An inhomogeneous variational model applied to predict the behaviour of isotropic polycrystalline ice [1]

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A MODEL FOR THE PREDICTION of the viscoplastic behaviour of polycrystalline ice is presented. This model is based on the minimization of the dissipation energy under the principle of minimal heterogeneity. The grain is supposed to behave as a linear transversely isotropic medium depending on one anisotropy parameter. Anisotropic textures can be considered, but the present numerical results are for an isotropic texture. The model then predicts a linear isotropic behaviour involving an effective viscosity. The latter depends on the prescribed value for the strain-rate heterogeneity and on the grain anisotropy parameter. The present model is compared with a self-consistent model built under the same assumptions for the grain behaviour. The deviation from the no-correlation condition is studied.

1. Introduction

IN ORDER TO UNDERSTAND the evolution of the polar ice sheets and their response to climatic changes, it is necessary to build thermomechanical models of the flow of ice sheet under gravity. Due to the large depth, the internal layers of the sheet are subjected to very large compression strains that lead to the development of a strong crystallographic texture (or "fabric") in the polycrystalline ice. Moreover, the anisotropy of the constituent crystals is rather extreme: the rate of creep of a single crystal by basal glide is roughly 10^4 times faster, at a given stress, than that of a single crystal oriented such that the resolved shear stress on the basal plane is negligible [1]. The single crystal of ice deforms mainly by dislocation glide on the basal plane, normal to the hexagonal symmetry c−axis. This makes the textured polycrystal strongly anisotropic. As shown by MANGENEY *et al.* [2, 3], this macroscopic anisotropy must be accounted for in the mechanical model, because it strongly influences the flow of the sheet. But, since the macroscopic anisotropy is due to the texture development, hence to the flow itself, one should

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include the polycrystal texture and its evolution in the constitutive equation –
in other words, it seems that one should use a micro-macro approach for the
constitutive relation. One is then faced with the important computation cost
needed to implement a polycrystal model in a finite element code. For this reason,
a finite-element thermomechanical model of an ice sheet has been based on the
"static" model, that assumes a uniform stress in a volume element of polycrystal
[4]. The use of the static model for ice, as opposed to using the Taylor model that
assumes uniform strain-rate, was suggested by a comparison between "static" and
"self-consistent" predictions, due to CASTELNAU et al. [5].

It is, however, useful to first use the more complex and more exact models to
predict the constitutive relation and the texture evolution for a given deformation
history. This also has a short-term benefit, which is to assess the error involved
in using the simpler (static) model.

In the present paper, a recently proposed micro-macro model is used [6, 7].
It is based on a minimum problem with two constraints and allows a continuous
transition between the extreme models (Voigt-Taylor and "static"), see Sec. 3.1 for
a motivation of using that model. In the present work, the model is adapted to a
linear viscoplastic grain, which allows analytical developments (see Sec. 2). A new
numerical approach is used (see Sec. 3.4) to solve the minimization problem.

The numerical results of the present study are restricted to the prediction
of the effective potential of an isotropic polycrystal, i.e., a randomly textured
polycrystal is considered. However, the present implementation of the micro-
macro model allows also to consider textured polycrystals [8], as observed in ice
sheets.

2. Single crystal behaviour

Since the ice crystal is incompressible, both strain-rate and deviatoric stress
tensors can be expressed as vectors in a 5-D space, respectively $\mathbf{D}^g$ and $\mathbf{S}^g$ [9, 10].
Here we shall use the transformation proposed by LEQUEU et al. [10]:

$$(2.1) \qquad \mathbf{X} = [(X_{22} - X_{11})/\sqrt{2}, \sqrt{3/2}X_{33}, \sqrt{2}X_{23}, \sqrt{2}X_{31}, \sqrt{2}X_{12}].$$

Because the crystal of ice has an hexagonal symmetry axis, it is assumed
to behave as a transversely isotropic medium. At low temperature (lower than
$-10°C$) and for the deviatoric stress magnitude typical in polar ice (less than
0.05 MPa), there are some indications from data analysis for a behaviour close
to linear behaviour [11]. Therefore, following MEYSSONNIER and PHILIP [12], we
will assume in what follows that the ice crystal behaves as a linear transversely
isotropic medium.

In the case of power-law viscoplastic behaviour with rate-sensitivity m, the potential Φ_D^g giving the stress as function of the strain-rate is given by

$$(2.2) \qquad \Phi_D^g = W^g(\mathbf{D}^g)/(m+1),$$

where $W^g(\mathbf{D}^g)$ is the energy dissipation per unit volume and unit time due to the viscous deformation, defined as

$$(2.3) \qquad W^g = \mathbf{D}^g \cdot \mathbf{S}^g.$$

In the particular case of the linear behaviour envisaged here ($m = 1$), the energy dissipation is twice as much as the dissipation potential $\Phi_D^g(\mathbf{D}^g)$. The deviatoric stress derives from $\Phi_D^g(\mathbf{D}^g)$ as

$$(2.4) \qquad \mathbf{S}^g = \frac{\partial \Phi_D^g}{\partial \mathbf{D}^g}.$$

Since the grain is transversely isotropic, only the direction x_3 of its rotational symmetry axis needs to be defined in order to fixe the grain reference frame relative to the fixed global reference frame. This is done by using two angles, the co-latitude θ and the longitude φ. The simplest expression for the dissipation potential $\Phi_D^g(\mathbf{D}^g)$, when expressed in the grain reference frame with rotational symmetry axis along the x_3 direction, is given by

$$(2.5) \qquad \Phi_D^g = \frac{1}{2} W^g = \frac{\eta}{\beta} \left[D_1^{g2} + D_2^{g2} + \beta \left(D_3^{g2} + D_4^{g2} \right) + D_5^{g2} \right],$$

where η is the viscosity for shear in the planes perpendicular to the plane of isotropy (x_1, x_2) ($\eta = 1/\psi$ in [13, 14], because the inverse law was used in the latter works) and β is the ratio of the shear viscosity in the planes perpendicular to the basal plane to that in the basal plane. The parameter β should be regarded as a measure of the grain anisotropy: when $\beta = 0$ the grain can deform only by basal glide, while $\beta = 1$ corresponds to an isotropic grain.

In the global reference frame, the relation (2.4) becomes

$$(2.6) \qquad \mathbf{S}^g = \eta^g(\theta, \varphi) \mathbf{D}^g,$$

where η^g is a 6-D fourth order tensor, symmetric, and with the dimension of a viscosity. Its expression can be inferred from Eqs. (2.4), (2.5) and by using the rotation matrix to pass from the grain reference frame to the global reference frame.

