_\mu^{vp}(x,t) = \sum_{s=1}^{3} \left(\frac{| \, \sigma_\mu(x,t) : m_s(x) \, |}{K_\mu} \right)^n \operatorname{sign} \left(\sigma_\mu(x,t) : m_s(x) \right) \, m_s(x). \tag{7}$$

The viscoplastic strain rate tensor $\dot{\varepsilon}_\mu^{vp}$ is a linear combination of the orientation tensors m_s, with coefficients depending on the resolved shear stress. We make the assumption that the parameters n and K_μ of the power-law are the same for all the grains. So, as mentioned above, the heterogeneity from one grain to another one just comes from the fact that the orientation tensors $m_s(x)$ are not the same.

So, the constitutive relation inside a grain reads

$$\dot{\varepsilon}_\mu(x,t) = \dot{\varepsilon}_\mu^e(x,t) + \dot{\varepsilon}_\mu^{vp}(x,t). \tag{8}$$

Recasting (8) in the form of (4), we see that, in our case, the microscopic

stress potentials (introduced in (4)) read

$$U_\mu^e(\dot{\sigma}_\mu) = \frac{1}{2}\dot{\sigma}_\mu \cdot \Lambda \cdot \dot{\sigma}_\mu,$$

$$U_\mu^{vp}(x, \sigma_\mu) = \frac{1}{n+1}\left(\frac{1}{K_\mu}\right)^n \sum_{s=1}^{3} |\sigma_\mu : m_s(x)|^{n+1}.$$

(9)

Solving the microscopic model consists in searching for the displacement field $u_\mu(x,t)$ solution to the equilibrium equation

$$\forall x \in \Omega, \ \forall t \in [0, T], \qquad \text{div}\,\sigma_\mu(x, t) = 0, \tag{10}$$

along with the constitutive laws (6 - 7 - 8), the compatibility equation (2), and convenient initial and boundary conditions.

Quantitatively, we use the following numerical values:

$$E = 105\,000 \text{ MPa}, \qquad \nu = 0.43, \qquad K_\mu = 178 \text{ MPa}, \qquad n = 6.5$$

3 The homogenization procedure

In Section 3.1, we first briefly recall the classical homogenization procedure [11] used in the stationary case when the stress-strain relation can be written by using a single potential. Next, we detail some time-dependent cases for which we can use this procedure: these are the quasistatic cases. Finally, in Section 3.3 , we use the procedure to determine the analytical expression, up to some parameters, of the effective behaviour of the polycrystal. Henceforth, there are no body forces.

3.1 Classical homogenization procedure

Let us consider an hyperelastic material (see Section 1) in the stationary case, described by an heterogeneous microscopic stress potential $U_\mu(x, \sigma_\mu)$. The constitutive law is given by

$$\varepsilon(x) = \frac{\partial U}{\partial \sigma}(x, \sigma(x)). \tag{11}$$

We suppose that U_μ is strictly convex of σ_μ. The microscopic *deformation potential* $W_\mu(x, \varepsilon_\mu)$ is defined as the Legendre transform of U_μ with respect to

σ_μ (let us note that U_μ is convex of σ_μ):

$$W_\mu(x, \varepsilon_\mu) = \sup_{\sigma_\mu}\ \sigma_\mu : \varepsilon_\mu - U_\mu(x, \sigma_\mu).$$

As U_μ is strictly convex of σ_μ, the potential $W_\mu(x, \varepsilon_\mu)$ is strictly convex of ε_μ. The constitutive law (11) can be recast into

$$\sigma_\mu(x) = \frac{\partial W_\mu}{\partial \varepsilon_\mu}(x, \varepsilon_\mu(x)). \tag{12}$$

We can first work with the displacement as the unknown. The energy of the material as a function of the displacement is given by

$$E(u_\mu) = \int_\Omega W_\mu(x, \varepsilon_\mu(x))\, dx, \tag{13}$$

where the strain tensor ε_μ is defined from the displacement field u_μ by (2). As $W_\mu(x, \varepsilon_\mu)$ is strictly convex of ε_μ, the energy $E(u_\mu)$ is strictly convex of u_μ. The displacement at equilibrium, under given displacement u^0 at the boundary $\partial\Omega$, is the solution of the minimization problem

$$\inf\ \left\{ E(u_\mu), \quad \forall x \in \partial\Omega \ \ u_\mu(x) = u^0(x) \right\}. \tag{14}$$

