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Creep and recrystallization of large polycrystalline masses Part III: Continuum theory of ice sheets

by

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Creep and recrystallization of large polycrystalline masses Part III: continuum theory of ice sheets†

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This work sets forth the first thermodynamically consistent constitutive theory for ice sheets undergoing strain-induced anisotropy, polygonization and recrystallization effects. It is based on the notion of a mixture with continuous diversity, by picturing the ice sheet as a 'mixture of lattice orientations'. The fabric (texture) is described by an orientation-dependent field of mass density which is sensitive not only to lattice spin, but also to grain boundary migration. No constraint is imposed on stress or strain of individual crystallites, aside from the assumption that basal slip is the dominant deformation mechanism on the grain scale. In spite of the fact that individual ice crystallites are regarded as micropolar media, it is inferred that couples on distinct grains counteract each other, so that the ice sheet behaves on a large scale as an ordinary (non-polar) continuum. Several concepts from materials science are translated to the language of continuum theory, like e.g. *lattice distortion energy*, *grain boundary mobility* and *Schmid tensor*, as well as some fabric (texture) parameters like the so-called degree of orientation and spherical aperture. After choosing suitable expressions for the stored energy and entropy of dislocations, it is shown that the driving pressure for grain boundary migration can be associated to differences in the *dislocation potentials* (viz. the Gibbs free energies due to dislocations) of crystallites with distinct c-axis orientations. Finally, the generic representation derived for the Cauchy stress is compared with former generalizations of Glen's flow law, namely the Svendsen–Gödert–Hutter stress law and the Azuma–Goto-Azuma flow law.

Keywords: ice; thermodynamics; mechanics; continuous diversity; recrystallization; polygonization

1. Motivation

Ice sheets are huge ice masses of continental size. Presently there exist only two of them on the poles, covering Antarctica and Greenland, but there are indisputable evidences for the past existence of other equally large ice sheets covering extensive regions of North America, Europe and Asia about 100–20 thousand years ago (Siegert 2001). By the time of maximal volume, these ice sheets might have contained more than three times the actual amount of ice found on Earth. Clearly, the withdrawal of such a gigantic mass of ice cannot be explained simply

† Dedicated to Kolumban Hutter on the occasion of his 65th birthday.

by melting —the ice had to have flowed away towards the ocean, under the action of its own weight, creeping like a viscous fluid along the millennia. And it continues to flow from the remaining ice sheets, at a pace ranging from a few up to some hundreds of metres per year.

Among the greatest complications in the modelling of ice sheet dynamics are the huge time scales and the relatively high temperatures involved in the creeping process, which permit a ceaseless changing of the ice microstructure by flow-induced anisotropy and recrystallization phenomena. Such microstructural changes may enhance the ice flow rate by three fold or more (Budd & Jacka 1989). In spite of the fact that recrystallization phenomena have essentially a thermodynamic character, most polycrystalline ice sheet models proposed so far have been based on ad hoc theories, without corroboration of a rigorous thermodynamic analysis (e.g. Van der Veen & Whillans 1994; Castelnau *et al.* 1997; Staroszczyk & Morland 2001). The objective of the present study is to fill this gap, by setting forth a novel approach to the thermomechanics of polycrystalline ice sheets, based on the continuum theory of polycrystalline media described in Parts I and II of this series (Faria 2006; Faria *et al.* 2006). The cornerstone of the current approach is the characterization of the polycrystal as a mixture with continuous diversity (Faria 2001), more precisely a 'mixture of lattice orientations'. Details of this characterization and its fundamental equations have already been discussed in Parts I and II. Therefore, for conciseness, they will not be repeated here.

The notation follows the scheme outlined in Appendix A of Part I. In particular, when some reference to equations from the parts I and II is needed, the superscripts 'I' and 'II' will be added to the respective equation tags: e.g. $(3.1)^{\mathrm{II}}$ refers to the first equation of the third section of Part II.