3. Polycrystal behaviour

3.1. Motivation of the micro-macro model under consideration

A well-known approach to defining more accurate models than the extreme models is the self-consistent approach, initiated almost fifty years ago for lin-

early elastic aggregates by Hershey [15] and independently by Kröner [16]. These models start from the consideration of an ellipsoidal inclusion embedded in a space-filling matrix material, as envisaged by Eshelby [17, 18]: in the self-consistent model, the strain and stress in a given constituent are assumed to be the same as if that constituent were an ellipsoidal inclusion embedded in a space-filling matrix endowed with the effective macroscopic behaviour which is sought. A specific feature of Eshelby's exact solution to the problem of the linear elastic inclusion [18] is the fact that the inclusion undergoes a uniform strain state, hence also a uniform stress state. If one considers, not an ellipsoidal inclusion in a homogeneous matrix, but instead an aggregate of arbitrarily-shaped constituents, it is in practice impossible that any constituent may undergo a uniform strain state. Indeed it is easy to prove the following result [19]: If the strain-rate field has the uniform value $\mathbf{D}$ in the domain Ω and the uniform value $\mathbf{D}'$ in the contiguous domain Ω', and if the boundary between Ω and Ω' is not plane, then the strain-rate field can be derived from a continuous velocity field only if $\mathbf{L} = \mathbf{L}'$, where $\mathbf{L}$ and $\mathbf{L}'$ are the (necessarily uniform) values of the velocity gradient in Ω and Ω' (thus, not merely the strain-rates but also the rotation rates must be the same in Ω and Ω'). This result holds true, of course, if one substitutes "small-strain tensor" for "strain-rate tensor", and "displacement" for "velocity". It means that the strain-rate tensors $\mathbf{D}^1, ..., \mathbf{D}^N$, which are predicted in the constituents $\Omega^1, ..., \Omega^N$ of some aggregate, e.g. by a self-consistent model, have to be interpreted as volume averages of the strain-rate field in the different constituents. Accepting this interpretation for the predicted distribution $(\mathbf{L}^k)_{k=1,...,N}$ of the velocity gradient, then the "compatibility problem" may always be solved, in the sense that, given any (reasonable or unreasonable) distribution $(\mathbf{L}^k)_{k=1,...,N}$, it is always possible to construct a regular velocity field $\mathbf{V}$ such that, for all k, the volume average of grad $\mathbf{V}$ in domain Ω^k is $\mathbf{L}^k$ [19]. Thus no model can be preferred to another one as regards the compatibility problem for the strain distribution – except, of course for the Voigt-Taylor model: but, for the latter, the incompatibility is found in the stress distribution. In the same way, one should be able to show that the compatibility problem may always be solved for the stress distribution in the sense of the volume average.

Furthermore, the self-consistent model provides a particular solution between the extreme models of Voigt (assuming uniform strain) and of Reuss (assuming uniform stress; when extended to non-linear behaviour, this is also called the "static model"). As found by Kröner [20], the self-consistent model for a linearly elastic aggregate is likely to correspond to the ideal statistical situation called "perfect disorder", in which knowledge of the volume fractions of the different constituents in the aggregate is sufficient to determine the effective macroscopic behaviour, due to the vanishing of all higher-order correlations. It is unlikely that this ideal situation could always be representative for real materials. In

the present paper, it will be shown that, for an isotropic aggregate of linearly viscous ice crystals, the self-consistent solution is indeed not very close to the likely effective behaviour.

Finally, following Kröner [21], various extensions of the self-consistent model have been proposed for the non-linear constitutive relations that describe elasto-plastic, viscoplastic or other behaviours. These extensions use different kinds of linearizations of the constitutive relations of the constituent phases. As shown by Gilormini [22], the most classical extension, based on an incremental linearization due to Hill [23], exceeds the tighter upper bound derived by Ponte Castañeda [24] (more precisely, this has been shown for an isotropic two-phase aggregate of incompressible power-law elastic spheres [22]. This shortcoming of the classical extensions of the self-consistent model will not be relevant in the present paper, however, because a linearly viscous behaviour will be assumed on experimental grounds).

Despite the foregoing arguments, it is acknowleged, of course, that the self-consistent approach has proved very useful in providing many micro-macro models capable of capturing observed features in real heterogeneous materials [25, 26, 27, 28]. But these arguments add appeal to a different model, namely the "inhomogeneous variational model" [6, 7]: *i*) This model is based on a rigorous statistical framework and accounts explicitly for the fact that distributions only of the volume averages of the stress and strain in the different constituents are sought [6]. *ii*) It leads to a continuous transition between the two extreme (Voigt-Taylor and "static") models. *iii*) It makes no use of any linearization nor any perturbation treatment, and it applies to any behaviour that derives from a convex potential. Thus it is likely to be appropriate for the modelling of strongly heterogeneous materials (as is polycrystalline ice), for which perturbation techniques do not seem to be best suited. These advantages must have a price, and this is the fact that the heterogeneity parameter r, allowing the continuous transition between the extreme bounds (see Sec. 3.2), cannot be predicted from microstructural information and instead must be phenomenologically adjusted. This does not prevent the model from exhibiting a predictive capacity, however: this has been verified already for deformation textures in steels [7] and for the overall behaviour of fiber-reinforced composites [29].

3.2. Formulation of the micro-macro model under consideration

The micro-macro model formulated by Arminjon and Imbault [7] is based on the minimization of the average potential under the principle of minimal heterogeneity. Because of the viscoplastic linear behaviour, it is equivalent here to consider the energy dissipation W instead of the potential Φ_D. Let us first introduce some general definitions that are useful for the presentation of the

model. In the following, the polycrystal is assumed to be made of N constituents. Each constituent (k) $(k = 1, .., N)$ occupies the spatial domain Ω_k where the crystal orientation has some given value (θ_k, φ_k). Note that Ω_k is in general not a connected domain, i.e., the zone with given orientation is in several pieces. The texture is described in the global reference frame by the set of the orientations (θ_k, φ_k) and the associated volume fractions f_k. When some quantity Y^k is defined for each constituent (k), we shall denote the weighted average of the distribution $(Y^k)_{k=1,..,N}$ by:

$$(3.1) \qquad Y^{\mathrm{av}} = \langle Y^k \rangle = \sum_{k=1}^{N} f_k Y^k .$$

The average heterogeneity function h of some distribution (strain-rate, stress) $(\mathbf{Y}^k)_{k=1,..,N}$ around the macroscopic quantity $\mathbf{Y}$ is defined as

$$(3.2) \qquad h((\mathbf{Y}^k)) = \left[\sum_{k=1}^{N} f_k |\mathbf{Y}^k - \mathbf{Y}^{\mathrm{av}}|^2 \right]^{1/2} ,$$

where $|\mathbf{Y}| = [\mathrm{tr}\mathbf{Y}^2]^{1/2} = [Y_i Y_i]^{1/2}$.