Let us now define the so-called *effective deformation potential* W_M. For a given symmetric constant tensor ε_M, $W_M(\varepsilon_M)$ is defined by

$$W_M(\varepsilon_M) = \inf_{\varepsilon_\mu(x)\ \in\ K(\varepsilon_M)} \langle\, W_\mu(x, \varepsilon_\mu(x))\,\rangle, \tag{15}$$

where $\langle\,\cdot\,\rangle$ is the average over Ω and the minimization space is defined by

$$K(\varepsilon_M) = \left\{ \begin{array}{l} \varepsilon_\mu(x)\,;\ \exists\, u_\mu(x) \text{ satisfying (2) in } \Omega \\[4pt] \text{and } u_\mu(x) = \varepsilon_M \cdot x \text{ on } \partial\Omega \end{array} \right\}.$$

Note that, as a consequence of (2), all strain tensors ε_μ in $K(\varepsilon_M)$ satisfy $\langle\, \varepsilon_\mu(x)\,\rangle = \varepsilon_M$.

We thus look at the equilibrium of the material with special displacement boundary conditions. Let $\bar\varepsilon_\mu(x)$ be the minimizer of problem (15). The microscopic stress field at equilibrium is (see (12))

$$\bar\sigma_\mu(x) = \frac{\partial W_\mu}{\partial \varepsilon_\mu}(x, \bar\varepsilon_\mu(x)).$$

The effective strain and stress tensors are defined as the average over Ω of the microscopic tensors. We have already noticed that the effective strain tensor is ε_M. We set $\sigma_M = \langle \overline{\sigma}_\mu(x) \rangle$. One can show that the effective tensors and the effective potential are linked by

$$\sigma_M = \frac{\partial W_M}{\partial \varepsilon_M}(\varepsilon_M). \tag{16}$$

For completeness, let us mention that there are other ways to define an effective potential. We have so far worked with the deformation potential $W_\mu(x, \varepsilon_\mu)$, we may alternatively work with the stress potential $U_\mu(x, \sigma_\mu)$, the stress field being the unknown. The energy of the material as a function of the stress tensor is given by

$$E^*(\sigma_\mu) = \int_\Omega U_\mu(x, \sigma_\mu(x))\, dx,$$

and the stress at equilibrium, under given surfacic force T^0 at the boundary $\partial\Omega$, is the solution of the minimization problem

$$\inf \left\{ E^*(\sigma_\mu), \quad \text{div } \sigma_\mu = 0 \text{ on } \Omega, \quad \sigma_\mu(x) \cdot n(x) = T^0(x) \text{ on } \partial\Omega \right\}.$$

The so-called *effective stress potential* U_M is defined by

$$U_M(\sigma_M) = \inf_{\sigma_\mu(x) \in S(\sigma_M)} \langle U_\mu(x, \sigma_\mu(x)) \rangle, \tag{17}$$

where σ_M is a given symmetric constant tensor, and where the minimization space is defined by

$$S(\sigma_M) = \left\{ \begin{array}{c} \sigma_\mu(x)\, ;\, \sigma_\mu(x) \cdot n(x) = \sigma_M \cdot n(x) \text{ on } \partial\Omega \\ \text{and } \text{div } \sigma_\mu = 0 \text{ in } \Omega \end{array} \right\}.$$

We thus look at the equilibrium of the material with special surfacic force boundary conditions. Let $\overline{\sigma}_\mu(x)$ be the minimizer of problem (17). The microscopic strain field at equilibrium is (see (11))

$$\overline{\varepsilon}_\mu(x) = \frac{\partial U_\mu}{\partial \sigma_\mu}(x, \overline{\sigma}_\mu(x)).$$

Again, effective tensors are defined as averages over Ω of microscopic tensors. All stress tensors $\sigma_\mu(x)$ in $S(\sigma_M)$ satisfy $\langle \sigma_\mu(x) \rangle = \sigma_M$, so the effective stress

tensor is σ_M. We set $\varepsilon_M = \langle \bar{\varepsilon}_\mu(x) \rangle$. As in the first case, one can show that the effective tensors and the effective potential are linked by

$$\varepsilon_M = \frac{\partial U_M}{\partial \sigma_M}(\sigma_M).$$

One says that the material follows an *effective stress-strain relation* if the effective stress potential U_M defined by (17) is the Legendre transform, with respect to the macroscopic strain tensor ε_M, of the effective deformation potential W_M defined by (15).