2. Basic assumptions

From a thermomechanical point of view, polar ice grains manifest transversely isotropic response (figure 1), which stems from a combination of their lattice symmetry (hexagonal system, dihexagonal dipyramidal class) with the peculiar behaviour of dislocations in ice (Hobbs 1974; Hondoh 2000). Consequently, in thermomechanical applications just one crystallographic axis, called *c-axis*, completely describes the orientation of the ice lattice. By adopting this characterization, we are in practice conforming with the standard belief that the deformation of polar ice is dominated by *basal slip* (Duval 2000; Faria & Kipfstuhl 2004), i.e. by dislocation glide along planes orthogonal to the local c-axis direction. These facts indicate that the constitutive theory developed in Part II is well-suited for ice sheets. However, to yield a tractable theory we need to introduce appropriate simplifying assumptions.

(*a*) *Thermodynamic processes in polycrystalline ice sheets*

In the simplest description of an ice sheet as a cold,† amorphous, isotropic and incompressible medium (Hutter 1983), a thermodynamic process is determined by the specification of four scalar fields, viz. the temperature $T(x_i, t)$ and the three components of the velocity vector $v_i(x_j, t)$, at every point x_j and time instant t.

† As usual, 'cold ice' means ice without melt water. The modelling of ice with melt water (viz. 'temperate ice') would require a multiphase theory which is out of the scope of this work.

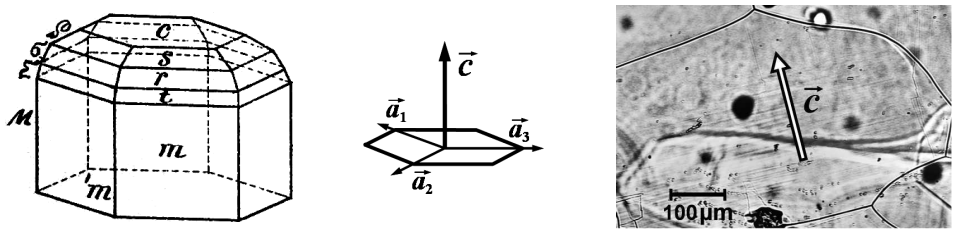

Figure 1. *Left*: crystallographic planes of ice drawn by Nordenskjöld (1861). Basal planes, denoted by 'c', lie orthogonal to the main symmetry axis of the lattice, the *c-axis*. Slip activity in polar ice is believed to be concentrated in such planes. Further planes identified in the drawing are the prismatic (denoted by 'm') and the pyramidal (inclined, denoted by 'r', 's', 't'). *Centre*: Sketch of the basal plane and principal crystallographic axes. *Right*: ice crystallite in an Antarctic sample from 1156 m depth of the EPICA–DML ice core. Basal planes are visible in series of *slip bands* (faint fringes) formed during in situ deformation.

Nevertheless, the high-temperature creep of ice sheets is in fact very sensitive to the *fabric* (or *texture*‡) of the material, i.e. to the orientational distribution of c-axes. Hence, a precise description of the ice sheet dynamics requires the consideration of evolving anisotropy, which results from changes in the microstructure via *lattice rotation*, *recovery* and *recrystallization*. All these effects have already been considered in the general constitutive theory for polycrystals developed in Part II (Faria *et al.* 2006), so that we may follow the same scheme here by supposing that a *thermodynamic process* in a polycrystalline ice sheet is characterized by the nine basic fields of

$$\begin{array}{ll} \varrho^*(x_i,t,n_j) & \text{mass density,} \\ \rho^*_{\mathrm{D}}(x_i,t,n_j) & \text{dislocation density,} \\ s^*_i(x_j,t,n_k) & c\text{-axis spin velocity,} \\ v_i(x_j,t) & \text{translational velocity,} \\ T\,(x_i,t) & \text{absolute temperature,} \end{array} \tag{2.1}$$