This micro-macro model consists in determining the distribution of the average strain-rates $\mathbf{D}^k$ (in the constituents (k), $k = 1, .., N$) by solving a minimum problem with two constraints. Namely, we have to find the minimum of the average viscoplastic dissipation energy W^{av} under the two conditions that (i) the average strain-rate $\mathbf{D}^{\mathrm{av}}$ over the N constituents is the macroscopic strain-rate $\mathbf{D}$ (consistency condition) and (ii) the average heterogeneity of the strain-rate distribution $h((\mathbf{D}^k))$ does not exceed a prescribed value r, thus:

$$(3.3) \qquad W_r(\mathbf{D}) \equiv \min_{\mathbf{D}^k} \left[\sum_{k=1}^{N} f_k W^k(\mathbf{D}^k) \right] ,$$

under constraints

$$(3.4) \qquad (i) \quad \sum_{k=1}^{N} f_k \mathbf{D}^k = \mathbf{D} \quad \text{and} \quad (ii) \quad h((\mathbf{D}^k)) \leq r .$$

In Eq. (3.3), $W^k(\mathbf{D}^k)$ is the energy dissipation (2.5) in the constituent $g = k$, assuming that the N constituents of the polycrystal have the same behaviour in their respective axes $(\eta = \eta^k$ and $\beta = \beta^k$ for all $k)$.

3.3. The lower and upper bounds in the model considered

The proposed formulation allows the passage from the upper bound to the lower bound in a continuous manner. Since the upper bound corresponds to a uniform strain-rate distribution (i.e., $\mathbf{D}^k = \mathbf{D}$ for all k), it appears from Eq. (3.2)

that this bound is obtained when the average strain-rate heterogeneity is null (i.e., for the heterogeneity parameter $r = 0$). ARMINJON [6] has shown that the lower bound corresponds to the static model (i.e. a uniform distribution of stress, $\mathbf{S}^k = \mathbf{S}$ for all k) and that this bound is obtained when the heterogeneity parameter r reaches a critical value R. This critical value depends on the grain anisotropy parameter β.

When the polycrystal texture is isotropic, analytical expressions of the dissipation potential can be obtained for both the upper and lower bounds. This is done by using a continuous description of the texture with the, so-called, Orientation Distribution Function (ODF). The ODF $f(\theta, \varphi)$ gives the relative density of grains whose rotational symmetry axis x_3 have the orientation (θ, φ). With the use of the ODF, a macroscopic quantity Y^{av} is defined similar to (3.1):

$$(3.5) \qquad Y^{\mathrm{av}} = \langle Y(\theta, \varphi) \rangle = \frac{1}{2\pi} \int\limits_{0}^{2\pi} \int\limits_{0}^{\pi/2} Y(\theta, \varphi) f(\theta, \varphi) \sin\theta \, d\theta \, d\varphi \,.$$

Using this definition for the weighted average, the average of the energy dissipation, W^{av}, is defined as

$$(3.6) \qquad W^{\mathrm{av}} = \langle W(\mathbf{D}^{\mathrm{loc}}(\theta, \varphi)) \rangle \,,$$

where W is given by Eq. (2.5) in the grain reference frame and $\mathbf{D}^{\mathrm{loc}} = \mathbf{D}^{\mathrm{loc}}(\theta, \varphi)$ is the distribution of the strain-rate as function of the orientation. For an isotropic texture $f(\theta, \varphi) = 1$ and, therefore, after some straightforward integrations, the analytical expression of the upper bound is found to be

$$(3.7) \qquad W_{\mathrm{sup,iso}} \equiv \langle W(\mathbf{D}) \rangle = \eta \frac{6 + 4\beta}{5\beta} \mathrm{tr}\mathbf{D}^2 \,,$$

and that of the lower bound is

$$(3.8) \qquad W_{\mathrm{inf,iso}} \equiv \inf(W^{\mathrm{av}}; \langle \mathbf{D}^{\mathrm{loc}}(\theta, \varphi) \rangle = \mathbf{D}) = \eta \frac{10}{2 + 3\beta} \mathrm{tr}\mathbf{D}^2 \,.$$

For an isotropic grain (i.e., $\beta = 1$) the two bounds are identical and $W_{\mathrm{sup,iso}} = W_{\mathrm{inf,iso}} = 2\eta \mathrm{tr}\mathbf{D}^2$. The difference between the two bounds increases as the anisotropy of the grain increases (i.e., as the anisotropy parameter β decreases). Since $W_{\mathrm{sup,iso}} = \infty$ when $\beta = 0$, the difference between the two bounds is infinite when the grain deforms only by slide in its isotropic plane.

The analytical values of the energy dissipation (3.7) and (3.8) will be used to check the numerical implementation of the model.

3.4. Numerical method for the calculation of the microscopic distributions

We have to solve the convex minimum problem (3.3) involving one linear constraint (3.4) $i4andoneconvexinequality(3.4)ii4$. We use the problem formu-

lation of [30]. The linear constraint (3.4) i is used to eliminate the strain-rate of the last constituent ($k = N$), so that the list of the optimization variables is $\mathbf{Y} = (\mathbf{D}^k)_{k=1,..,N-1}$ (thus $5(N-1)$ variables). From (3.4) i, we get

$$(3.9) \qquad \mathbf{D}^N = \left(\mathbf{D} - \sum_{k=1}^{N-1} f_k \mathbf{D}^k \right) / f_N \,.$$

The function to minimize is then written as:

$$(3.10) \qquad F(\mathbf{Y}) = \sum_{k=1}^{N-1} f_k W^k(\mathbf{D}^k) + f_N W^N \left[\left(\mathbf{D} - \sum_{k=1}^{N-1} f_k \mathbf{D}^k \right) / f_N \right] \,,$$

and the heterogeneity function (3.2) is rewritten as a function of the list $\mathbf{Y}$:

$$(3.11) \qquad h(\mathbf{Y}) = \left[\sum_{k=1}^{N-1} f_k \left| \mathbf{D}^k - \mathbf{D} \right|^2 + \frac{1}{f_N} \left| \sum_{k=1}^{N-1} f_k (\mathbf{D}^k - \mathbf{D}) \right|^2 \right]^{1/2} \,.$$