3.2 Homogenization procedure in some time-dependent cases

The homogenization procedure we have just recalled is based on calculus of variations. No quantity depends on time. In this section, we detail some time-dependent cases for which we can still use the same procedure.

We consider the same hyperelastic material as previously, described by the convex microscopic deformation potential $W_\mu(x, \varepsilon_\mu)$: its constitutive law is

$$\sigma_\mu(x, t) = \frac{\partial W_\mu}{\partial \varepsilon_\mu}(x, \varepsilon_\mu(x, t)). \tag{18}$$

Let $\rho(x)$ be the mass density of the material. We suppose that the material is subjected to a given time-dependent displacement $u^0(x, t)$ at the boundary $\partial\Omega$. The dynamics is ruled by

$$\forall x \in \Omega, \ \forall t \in [0, T], \qquad \rho(x)\, \partial_{tt} u_\mu(x, t) = \operatorname{div} \sigma_\mu(x, t),$$

along with the constitutive law (18), the compatibility equation (2), the boundary conditions $u_\mu(x, t) = u^0(x, t)$ on $\partial\Omega$ for all $t \in [0, T]$, and convenient initial conditions.

We make the approximation that the problem is quasistatic: we can neglect the acceleration $\rho\, \partial_{tt} u_\mu$, which is small compared to the internal forces. Thus, the system to solve becomes

$$\forall x \in \Omega, \ \forall t \in [0, T], \qquad \operatorname{div} \sigma_\mu(x, t) = 0, \tag{19}$$

along with (2), (18) and the same boundary conditions as previously. The unknown is $u_\mu(x, t)$. At a given time t, this system is exactly the Euler-Lagrange

equation of the problem

$$\inf \left\{ E(u_\mu), \quad \forall x \in \partial\Omega \;\; u_\mu(x) = u^0(x,t) \right\},$$

with $E(u_\mu)$ defined by (13). Since W_μ is convex, solving (19) is equivalent to solving the previous variational problems for all $t \in [0, T]$.

In this case (working with an hyperelastic material and in the quasistatic regime), we can still define an effective deformation potential and an effective stress potential, which are again given by (15) and (17). The material follows an effective stress-strain relation if these two effective potentials are the Legendre transform one of each other.

3.3 Homogenization of the polycrystal law

We now proceed to the homogenization of the polycrystal model presented in Section 2. Constitutive laws are (6 - 7 - 8), corresponding potentials are defined by (9), and the equilibrium equation is (10). When writting this equation, we have neglected the acceleration. As two potentials are involved, and as the constitutive law is time-dependent (it involves an ODE), we cannot directly use the theory we have just recalled. However, we can apply the theory separately on the elastic stress potential and on the viscoplastic stress potential. Indeed, if we only consider one potential, we are in the quasistatic setting detailed in Section 3.2. Actually, the procedure is immediate for the elastic potential as elastic properties are homogeneous in the polycrystal (the tensor Λ does not depend on x). We thus focus on the viscoplastic stress potential. To simplify the notation, let $d_\mu = \dot{\varepsilon}_\mu^{vp}$ denote the microscopic viscoplastic strain rate tensor.