where the superscript '$*$' tags those fields that depend not only on position and time, but also on c-axis orientation. The latter is denoted by the unit *orientation vector* $n_i \in \mathcal{S}^2$, which is the counterpart of the position vector $x_i \in \mathbb{R}^3$ in the *orientation space* $\mathcal{S}^2$ (see §2c of Part I). Following the terminology of Parts I and II, orientation-dependent fields are also named *species fields*. On this account, the species mass density ϱ^* portrays the fabric by standing for the net mass of all crystallites whose c-axes are parallel to n_i, within a unit polycrystalline volume. The rotation rate of the lattice is measured by the c-axis spin velocity s^*_i, while ρ^*_{D} represents the total length of dislocations, per unit polycrystalline volume, found in those grains with c-axes directed to n_i. Finally, the fields of velocity v_i and temperature T describe the ordinary thermomechanics of the ice sheet, already mentioned.

Remark 2.1. The current theory may be classified as a 'macroscopic' continuum model, in which the deformation of individual grains is *neither controlled nor determined*. Indeed, each ice-sheet particle should by definition contain a huge number of grains (cf. footnote 2 in §1 of Part I), so that inhomogeneities on the grain

‡ As in the former parts of this series, the terms *texture* and *fabric* are used as synonyms to the preferred orientations of the lattice. No particular word is adopted for grain sizes and shapes.

scale are smeared out within every particle and are therefore irrelevant for the large-scale description. In this regard, the *assumption of negligible grain shifting*, $v_i^*(x_j, t, n_k) \equiv v_i(x_j, t)$, has *no relation at all* to any kind of 'Taylor-type' constraint on the deformation of individual grains, seeing that v_i^* is just a *'macroscopic' average* (over an ice-sheet particle) of the velocities of all grains with c-axes in the n_i-direction. Rather, the assumption $v_i^* = v_i$ simply states that ice grains do not permeate through the polycrystalline matrix, which is certainly valid for polar ice sheets *as long as they do not flow in a superplastic regime* (cf. remark 3.5 of Part I; Duval 2000; Duval & Montagnat 2002; Faria *et al.* 2003).

(*b*) *Thermomechanical simplifications*

In order to determine the basic fields (2.1) we need suitable field equations. In principle, such equations should stem from a combination of the balance equations $(2.2)^{\text{II}}$–$(2.6)^{\text{II}}$ with the constitutive relations $(3.61)^{\text{II}}$–$(3.64)^{\text{II}}$ presented in Part II. Nevertheless, in spite of the fact that the constitutive relations $(3.61)^{\text{II}}$–$(3.64)^{\text{II}}$ are quite general and rigorous, they are definitely too complex to be adopted in practical applications. For instance, there is an abundance of transport coefficients —many of them tensor-valued— the explicit forms of which can hardly be determined by experiments or guesswork. Further simplifications are still needed, fortunately many are sensible for ice sheet flow, as described below.

1. Negligible c*-axis inertia.* This is not particular to ice, but rather a general feature of all crystalline solids: crystallographic axes do not continue rotating after cessation of the couples acting on them. Hence, we may set $I = 0$ in $(2.2)^{\text{II}}$–$(2.6)^{\text{II}}$.

2. On external supplies. In ice-sheet dynamics, relevant body supplies are due to gravity and solar/geothermal radiation. It is obvious that gravity acts equally upon all grains, regardless of c-axis orientation. Likewise, the absorption of radiation energy by polar ice can be considered (for the purposes of this theory) virtually independent of the fabric (Hobbs 1974; Faria *et al.* 2003). Consequently, the external supplies appearing in $(2.2)^{\text{II}}$–$(2.6)^{\text{II}}$ and $(2.9)^{\text{II}}$ reduce to $c_i^* = 0$, $g_i^* = g_i$, and $r^* = r$, with an entropy supply in the ordinary form $s^* = s = r/T$.