The optimization problem is: find $\mathbf{Y}_0$ making $F(\mathbf{Y})$ a minimum, among the $\mathbf{Y}$'s satisfying the constraint $C(\mathbf{Y}) = h(\mathbf{Y})^2 - (r|\mathbf{D}|)^2 \le 0$. The saddle point theorem characterizes the solution of this problem as follows:

$$(3.12)$$
$$\exists \lambda \ge 0 \quad \text{such that:}$$
$$(i) \qquad \nabla F(\mathbf{Y}_0) + \lambda \nabla C(\mathbf{Y}_0) = \mathbf{0} \quad \text{and} \quad (ii) \quad \lambda C(\mathbf{Y}_0) = 0 \,.$$

In this work, the optimization problem is solved by seeking the saddle point $(\mathbf{Y}_0, \lambda_0)$ of the Lagrangian function

$$(3.13) \qquad L(\mathbf{Y}, \lambda) = F(\mathbf{Y}) + \lambda C(\mathbf{Y}) \,,$$

instead of using a classical penalty method as in [7, 30]. This saddle point is defined as

$$(3.14) \qquad L(\mathbf{Y}_0, \lambda_0) = \min_{\mathbf{Y}} L(\mathbf{Y}, \lambda_0) = \max_{\lambda} \min_{\mathbf{Y}} L(\mathbf{Y}, \lambda) \,.$$

By introducing the function $G(\lambda)$ defined as

$$(3.15) \qquad G(\lambda) = \min_{\mathbf{Y}} L(\mathbf{Y}, \lambda) \,,$$

the saddle point corresponds to the maximum of $G(\lambda)$.

Numerically, for a given value of λ, the value of the function $G(\lambda)$ is obtained by using the conjugate gradient method. The maximum value of $G(\lambda)$ is then

sought by an inverse parabolic interpolation. Since the function $G(\lambda)$ is smooth, this method has been found to be more efficient than the Uzawa algorithm.

When $r \geq R$, the Lagrange multiplier λ is equal to zero and the optimization problem reduces to finding the minimum of the function $F(\mathbf{Y})$. To obtain convergence of the algorithm in the case $r \geq R$, the function $G(\lambda)$ (3.15) is transformed into:

$$(3.16) \qquad G(\lambda) = \begin{cases} \min_{\mathbf{Y}} [F(\mathbf{Y}) + \lambda C(\mathbf{Y})] & \text{if } \lambda > 0 \\ \min_{\mathbf{Y}} [F(\mathbf{Y})] - \lambda & \text{if } \lambda \leq 0, \end{cases}$$

4. Results

4.1. Numerical tests of the saddle point solution

In Fig. 1 is presented the evolution of the function $G(\lambda) = L(\mathbf{Y}_0(\lambda), \lambda)$ Eq. (3.16) for a given grain anisotropy parameter $\beta = 0.01$ and a given heterogeneity parameter $r = 0.5$. The condition (3.12) i is verified for every λ (for each λ, it is verified with the solution $\mathbf{Y}_0(\lambda)$ of the minimization problem (3.15), but it appears in this figure that the condition (3.12) ii (i.e., $\lambda C(\mathbf{Y}_0) = 0$) is confirmed for only one value $\lambda = \lambda_0$, which corresponds to the the saddle point solution.
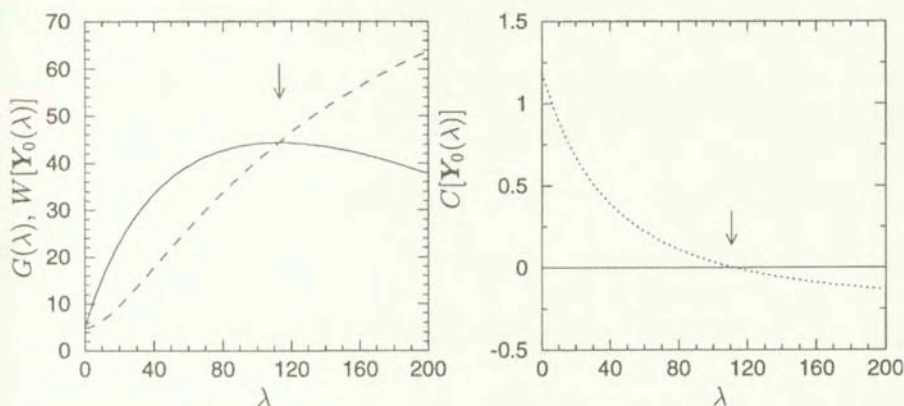

FIG. 1. Evolution of $G(\lambda) = L(\mathbf{Y}_0(\lambda), \lambda)$ (solid line), the energy dissipation $F[\mathbf{Y}_0(\lambda)]$ (dashed line) and the constraint $C[\mathbf{Y}_0(\lambda)]$ (dotted line) as a function of the Lagrange multiplier λ for $\beta = 0.01$ and $r = 0.5$. The arrows show the value of λ_0 corresponding to the maximum of $G(\lambda)$ (i.e., the saddle point solution).

This value λ_0 depends on the grain anisotropy parameter β and on the heterogeneity parameter r. Figure 2 shows the evolution of the calculated Lagrange multiplier λ_0 as a function of the heterogeneity parameter r. Theoretically, we

should get an infinite value for λ_0 when the heterogeneity parameter is zero (upper bound). Numerically, the convergence of the method is not achieved when the value of r is lower than the precision expected on the constraint $C(\mathbf{Y}_0)$. On the other hand, with the adopted function (3.16), the lower bound can be calculated, even when $r > R$. Numerically, when $r > R$ the constraint becomes negative, but the Lagrange multiplier is very close to zero (of the order of 10^{-14}).
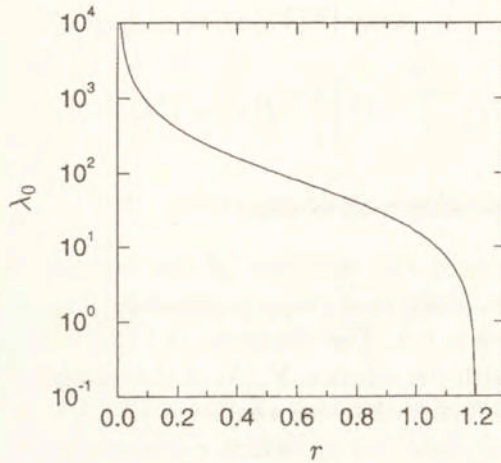

FIG. 2. Evolution of the Lagrange multiplier λ_0 corresponding to the saddle point solution as a function of the strain-rate heterogeneity parameter r for $\beta = 0.01$.

Numerically, with a relative precision of about 10^{-7}, it is found that the Lagrange multiplier verifies the relation

$$(4.1) \qquad \lambda_0 = \frac{h((\mathbf{S}_0^k))}{h((\mathbf{D}_0^k))},$$

where $(\mathbf{S}_0^k)$ and $(\mathbf{D}_0^k)$ are the microscopic stress and strain-rate distributions, respectively, corresponding to the solution of the optimization problem.