3.3.1 The viscoplastic term

We first note that, because of their definition (see (5)), the orientation tensors m_s have the following very particular expression

$$m_s = \begin{pmatrix} u_s & v_s & 0 \\ v_s & -u_s & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The same form also holds for d_μ, which therefore only depends on two scalar variables, d_μ^{xx} and d_μ^{xy}. We also check that, for any symmetric microscopic

stress tensor σ_μ, we have

$$\sigma_\mu(x) : m_s(x) = \alpha_\mu(x)u_s(x) + \beta_\mu(x)v_s(x),$$

where we set

$$\alpha_\mu = \sigma_\mu^{xx} - \sigma_\mu^{yy} \quad \text{and} \quad \beta_\mu = 2\,\sigma_\mu^{xy}.$$

So the only variables to consider are d_μ^{xx}, d_μ^{xy}, α_μ and β_μ. The potential $U_\mu^{vp}(x, \sigma_\mu)$ that we introduced in (9) is not strictly convex of σ_μ, but if we rewrite it in terms of (α_μ, β_μ),

$$U_\mu^{vp}(x, \alpha_\mu, \beta_\mu) = \frac{1}{n+1} \left(\frac{1}{K_\mu}\right)^n \sum_{s=1}^{3} |\,\alpha_\mu u_s(x) + \beta_\mu v_s(x)\,|^{n+1},$$

it turns out to be a convex function of (α_μ, β_μ), and (7) can be recast into

$$d_\mu^{xx} = \frac{\partial U_\mu^{vp}}{\partial \alpha_\mu} \quad \text{and} \quad d_\mu^{xy} = \frac{\partial U_\mu^{vp}}{\partial \beta_\mu}.$$

Let $W_\mu^{vp}(x, d_\mu^{xx}, d_\mu^{xy})$ be the Legendre transform of U_μ^{vp} with respect to (α_μ, β_μ). It holds that

$$\alpha_\mu = \frac{\partial W_\mu^{vp}}{\partial d_\mu^{xx}} \quad \text{and} \quad \beta_\mu = \frac{\partial W_\mu^{vp}}{\partial d_\mu^{xy}}.$$

As U_μ^{vp} is homogeneous of degree $n+1$ of the pair (α_μ, β_μ), the potential W_μ^{vp} is homogeneous of degree $1 + 1/n$ of the pair (d_μ^{xx}, d_μ^{xy}).

We now turn to the derivation of an effective model. Following the general procedure recalled in Section 3.2, we define the effective potential W_M^{vp} by

$$W_M^{vp}(d_M^{xx}, d_M^{xy}) = \inf_{(d_\mu^{xx}, d_\mu^{xy}) \,\in\, K(d_M^{xx}, d_M^{xy})} \langle\, W_\mu^{vp}(x, d_\mu^{xx}, d_\mu^{xy})\,\rangle,$$

where $K(d_M^{xx}, d_M^{xy})$ is defined by

$$K(d_M^{xx}, d_M^{xy}) = \left\{ \begin{array}{l} (d_\mu^{xx}(x), d_\mu^{xy}(x)) \,;\; \exists\, u_\mu(x) \text{ such that } u_\mu(x) = \gamma(d_M^{xx}, d_M^{xy}) \cdot x \\[1.5em] \text{on } \partial\Omega \text{ and } \dfrac{1}{2}\left(\nabla u_\mu + {}^t\nabla u_\mu\right) = \gamma(d_\mu^{xx}(x), d_\mu^{xy}(x)) \text{ in } \Omega \end{array} \right\},$$

the function γ being defined by

$$\gamma : (u, v) \in \mathbb{R}^2 \mapsto \begin{pmatrix} u & v & 0 \\ v & -u & 0 \\ 0 & 0 & 0 \end{pmatrix} \in \mathcal{M}_3(\mathbb{R}).$$

Just as (16) holds, it holds that

$$\alpha_M = \sigma_M^{xx} - \sigma_M^{yy} = \frac{\partial W_M^{vp}}{\partial d_M^{xx}},$$

$$\beta_M = 2\sigma_M^{xy} = \frac{\partial W_M^{vp}}{\partial d_M^{xy}}. \tag{20}$$

The macroscopic potential W_M^{vp} is homogeneous of degree $1 + 1/n$ of (d_M^{xx}, d_M^{xy}). To use this fact, we need to change of variables: instead of working with the cartesian variables d_M^{xx} and d_M^{xy}, let us work with the polar coordinates associated to them, the radius

$$R_M = \sqrt{(d_M^{xx})^2 + (d_M^{xy})^2}$$

and the angle θ_M. These variables present the advantage that R_M is homogeneous of degree 1 of (d_M^{xx}, d_M^{xy}), whereas θ_M is homogeneous of degree 0. So W_M^{vp} reads

$$W_M^{vp}(R_M, \theta_M) = R_M^{1+1/n} C(\theta_M),$$

where C is an unknown function.