3. Conservation of species linear momentum. As explained in §3b of Part I, the vectors κ_i^* and $\partial_j \tau_{ij}^*$ appearing in $(3.23)^{\text{I}}$ and $(2.5)^{\text{II}}$ can be interpreted as production rates of linear momentum associated to high- and low-angle interactions, respectively. Such productions should play an important role when grain shifting is relevant, viz. $v_i^* \neq v_i$. However, for ice sheets this is not the case (cf. remark 2.1) and therefore the relevance of κ_i^* and τ_{ij}^* becomes doubtful. Furthermore, from $(3.63)^{\text{II}}_{13}$ and $(3.64)^{\text{II}}_{5}$ we realize that —in the absence of grain shifting— the constitutive equations for κ_i^* and τ_{ij}^* are demoted to productions of linear momentum by gradients of temperature: a kind of thermomechanical coupling irrelevant for ice sheets. On these grounds it makes sense to impose $\kappa_i^* = \tau_{ij}^* = 0$.

4. Non-linearity of dislocation production by straining. As stated in remark 3.3 of Part II, the production of dislocations by straining along the c-axis direction should be strongly dependent on the slip activity in pyramidal planes, so that it is expected to vanish in materials whose pyramidal slip systems are hardly active, like polar ice (Hondoh 2000). Thus, for ice sheets we may set $\Pi_{\text{D}}^{*(2)} = 0$ in $(3.64)^{\text{II}}_{2}$.

5. On interspecies fluxes. The interspecies fluxes ξ_i^* and φ_i^* appearing in $(2.6)^{\text{II}}$ and $(2.9)^{\text{II}}$ should describe the transport of energy and entropy by dislocations

moving along bent crystallites and through subgrain boundaries, i.e. they should be proportional to the interspecies flux of dislocations $j^*_{\mathrm{D}\,i}$ (cf. $(2.3)^{\mathrm{II}}$). In ice sheets, bent crystallites and subgrain boundaries may indeed be found throughout (Faria & Kipfstuhl 2004), but most dislocations are expected to be *geometrically necessary* (Montagnat *et al.* 2003) and consequently not freely mobile. Thus, it seems fair to suppose that $j^*_{\mathrm{D}\,i} = \xi^*_i = \varphi^*_i = \iota^*_i = 0$ holds for polar ice. As a consequence, it follows from $(3.63)^{\mathrm{II}}_{12}$ that $\pi_{ij} = 0$.

6. Exclusion of crossed products of non-equilibrium variables. Even after all the simplifications discussed so far, the set of field equations derived from $(2.2)^{\mathrm{II}}$–$(2.6)^{\mathrm{II}}$, $(2.9)^{\mathrm{II}}$ and $(3.61)^{\mathrm{II}}$–$(3.64)^{\mathrm{II}}$ is still formidable. The reason is the presence of crossed products like $D_{\langle ij\rangle}H^*_{jk}$, $D_{\langle ij\rangle}T_{,j}$, etc. Such products are difficult to interpret physically and make the mathematics quite involved. Therefore, for practical reasons it is advisable to discard crossed terms from all constitutive equations listed in $(3.61)^{\mathrm{II}}$–$(3.64)^{\mathrm{II}}$. It should be noticed that this exclusion does not remove entirely the couplings between the field equations. Moreover, the non-linearity of the constitutive functions remains in self-products like $D_{\langle ik\rangle}D_{\langle kj\rangle}$, $(\Gamma^*)^{2/3}$, etc.

3. A simple continuum theory for polycrystalline ice sheets

The simplifications discussed in the last section are listed in reversed order of generality: the first ones are quite obvious and general, whereas the last ones are somewhat more restrictive and specialized. In particular, the last assumption applied to $(3.60)^{\mathrm{II}}$ yields conspicuous restrictions upon the constitutive relations for σ^*_{ij}, $t^*_{[ij]}$, q^*_i and P^*, since crossed products of non-equilibrium variables are excluded from $(3.60)^{\mathrm{II}}$. The results of these simplifications are listed below.