4.2. Macroscopic behaviour of isotropic polycrystalline ice

In this section, the mechanical response of isotropic ice is analysed as a function of the strain-rate heterogeneity parameter r and the grain anisotropy parameter β. The value of the viscosity parameter η has no influence on the strain-rate distribution and merely acts as a scaling parameter on the stresses. Therefore, all the numerical results presented have been obtained for an applied macroscopic strain-rate such that $\eta\mathrm{tr}\mathbf{D}^2 = 1$. The polycrystal is made up of $N = 200$ randomly distributed grains and then the number of optimization variables is 995.

In Fig. 3a is presented the evolution of the calculated strain-rate and deviatoric stress heterogeneities as functions of the imposed heterogeneity parameter r. The calculated strain-rate heterogeneity h is equal to the heterogeneity parameter r until the maximum value of h, i.e. $R = 1.2$, is reached. As for the strain-rate heterogeneity, the stress heterogeneity evolution is linear, but it decreases from the maximum value 96.8 when $r = 0$ to zero when $r \geq R$. As expected, the stress heterogeneity function $h((\mathbf{S}^k)) = 0$ when $r \geq R$, which means that the (average) deviatoric stress is the same in all the constituents (static model).
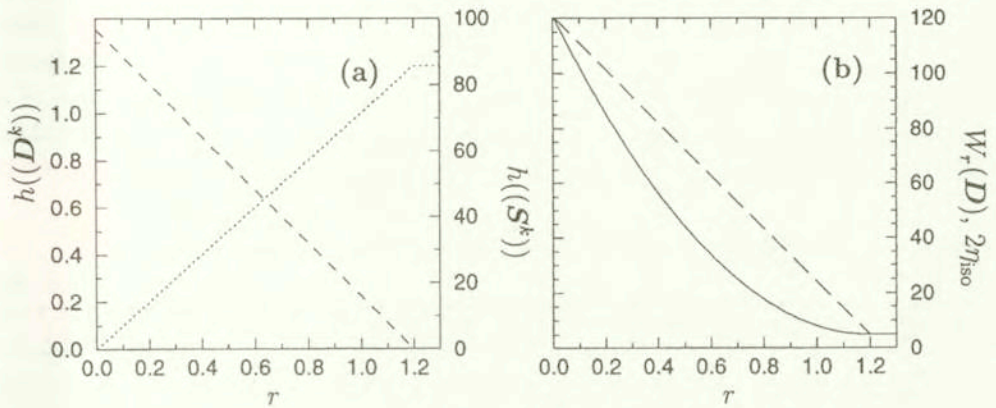

FIG. 3. Evolution of (a) the calculated strain-rate and stress heterogeneities, $h((\mathbf{D}^k))$ and $h((\mathbf{S}^k))$, (dotted and dashed lines, respectively) and (b) the average of the dissipation potential $W_r(\mathbf{D})$ (solid line) and the viscosity for isotropic ice η_{iso} (long dashed line) as a function of the imposewd heterogeneity parameter r for $\beta = 0.01$.

By testing twenty different $\mathbf{D}$ tensors, we have found numerically that the stress response $\mathbf{S}$ is very nearly proportional to the strain-rate direction $\mathbf{D}$ and, moreover, the proportionality coefficient does not depend on the investigated $\mathbf{D}$ tensor. In other words, the macroscopic response of the isotropic polycrystal is numerically found to be of the form:

$$(4.2) \qquad \mathbf{S} = 2\eta_{iso}\mathbf{D},$$

where η_{iso} is an effective viscosity of isotropic ice. The numerical departure from this exact equation is found to be smaller than 1%. This departure can be attributed to the randomly created texture, which is not *exactly* isotropic.

Figure 3b shows the evolution of the energy dissipation as a function of the heterogeneity parameter r. For $\beta = 0.01$, the analytical values of the upper and lower bounds (3.7) and (3.8) are $W_{sup,iso} = 120.8$ and $W_{inf,iso} = 4.92$. As shown in Fig. 3a, the calculated potential reaches these two values for $r = 0$ and $r \geq R = 1.2$, respectively. The upper bound was calculated for $r = 10^{-10}$

since for $r = 0$ the convergence is not achieved with the algorithm used here. Of course, the programming of the Taylor model is trivial and can be included, so as to take into account the case $r = 0$.

Because there are very few reliable experimental results on ice crystals and also because the constituent in a micro-macro model does not behave as a single isolated ice crystal, it is more convenient to determine the rheological values of the constituent (here the values of η and β) by using experimental results on polycrystalline ice.

According to the experimental results of Pimienta *et al.* [31], a polycrystal with all its grain symmetry axes parallel, undergoing simple shear in a plane perpendicular to the grain symmetry $c-$axes, would deform 10 ± 2 times faster than an isotropic polycrystal. Since in a micro-macro model the response of a polycrystal in which all the constituents have the same orientation is equal to the response of a single constituent, this leads to the relation:

$$(4.3) \qquad \frac{\eta_{\text{iso}}}{\eta} = 10 \pm 2.$$

As shown in Fig. 3b, $\eta_{\text{iso}}\text{tr}\mathbf{D}^2$ is numerically found to decrease linearly as a function of the heterogeneity parameter r, from the Taylor value to the static one. Taking benefit of this linearity (assumed exact), and using the analytical solutions (3.7) and (3.8) for the two bounds, one can easily derive the following analytical relation between the grain viscosity for shear in the plane perpendicular to the basal plane, η, and the effective viscosity for isotropic ice, η_{iso}:

$$(4.4) \qquad \frac{\eta_{\text{iso}}}{\eta} = \frac{3 + 2\beta}{5\beta} - \frac{6(1 - \beta)^2}{5\beta(2 + 3\beta)} \frac{r}{R},$$

where R can be approximated from numerical results by $R = \beta^2 - 2.23\beta + 1.23$.