As this point, we introduce the following simplification. Considering that, first, all the orientations of the grains occur with equal probability, and second, that the geometry of the grains and of the polycrystal is isotropic, we postulate, without any rigorous justification of this fact, that the response of the polycrystal is isotropic, at least when the number of grains is large enough. We therefore simplify the previous expression of W_M^{vp}, setting $C(\theta_M)$ as an (unknown) constant C, for θ_M is an anisotropic variable whereas R_M is

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an isotropic variable. Writting (d_M^{xx}, d_M^{xy}) as a function of (α_M, β_M), we get

$$d_M^{xx} = C \left(\sqrt{\alpha_M^2 + \beta_M^2} \right)^{n-1} \alpha_M,$$

$$d_M^{xy} = C \left(\sqrt{\alpha_M^2 + \beta_M^2} \right)^{n-1} \beta_M.$$

(21)

To agree with a usual normalization, we prefer to recast these equations into a slightly different expression. We set

$$J(\sigma_M) = \sqrt{\frac{3}{2}} \sqrt{(\tilde{\sigma}_M^{xx})^2 + (\tilde{\sigma}_M^{yy})^2 - \frac{1}{2} (\tilde{\sigma}_M^{zz})^2 + 2 (\sigma_M^{xy})^2}, \qquad (22)$$

where $\tilde{\sigma}_M = \sigma_M - \left(\frac{1}{3} \mathrm{tr}\, \sigma_M \right) 1$ is the *deviatoric part* of σ_M. Then equations (21) can be written as

$$\dot{\varepsilon}_M^{vp} = \left(\frac{J(\sigma_M)}{K_M} \right)^n \frac{\partial J}{\partial \sigma_M}, \qquad (23)$$

where K_M is an unknown parameter (playing the role of the constant C used above) that we will determine by numerical computations in Section 4.

3.3.2 Postulated macroscopic model for the polycrystal

In the previous part, we have made use of the classical homogenization procedure to obtain separately an elastic effective potential and a viscoplastic effective potential. We postulate, again without any rigorous justification of this fact, that the effective constitutive law for the polycrystal is the sum of the elastic effective term with the viscoplastic effective term. So the effective constitutive law that we use is

$$\dot{\varepsilon}_M(x,t) = \Lambda : \dot{\sigma}_M(x,t) + \left(\frac{J(\sigma_M(x,t))}{K_M} \right)^n \frac{\partial J}{\partial \sigma_M}, \qquad (24)$$

where J is defined by (22). Solving the effective model consists in searching for the displacement field $u_M(x,t)$ solution to the equilibrium equation

$$\forall x \in \Omega, \ \forall t \in [0,T], \qquad \mathrm{div}\, \sigma_M(x,t) = 0, \qquad (25)$$

along with the constitutive law (24), the compatibility equation (2), and convenient initial and boundary conditions.

The whole microscopic constitutive law involves an ODE, and the procedures detailed in Section 3.1 and 3.2 do not apply in this case. With the numerical tests described in the following, we check whether this approximation may be sensible.

4 Numerical results

In the previous part, working with the deformation potential, we have found an effective model for the polycrystal, *up to the knowledge of the constant K_M* (see (24)). In order to determine a value for K_M, we use numerical computations on different polycrystals [2,5], with several linear displacement boundary conditions. In the following, we check that there exists a single value for K_M such that macroscopic computations agree with microscopic computations for all test problems (that is, macroscopic tensors are equal to the mean of microscopic tensors over the polycrystal Ω).

One can also work with the microscopic stress potential to obtain an effective stress potential. One finds the same result as in (23), with a *a priori* different constant K_M^s. To numerically determine a value for K_M^s, one would follow the same procedure as before, except that one would work with linear surfacic force boundary conditions. If the value found for K_M^s is the same as the value found for K_M (with linear displacement boundary conditions), then the effective stress potential is the Legendre transform of the effective deformation potential, and the polycrystal actually obeys an effective stress-strain relation (see Section 3.2). We did not made this kind of test, since, when one uses surfacic force boundary conditions, the displacement at equilibrium is only determined up to a rigid body motion.