(*a*) *Constitutive equations for polycrystalline ice sheets*

From the simplifications put forward in the last section, we conclude that $(3.61)^{\mathrm{II}}$–$(3.64)^{\mathrm{II}}$ reduce to (see also Appendix A of Part I)

⇛ fundamental scalar relations:

$$\begin{gathered}
e^* = e^*(\varrho^*, \rho^*_{\mathrm{D}}, T)\,, \qquad \eta^* = \eta^*(\varrho^*, \rho^*_{\mathrm{D}}, T)\,, \qquad \psi^* := e^* - T\eta^*\,,\\
c^*_{\mathrm{D}} := \frac{\rho^*_{\mathrm{D}}}{\varrho^*}\,, \qquad \Psi^*(\varrho^*, c^*_{\mathrm{D}}, T) := \psi^*(\varrho^*, \varrho^* c^*_{\mathrm{D}}, T)\,, \qquad \eta^* = -\frac{\partial\Psi^*}{\partial T} = -\frac{\partial\psi^*}{\partial T}\,,\\
p^* = \varrho^{*2}\frac{\partial\Psi^*}{\partial\varrho^*} = \varrho^*\left(\varrho^*\frac{\partial\psi^*}{\partial\varrho^*} + \rho^*_{\mathrm{D}}\frac{\partial\psi^*}{\partial\rho^*_{\mathrm{D}}}\right)\,, \qquad \mu^*_{\mathrm{D}} := c^*_{\mathrm{D}}\frac{\partial\Psi^*}{\partial c^*_{\mathrm{D}}} = \rho^*_{\mathrm{D}}\frac{\partial\psi^*}{\partial\rho^*_{\mathrm{D}}}\,,\\
h^* := e^* + p^*/\varrho^*\,, \qquad g^* := h^* - T\eta^* = \frac{\partial\varrho^*\psi^*}{\partial\varrho^*} + \mu^*_{\mathrm{D}}\,,\\
\mathrm{d}\eta^* = \frac{1}{T}\left(\mathrm{d}e^* - \frac{p^*}{\varrho^{*2}}\mathrm{d}\varrho^* - \frac{\mu^*_{\mathrm{D}}}{c^*_{\mathrm{D}}}\mathrm{d}c^*_{\mathrm{D}}\right)\,,
\end{gathered} \tag{3.1}$$

⇛ dislocation parameter:

$$\gamma^* = \gamma^*(n_k n_s; \varrho^*, \rho^*_{\mathrm{D}}, \beta^*_{\varkappa}, \Gamma^*, H^*_{lm}; T, D_{\langle pq\rangle}, T_{,r}\,)\,, \tag{3.2}$$

$\Rrightarrow$ fluxes and stresses:

$$
\begin{gathered}
t^*_{ij} = -p^*\delta_{ij} + \sigma^*_{ij} + t^*_{[ij]} \ , \qquad \sigma^*_{ij} = \mu^*_{ijkl} D_{\langle kl\rangle} \ , \qquad t^*_{[ij]} = \theta^*_{ijkl} H^*_{kl} \ , \\
m^*_{ij} = \varphi^*_i = \xi^*_i = j^*_{\mathrm{D}\,i} = \tau^*_{ij} = 0 \ , \\
\phi^*_i = \frac{q^*_i}{T} \ , \qquad q^*_i = -k^*_{ij}\frac{\partial T}{\partial x_j} \ , \qquad \varpi^*_{ij} = p^*\epsilon_{ijk} n_k \ ,
\end{gathered}
\tag{3.3}
$$

$\Rrightarrow$ production rate terms:

$$
\begin{gathered}
\varepsilon^* = h^*\Gamma^* + \varepsilon^*_{\mathrm{NL}} \ , \qquad \Pi^*_{\mathrm{D}} = \rho^*_{\mathrm{D}}\Gamma^* + \Pi^*_{\mathrm{D\,NL}} \ , \qquad \delta^* = \eta^*\Gamma^* + \delta^*_{\mathrm{NL}} \ , \\
\varrho^*\left(\varepsilon^*_{\mathrm{NL}} - T\delta^*_{\mathrm{NL}} - \frac{\mu^*_{\mathrm{D}}}{\rho^*_{\mathrm{D}}}\Pi^*_{\mathrm{D\,NL}}\right) = P^*\Gamma^* \ , \\
\kappa^*_i = 0 \ , \qquad \nu^*_i = \epsilon_{ijk}\nu^{*(1)}_{lj} H^*_{kl} + N^*_i \ , \qquad N^*_i := \epsilon_{ijk}\nu^{*(2)}_{lj} D_{\langle kl\rangle} \ ,
\end{gathered}
\tag{3.4}
$$