The contours of the ratio η_{iso}/η (??) from 4 to 20 by step of 2 are drawn in Fig. 4 as a function of the grain anisotropy parameter β and the heterogeneity ratio r/R. If the grain anisotropy parameter β decreases, then to get the same value of the ratio η_{iso}/η, the strain-rate heterogeneity has to increase. If the grain anisotropy parameter is between 0.001 and 0.01, which seems to be a reasonable range of values for ice [31], then the value $\eta_{\text{iso}}/\eta = 10$ corresponds to a range of heterogeneity parameter between $r = 0.87R$ and $r = 0.987R$, i.e. very close to the solution given by the static model ($r = R$). As shown in Fig. 4, the value $\eta_{\text{iso}}/\eta = 10$ can be obtained only if the grain anisotropy parameter β is lower than 0.0625. Figure 4 should be used to select a pair (β, r) corresponding to the required macroscopic anisotropy.
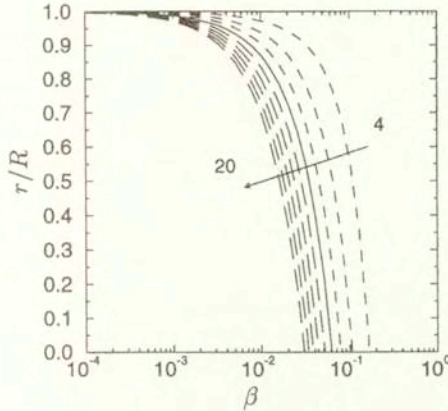
FIG. 4. Contours of the ratio η_{iso}/η from 4 to 20 by step of 2 as a function of the grain anisotropy parameter β and the heterogeneity ratio r/R (R is the heterogeneity obtained for the static solution).

4.3. Deviation from the no-correlation condition

In this section, the deviation from the following *no-correlation condition*:

$$(4.5) \qquad \langle \mathbf{D}^k \rangle . \langle \mathbf{S}^k \rangle = \langle \mathbf{D}^k . \mathbf{S}^k \rangle ,$$

is studied as a function of the heterogeneity parameter r and the grain anisotropy parameter β. To this goal, we compare the calculated macroscopic dissipation energy

$$(4.6) \qquad \mathbf{D}.\mathbf{S} = \langle \mathbf{D}^k \rangle . \langle \mathbf{S}^k \rangle ,$$

and the average of the dissipation energy (used previously for the minimization problem)

$$(4.7) \qquad W^{av} = \langle W^k \rangle = \langle \mathbf{D}^k . \mathbf{S}^k \rangle .$$

When formulating the model used here [6, 7], it was assumed that condition (4.5) applies when $\mathbf{D}^k$ and $\mathbf{S}^k$ are the respective average values of the *actual* field of strain-rate, $\mathbf{d}$, and of the *actual* field of deviatoric stress, $\mathbf{s}$, in the volume occupied by constituent (k):

$$(4.8) \qquad \mathbf{D}^k_{act} = \int_{\Omega_k} \mathbf{d} \, dV / V(\Omega_k) \quad \text{and} \quad \mathbf{S}^k_{act} = \int_{\Omega_k} \mathbf{s} \, dV / V(\Omega_k) .$$

Furthermore, the model assumes that, for the relevant value r_0 of the heterogeneity parameter r, the strain-rate distribution $(\mathbf{D}^k)$ solution of the minimum problem (3.3) – (3.4) is equal to the actual distribution $(\mathbf{D}^k_{act})$. It is well known

that condition (4.5) applies trivially when the extreme models are used: either the upper bound model ($\mathbf{D}^k = \mathbf{D} \,\forall\, k$) or the lower bound model ($\mathbf{S}^k = \mathbf{S} \,\forall\, k$). Now it is apparent in Fig. 5 that, except for these extreme models (which corresponds respectively to $r = 0$ and $r = R$), the strain-rate distribution ($\mathbf{D}_r^k$) does not fulfil condition (4.5). Therefore, at least one among the following three possibilities is true:

(*i*) The actual distribution does not fulfil condition (4.5). This could be due to the strong heterogeneity of the polycrystal (due to the strong anisotropy of the crystals) and it would mean that using a one-point model is not well justified.

(*ii*) The proposed variational model does not predict correctly the actual strain-rate distribution when the polycrystal heterogeneity is too large. Again, this would mean that using a one-point model, such as the present model, is not wise for strong material heterogeneity.

(*iii*) One of the two extreme models (Static or Voigt-Taylor) corresponds to the actual solution. This possibility does not seem to be very realistic.

In any case, it should be emphasized that the no-correlation condition (4.5) is different from Hill's macrohomogeneity condition [32, 33]. The latter must be written in terms of the microscopic fields and their volume averages in the representative volume element Ω of the polycrystal (Ω is the union of the domains $\Omega_k, k = 1, .., N$):

$$(4.9) \qquad \overline{\boldsymbol{\sigma} : \mathbf{d}} \equiv \frac{1}{V(\Omega)} \int_\Omega \boldsymbol{\sigma} : \mathbf{d}\, dV$$

$$= \overline{\boldsymbol{\sigma}} : \overline{\mathbf{d}} \equiv \left(\frac{1}{V(\Omega)} \int_\Omega \boldsymbol{\sigma}\, dV \right) : \left(\frac{1}{V(\Omega)} \int_\Omega \mathbf{d}\, dV \right) .$$

In fact, ARMINJON [6], as well as ARMINJON and IMBAULT [7] derive condition (4.5) from Hill's condition (4.9) and using an additional assumption (Eq. (4.5) in [7]).

As shown in Fig. 5, the ratio $\langle \mathbf{D}^k . \mathbf{S}^k \rangle / (\mathbf{D}.\mathbf{S})$ decreases as the grain anisotropy increases (i.e., as β decreases) and the location of the maximum difference tends towards $r/R = 1$ with β.

MEYSSONNIER and PHILIP [12] have proposed a self-consistent "one-site" model (SC1) based on the same model for the grain behaviour, *i.e* linear transversely isotropic medium. In the SC1 model, the texture is described by the use of an ODF, and the linearity of the grain behaviour allows analytical developments of the strain-rate and stress fields as functions of the grain orientations.
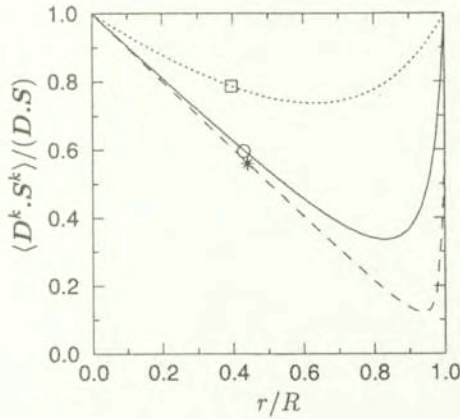
FIG. 5. Evolution of the ratio $\langle \mathbf{D}^k.\mathbf{S}^k \rangle / (\mathbf{D}.\mathbf{S})$ as a function of $r\{R\}$, for $\beta = 0.1$ (dotted line), $\beta = 0.01$ (solid line) and $\beta = 0.001$ (dashed line). In this figure is plotted the value find for the ratio $\langle \mathbf{D}^k.\mathbf{S}^k \rangle / (\mathbf{D}.\mathbf{S})$ by using the 1-site self-consistent model of [12] for $\beta = 0.1$ (square), $\beta = 0.01$ (circle) and $\beta = 0.001$ (star).