Finally, a third test is possible: one can use mixed boundary conditions (we impose on some part on the boundary the displacement and elsewhere the normal stress). Results of this kind of test are given in the following. The polycrystal actually obeys an effective stress-strain relation if the value previously found for K_M (using linear displacement boundary conditions) is also valid with these mixed boundary conditions.

We have performed numerical tests with three different polycrystals, one of 30 grains (first with a coarse mesh: 5 to 15 finite elements per grain; then with a finer mesh: finite element edges two times smaller), and two of 110 grains (the same grain geometry, but with two different orientation samples). We work in 2.5D (see Section 1), just simulating a 2D layer of the polycrystal of side surface $\mathcal{S}$ (see Fig. 5).
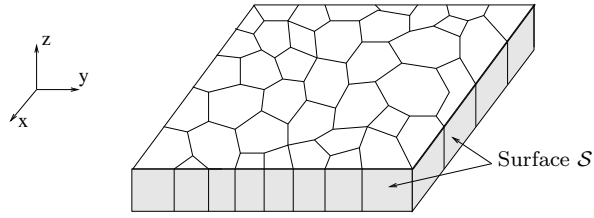
Fig. 5. Only a 2D layer of the polycrystal is simulated.

On the surface $\mathcal{S}$, we choose several different boundary conditions: linear displacement boundary conditions (*traction compression*, thus a strain denoted by a superscript TC; *shear*, a strain denoted S; *traction compression shear*, a strain denoted TCS), and also *mixed boundary conditions*, letting two opposite faces force free, imposing zero normal displacement on one face, and imposing a uniform traction displacement rate on the last face (test denoted T). For displacement boundary conditions, the strain tensors are

$$\varepsilon_M^{TC}(t) = \begin{pmatrix} \alpha\,t & 0 & 0 \\ 0 & -\alpha\,t & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \varepsilon_M^{S}(t) = \begin{pmatrix} 0 & \alpha\,t & 0 \\ \alpha\,t & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

and

$$\varepsilon_M^{TCS}(t) = \begin{pmatrix} \alpha_1\,t & \alpha_2\,t & 0 \\ \alpha_2\,t & -\alpha_1\,t & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

For brevity, we only detail here one test case, namely that of a polycrystal subjected to a shear load. The averaged microscopic strain tensor and the macroscopic strain tensor increase linearly as time increases. One can see on Fig. 6 the averaged microscopic stress $\langle\,\sigma_\mu(x,t)\,\rangle$ as a function of time (we have $\langle\,\sigma_\mu^{yy}\,\rangle = -\langle\,\sigma_\mu^{xx}\,\rangle$ and $\sigma_\mu^{zx}(x,t) = \sigma_\mu^{zy}(x,t) = \sigma_\mu^{zz}(x,t) = 0$), and the macroscopic stress $\sigma_M(t)$, which is uniform in this case. We make the assumption that, in the long-time limit, the stress tensors $\sigma_\mu(x,t)$ and $\sigma_M(x,t)$ converge to a limit, which thus corresponds to the stationary regime of (8) and (24). One can check that the limit $\lim_{t\to\infty}\sigma_M^{xy}(t)$ depends on K_M (for this shear load test, an analytical expression can be found). We choose K_M so that

$$\lim_{t\to\infty}\sigma_M^{xy}(t) = \lim_{t\to\infty}\langle\,\sigma_\mu^{xy}(x,t)\,\rangle,$$

which leads in this case to the numerical value $K_M = 347$ MPa. The previous equation enforces that, in the long-time limit, the effective law is consistent