where e^*, η^*, ψ^*, c^*_{D}, μ^*_{D}, h^* and g^* are the specific species fields of internal energy, entropy, Helmholtz free energy, concentration of dislocations, dislocation potential, free enthalpy and Gibbs free energy, respectively. Further, t^*_{ij}, p^*, σ^*_{ij}, m^*_{ij}, ϕ^*_i and q^*_i stand for the species fields of Cauchy stress, thermodynamic pressure, symmetric dissipative stress, Voigt couple stress, entropy and heat fluxes, while $D_{\langle ij\rangle}$ is the strain rate. Interspecies fluxes of entropy, heat, dislocations, linear and angular momenta are given by φ^*_i, ξ^*_i, $j^*_{\mathrm{D}\,i}$, τ^*_{ij} and ϖ^*_{ij}, respectively, while ε^*, Γ^*, Π^*_{D}, δ^*, κ^*_i and ν^*_i denote the specific production rates of internal energy, mass, dislocations, entropy, linear and angular momenta, with $(\cdot)_{\mathrm{NL}}$ indicating strictly non-linear dependence on dissipative variables. Finally, P^* is the driving pressure for recrystallization. (cf. Part II).

By combining condition 6 of §2b with $(3.60)^{\mathrm{II}}$, (3.3) and (3.4) we infer

$$
\left\{\mu^*_{ijkl}, \nu^{*(2)}_{ij}\right\} = \mathfrak{M}_\chi\left(\varrho^*, \rho^*_{\mathrm{D}}, \beta^*_\varkappa, T, D_{\langle ij\rangle}, n_i n_j\right) \ , \qquad \chi = 1, 2, \ldots 90 \ , \tag{3.5}
$$

$$
\left\{\theta^*_{ijkl}, k^*_{ij}, \nu^{*(1)}_{ij}\right\} = \mathfrak{N}_\lambda\left(\varrho^*, \rho^*_{\mathrm{D}}, \beta^*_\varkappa, T, n_i n_j\right) \ , \qquad \lambda = 1, 2, \ldots 99 \ . \tag{3.6}
$$

From (3.6) follow the explicit representations

$$
\begin{gathered}
\theta^*_{ijkl} = 2\,\theta^{*(1)}\delta_{ki}\delta_{jl} + \theta^{*(2)} n_k n_{[i}\delta_{j]l} \ , \\
k^*_{ij} = k^{*(1)}\delta_{ij} + k^{*(2)} n_i n_j \ , \qquad \nu^{*(1)}_{lj} = \nu^{*(1,1)}\delta_{lj} + \nu^{*(1,2)} n_l n_j \ ,
\end{gathered}
\tag{3.7}
$$

where the scalar coefficients $\theta^{*(\zeta)}$, $k^{*(\zeta)}$, $\nu^{*(1,\zeta)}$ $(\zeta = 1, 2)$ depend solely on ϱ^*, ρ^*_{D}, $\beta^*_\varkappa$, and T. In contrast, explicit expressions for μ^*_{ijkl} and $\nu^{*(2)}_{ij}$ are in general quite intricate, owing to their non-linear dependence on $D_{\langle ij\rangle}$ and n_i, so that they are useful only in specialized cases (cf. §4). Instead, it is often simpler to work with the dissipative stress σ^*_{ij} and the interaction couple N^*_i, which from $(3.3)_2$, $(3.4)_7$ and (3.5) have the general representations (cf. Liu 2002)