Since the SC1 model is based on the same model for the grain behaviour, it allows an objective comparison of both models. In Fig. 5, the value of the ratio $\langle \mathbf{D}^k.\mathbf{S}^k \rangle / (\mathbf{D}.\mathbf{S})$ obtained with the SC1 model is plotted for the corresponding calculated strain-rate heterogeneity (the latter is not imposed in the SC1 model). As shown in Fig. 5, for a given grain anisotropy, the solution obtained with the SC1 model corresponds exactly to one solution given by the present model. As shown in Fig. 6 for $\beta = 0.01$ and an applied compression $D_2 = 1$ and $D_1 = 0$, the strain-rate distribution given by the SC1 model is almost exactly the same as that given by the present model when the heterogeneity parameter r imposed for the present model is equal to the value h_{SC1} of the strain-rate heterogeneity, calculated with the SC1 model ($h_{SC1} = 0.52$). In other words, up to a negligible error, the strain-rate distribution predicted by the self-consistent model is (in this linear case) solution of the variational problem (3.3) – (3.4), for some particular value r. Howewer, that particular value $r = 0.52$ corresponds to $r/R \approx 0.42$ and gives an effective viscosity $\eta_{iso} \approx 36\eta$, which seems to be inconsistent with the experimental data $\eta_{iso}/\eta \approx 10$ of PIMIENTA et al. [31]. This latter value of the ratio is obtained with the SC1 model only for one value $\beta = 0.04$ [12]. The behaviour of polycrystalline ice is much closer to the static model than on would expect using the self-consistent model.

CASTELNAU et al. [34] found similar results with a 1-site self-consistent model but for a non-linear behaviour of the grains. By introducing an interaction coefficient α, which is used to constrain the interaction between grains and the matrix (a zero value of α corresponds to the Taylor model and an infinite value to the static model), these authors showed that the maximum deviation from the

no-correlation condition (4.5) is obtained for the classical tangent formulation of
the model ($\alpha = 1$). (It is recalled that, in the linear case studied here, there is
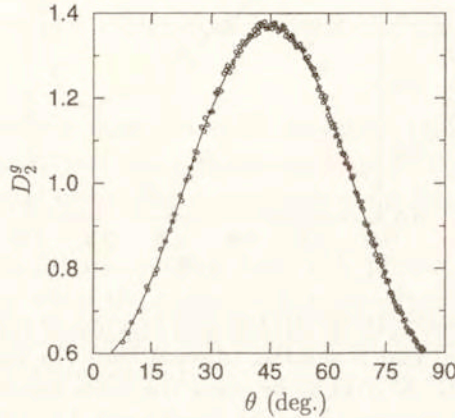only one self-consistent solution, i.e., there is no parameter like α).

FIG. 6. Evolution of the strain-rate D_2^g in the grains as a function of the grain orientation
angle θ, for $\beta = 0.01$, calculated with the present model for an imposed strain-rate
heterogeneity parameter $r = 0.52$ (circle) and with the CS! model (solid line).

5. Conclusions and discussion

A variational micro-macro model has been numerically implemented to pre-
dict the strain-rate distribution in polycrystalline ice, when the behaviour of the
constituent crystals is assumed linearly viscous (i.e., an anisotropic fluid). This
convenient assumption is suggested by an analysis of data resulting from deep
ice-cores [11]. The variational problem defining the model allows a continuous
transition between the extreme (Taylor-Voigt and Reuss-static) models, depend-
ing on the value of the strain-rate heterogeneity parameter r. In this work, the
numerical solution of this variational problem with constraints has been found
by using a saddle point method. This has proved more accurate and even more
efficient than the penalty method that was used previously, though it should
be remembered that the linear behaviour, as envisaged here, leads to a simpler
minimization problem.

From the strain-rate distribution, obtained as the solution of the minimization
problem, it is easy to deduce the stress distribution and the effective behaviour.
All three depend on: (i) the crystal behaviour, here characterized by the crys-
tal viscosity η and the crystal anisotropy parameter β, (ii) the heterogeneity
parameter r and (iii) the (current) texture or orientation distribution. In this
work, a uniform texture has been considered, thus leading to an isotropic effective
behaviour (for an application to non-uniform textures see [8]). The effective be-

haviour depends then only on η, β and r, and is found to be an isotropic linearly viscous behaviour, involving an effective viscosity η_{iso}. The ratio η_{iso}/η depends analytically on β and r (Eq. (4.4)). Since η_{iso}/η and β can be constrained from experimental data, this leads to an evaluation of the heterogeneity parameter r, which is found to be high: $r/R \approx 0.9$, where R is the strain-rate heterogeneity that corresponds to the static model. In contrast, the self-consistent model predicts $r/R \approx 0.4$, which seems incompatible with experimental data. Thus, the behaviour of polycrystalline ice seems to be much closer to the static model than is the self-consistent estimate. This is probably due to the strong material heterogeneity, which is likely to favour a behaviour close to the static model.

When using "one-point" (volume fractions) models like self-consistent models or that investigated here, one hopes that the discrete strain-rate and stress distributions calculated by the model are representative of the actual strain-rate and stress fields and, in particular, allow calculation of the macroscopic work-rate as the corresponding discrete average. This needs the no-correlation condition (4.5) to be fulfilled. However, it has been found that the distribution predicted by the model used here, and which depends on the heterogeneity parameter r, does not satisfy Eq. (4.5), except for the extreme models ($r = 0$ or $r = R$). The same is true for the self-consistent model (it has been found that the self-consistent model corresponds almost exactly to the model used here for a particular value of r). The analysis of this condition by ARMINJON [6] and by ARMINJON and IMBAULT [7], suggests that the use of a one-point model cannot be entirely satisfactory as the material heterogeneity (here the parameter $1/\beta$) is high. More precisely, it is less justified in that case to assume that the volume average of the stress field in a given constituent is related to the corresponding strain-rate average by a constitutive relation. If one keeps using a one-point model to get the effective behaviour, one should probably consider that the macroscopic work-rate is given by the left-hand side of Eq. (4,5), which is greater than the right-hand side. This would mean that some additional "accommodation work" is not included in the r.h.s. of Eq. (4.5), being due to the correlated heterogeneity of the microscopic fields c and d at the sub-constituent scale. There is also the possibility to use a model involving a description of the micro-geometry (see e.g. [29]), at the price of significantly increasing the computation time.

References

1. P. DUVAL, M. F. ASHBY, and I. ANDERMAN, *Rate-controlling processes in the creep of polycrystalline ice*, J. of Phys. Chem., **87**, 10, 4066–4074, 1983.