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with the microscopic law. The macroscopic stress displayed on Fig. 6 has been computed using this value of K_M. We also notice that $\sigma_M^{xx} = 0$, as expected. On the other hand, $\langle \sigma_\mu^{xx}(x,t) \rangle$ is not zero, however up to a small error.
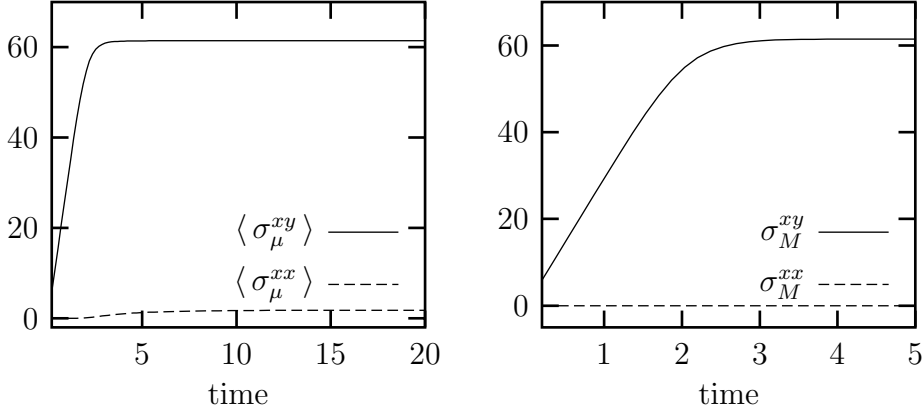

Fig. 6. Shear load on the 30 grain polycrystal: averaged microscopic stress (left), macroscopic stress (right).

For the other test problems, the situation is the same as the one we describe here. It is possible to find of value for K_M by adjusting the largest components of the stress and strain tensors (in the limit $t \to \infty$), and there is a small error on some components (xx and yy in shear load, xy in traction compression load). The values found for K_M are given in Tab. 1. We notice that, up to a 0.4 % error, the value depends neither on the type of boundary conditions, on the number of grains, on the mesh size nor on the orientation distribution sample. Thus the polycrystal obeys an effective constitutive law with $K_M = 346$ MPa.

	30 grains Coarse mesh	30 grains Fine mesh	110 grains Sample 1	110 grains Sample 2
T	345.6		347.1	
T C	345.6	345.6	347.1	345.3
S	347.25	347.25	344.6	344.6
TCS	346.1	346.0	346.62	345.4

Table 1
Values of K_M for different polycrystals with different loadings (the indicated value is the average on different boundary condition values).

In order to measure the error of the small components of the tensors with respect to the average value, we define some empiric estimators:

- for mixed boundary conditions, $\lim_{t \to \infty} \left(\langle \varepsilon_\mu^{xy} \rangle / \langle \varepsilon_\mu^{yy} \rangle \right)$;
- $\lim_{t \to \infty} \left(\langle \sigma_\mu^{xx} \rangle / \langle \sigma_\mu^{xy} \rangle \right)$ for shear load;
- for traction-compression load, $\lim_{t \to \infty} \left(\langle \sigma_\mu^{xy} \rangle / \langle \sigma_\mu^{yy} \rangle \right)$;

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- $\lim_{t\to\infty}\left(\langle\sigma_\mu^{xx}\pm\sigma_\mu^{xy}\rangle/\sigma_M^{xy}\right)$ for traction-compression-shear load, boundary conditions being so that $\lim_{t\to\infty}\sigma_M^{xx}\pm\sigma_M^{xy}=0$;

The values found for these estimators are given in Tab. 2. One can notice that all values are small, so the effective law is a good approximation of the microscopic model in most of the situations studied.

	30 grains Coarse mesh	30 grains Fine mesh	110 grains Sample 1	110 grains Sample 2
T	2%		0.9%	
T C	2.5%	2.5%	0.8%	1.2%
S	2.9%	2.9%	1.1%	1%
TCS	0.3%	0.3%	1.4%	1.3%

Table 2
Values of the error estimators for different polycrystals with different loadings.