2. A. MANGENEY, F. CALIFANO, and O. CASTELNAU, *Isothermal flow of an anisotropic ice sheet in the vicinity of an ice divide*, J. Geophys. Res., **101**, 12, 28, 189–28,204, 1996.

3. A. Mangeney, F. Califano, and K. Hutter, *A numerical study of anisotropic, low Reynolds number, free surface flow of ice sheet modeling*, J. Geophys. Res., **102**, B10, 22, 749–22,764, 1997.

4. O. Gagliardini and J. Meyssonnier, *Plane flow of an ice sheet exhibiting strain-induced anisotropy*, K. Hutter, Y. Wang, H. Beer [Eds.], Advances in Cold-Region Thermal Engineering and Sciences: technological, environmental and climatological Impact. Berlin, etc. Springer-Verlag, (Lecture Notes in Physics) **533**, 171–182, 1999.

5. O. Castelnau, P. Duval, R. A. Lebensohn, and G. Canova, *Viscoplastic modeling of texture development in polycrystalline ice with a self-consistent approach: Comparison with bound estimates*, J. Geophys. Res., **101**, 6, 13, 851–13,868, 1996.

6. M. Arminjon, *Limit distributions of the states and homogenization in random media*, Acta Mech., **88**, 27–59, 1991.

7. M. Arminjon and D. Imbault, *Variational micro-macro model and deformation textures predicted for steels*, Textures and Microstructures, **26-27**, 191–220, 1996.

8. O. Gagliardini, M. Arminjon and D. Imbault, *Predicting the macroscopic behaviour of anisotropic ice with a variational polycrystal model*, Proceedings of the 4th European Mechanics of Materials Conf., June 2000, Metz (E. Gautier, M. Clavel and F. Dunne, [Eds.]), to appear.

9. M. Arminjon and J. P. Boehler, *Comportement plastique et texture cristallographique des métaux anisotropes*, Comportement plastique des solides anisotropes (J. P. Boehler [Ed.]), Editions du CNRS, 133–155, Paris 1985.

10. Ph. Lequeu, P. Gilormini, F. Montheillet, B. Bacroix, and J. J. Jonas, *Yield surfaces for textured polycrystals –I. Crystallographic approach*, Acta Metall., **35**, 2, 439–451, 1987.

11. V. Ya. Lipenkov, A. N. Salamatin, and P. Duval, *Bubbly-ice densification in ice sheets: II. Applications*, J. Glaciol., **43**, 145, 397–407, 1997.

12. J. Meyssonnier and A. Philip, *A model for the tangent viscous behaviour of anisotropic polar ice*, Ann. Glaciol., **23**, 253–261, 1996.

13. O. Gagliardini and J. Meyssonnier, *Analytical derivations for the behaviour and fabric evolution of a linear orthotropic ice polycrystal*, J. Geophys. Res., **104**, B8, 17 797–17 809, 1999.

14. R. Staroszczyk and O. Gagliardini, *Two orthotropic models for strain-induced anisotropy of polar ice*, J. Glaciol., **45**, 151, 485 – 494, 1999.

15. A. V. Hershey, J. Appl. Mech., **21**, pp. 236 and 241, 1954.

16. E. Kröner, *Berechnung der elastischen Konstanten des Vielkristalls aus den Konstanten des Einkristalls*, Z. Phys., **151**, 504–518, 1958.

17. J. D. Eshelby, Phil. Trans. A, **244**, p. 87, 1951.

18. J. D. Eshelby, *The determination of the elastic field of an ellipsoidal inclusion, and related problems*, Proc. Roy. Soc. A, **241**, 376–396, 1957.

19. M. Arminjon, *Macro-homogeneous strain fields with arbitrary local inhomogeneity*, Arch. Mech., **43**, 191–214, 1991.

20. E. Kröner, *Self-consistent scheme and graded disorder in polycrystal elasticity*, J. Phys. F: Metal Phys., **8**, 2261–2267, 1978.

21. E. Kröner, *Zur plastischen Verformung des Vielkristalls*, Acta Metall., **9**, 155–161, 1961.

22. P. Gilormini, *A shortcoming of the classical non-linear extension of the self-consistent model*, C. R. Acad. Sci., **320**, Série IIb, 115–122, Paris 1995.

23. R. Hill, *Continuum micro-mechanics of elastoplastic polycrystals*, J. Mech. Phys. Solids, **13**, 89–101, 1965.

24. P. Ponte Castañeda, *The effective mechanical properties of nonlinear isotropic composites*, J. Mech. Phys. Solids, **39**, 45–71, 1991.

25. G. J. Weng, *Self-consistent determination of time-dependent behavior of metals*, J. Appl. Mech., **48**, 41–46, 1981.

26. A. Molinari, G. R. Canova and S. Ahzi, *A self-consistent approach of the large deformation polycrystal viscoplasticity*, Acta Metall., **35**, 12, 2983–2994, 1987.

27. P. Lipinski, M. Berveiller and F. Corvasce, *Statistical approach to elastoplastic behaviour of polycrystal at finite deformations*, Arch. Mech., **40**, 725–740, 1988.

28. G. J. Dvorak, *Micromechanics of inelastic composite materials: theory and experiment*, J. Engng. Mater. Technol., **115**, 327–338, 1993.

29. M. Arminjon and B. Guessab, *A model with two micro-scales for the effects of geometrical distribution of material inhomogeneity*, Acta Mechanica, **134**, 61–79, 1999.

30. M. Arminjon and D. Imbault, *On variational micro-macro models and their application to polycrystals*, Dynamical Plasticity and Structural Behaviors (Sh. Tanimura and A. S. Khan [Eds.]), Gordon and Breach, 245–248, Luxembourg 1995.

31. P. Pimienta, P. Duval and V. Y. Lipenkov, *Mechanical behaviour of anisotropic polar ice*, In International Association of Hydrological Sciences, Publication 170 (Symposium on The Physical Basis of Ice Sheet Modelling, Vancouver), 57–66, 1987.

32. J. F. W. Bishop and R. Hill, *A theory of the plastic distortion of a polycrystalline aggregate under combined stresses*, Phil. Mag., **42**, 414–427, 1951.

33. R. Hill, *The essential structure of constitutive laws for metal composites and polycrystals*, J. Mech. Phys. Solids, **15**, 79–95, 1967.

34. O. Castelnau, G. R. Canova, R. A. Lebensohn and P. Duval, *Modelling viscoplastic behavior of anisotropic polycrystalline ice with a self-consistent approach*, Acta. Mater., **45**, 11, 4823–4834, 1997.