It is also interesting to compute averages on grains of the stress or strain tensors, and not on the whole polycrystal. We want to know whether these averages are similar from one grain to another one, or very different. Let us focus on the traction-compression-shear load. At each time step, we compute, for each grain, the average over the grain of $(\varepsilon_\mu^{vp})^{yy}$ and of $\tilde{\sigma}_\mu^{yy}$ ($\tilde{\sigma}$ is the deviatoric part of σ). We work with the viscoplastic strain tensor and the deviatoric stress tensor since these are the natural variables for the viscoplastic term of the constitutive law. Results are displayed in Fig. 7. At the beginning, the averages for all grains are the same. As the viscoplastic term increases, grain responses become heterogeneous.
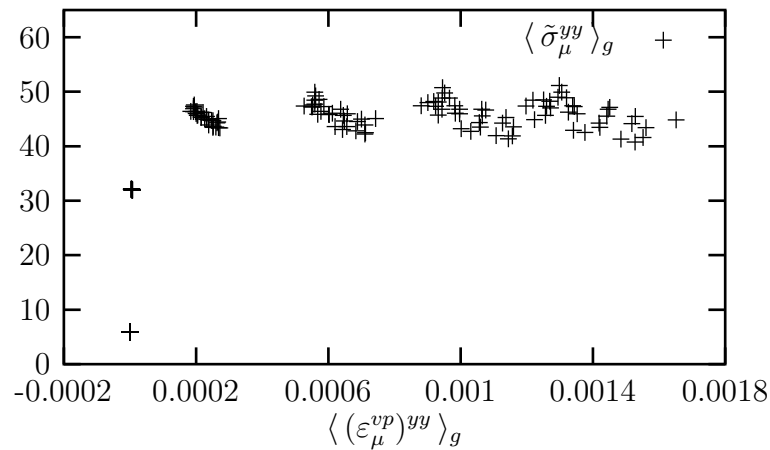

Fig. 7. Evolution of $\langle\tilde{\sigma}_\mu^{yy}\rangle_g$ as a function of $\langle(\varepsilon_\mu^{vp})^{yy}\rangle_g$ for the 30 grain polycrystal, traction-compression-shear load ($\langle\cdot\rangle_g$ is the average over the grain).

So far, we have just compared the responses in the limit $t\to\infty$ (in this

limit, the elastic part of the constitutive law cancels). We may also compare responses during the whole load process, to check whether microscopic and effective laws agree only in the viscoplastic limit or also when elastic and viscoplastic terms are of the same order of magnitude. We make such a comparison in Fig. 8. For the other test problems, the situation is alike: the effective law is in good agreement with the microscopic law (the difference is smaller than 1%).
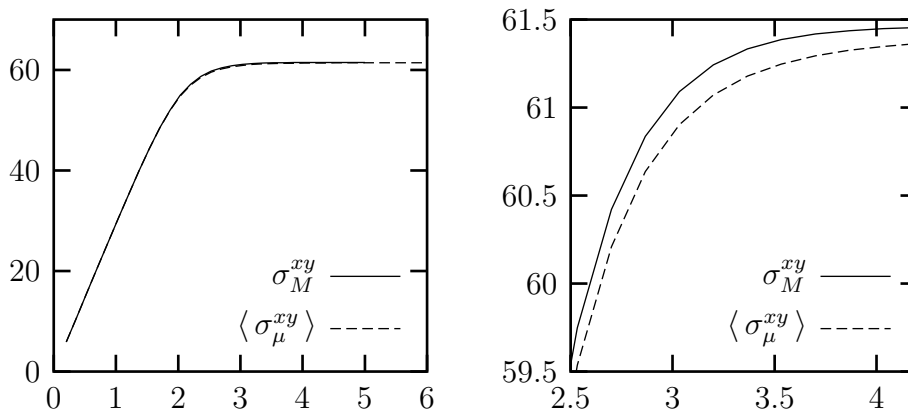

Fig. 8. Transient response of the 30 grain polycrystal, shear load. The effective law is in good agreement with the microscopic law (left). On the right-hand side, a zoom on the region where there are some differences.

This numerical result is very surprising. Starting from a microscopic constitutive law which is time-dependent and involves two potentials, we split it into two terms. We apply separately on each of them a procedure which is based on stationary calculus of variations. We fit K_M on the long-time limit of the system, which corresponds to the viscoplastic regime. The numerical result is that the effective law is in agreement with the microscopic one both in stationary and transient regime! We acknowledge the fact that there is no rigorous reason for this success: we just observe that the two laws are consistent.

5   Conclusions

We have dealt in this article with a simple model of a 2D heterogeneous elasto-viscoplastic polycrystal, for which no theoretical results on the effective law are available. We have succeeded in numerically identifying an effective law. We observe that this effective law is consistent with the microscopic law in both the stationary and transient regime, although it has been obtained by an homogenization procedure designed for stationary problems. We are unfortunately unable to provide any explanation for this fact but are currently working in that direction.

Acknowledgements

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