$$
\begin{aligned}
\sigma^*_{ij} = {} & \sigma^{*(1)}\delta_{ij} + \sigma^{*(2)} n_{\langle i} n_{j\rangle} + \sigma^{*(3)} D_{\langle ij\rangle} \\
& + \sigma^{*(4)} D_{\langle ik\rangle} D_{\langle kj\rangle} + \sigma^{*(5)} n_{\langle k} n_{(i} D_{\langle j)k\rangle} + \sigma^{*(6)} D_{\langle ik\rangle} D_{\langle jl\rangle} n_{\langle k} n_{l\rangle} \ ,
\end{aligned}
\tag{3.8}
$$

with $\sigma^{*(1)}\big|_{\mathrm{E}} = \sigma^{*(2)}\big|_{\mathrm{E}} = 0$, and

$$
\begin{aligned}
N^*_k = {} & N^{*(1)}\epsilon_{ijk}\, n_i D_{\langle jl\rangle} n_l \\
& + N^{*(2)}\epsilon_{ijk}\, n_i D_{\langle jl\rangle} D_{\langle lp\rangle} n_p + N^{*(3)}\epsilon_{ijk}\, n_q D_{\langle qi\rangle} D_{\langle jl\rangle} D_{\langle lp\rangle} n_p \ ,
\end{aligned}
\tag{3.9}
$$

where all scalar coefficients, viz. $\sigma^{*(\tau)}$ ($\tau = 1, \ldots, 6$) and $N^{*(\xi)}$ ($\xi = 1, 2, 3$), are functions of ϱ^*, ρ^*_{D}, $\beta^*_{\varkappa}$, T and the invariants $D_{\langle ij\rangle} D_{\langle ji\rangle}$, $D_{\langle ij\rangle} D_{\langle jk\rangle} D_{\langle ki\rangle}$, $D_{\langle ij\rangle} n_{\langle i} n_{j\rangle}$ and $D_{\langle ij\rangle} D_{\langle jk\rangle} n_{\langle k} n_{i\rangle}$. Additionally, by introducing the *species grain boundary mobility* M^*, defined in Appendix B, we conclude that the recrystallization pressure P^* can be written as

$$P^* = (f^*)^{\frac{1}{3}} \frac{Nb}{3M^*} \Gamma^* , \qquad \text{with} \qquad M^* = M^*(\varrho^*, \rho^*_{\mathsf{D}}, \beta^*_{\varkappa}, T; \Gamma^*) , \tag{3.10}$$

where $f^* := \varrho^*/\varrho$ is the *species mass fraction*, $b = 0.452$ nm is the magnitude of the *Burgers vector* of ice (Frost & Ashby 1982; Hondoh 2000) and $N \approx 2.21 \times 10^9$ (in SI units) is the number of Burgers vectors needed to form a unit length.

(*b*) *Energetics and arrangement of dislocations*

In Part II (Faria *et al.* 2006), the dislocation potential μ^*_{D} and the specific Gibbs free energy g^* have been introduced. Their difference was denoted by $g^*_{\mathsf{id}} := g^* - \mu^*_{\mathsf{D}}$ and interpreted as the specific Gibbs free energy in the absence of dislocations, i.e. in an aggregate of ideal crystallites. A similar decomposition can be now proposed for other quantities, e.g. (cf. $(3.1)_3$ and Appendix A of Part I)

$$\psi^*_{\mathsf{id}} + \psi^*_{\mathsf{D}} = (e^*_{\mathsf{id}} + e^*_{\mathsf{D}}) - T\,(\eta^*_{\mathsf{id}} + \eta^*_{\mathsf{D}}) \ , \tag{3.11}$$

in such a manner that, by definition, we may generally expect

$$\lim_{\rho^*_{\mathsf{D}} \to 0} (\,\cdot\,)^*_{\mathsf{D}} = 0 \qquad \text{and} \qquad \frac{\partial (\,\cdot\,)^*_{\mathsf{id}}}{\partial \rho^*_{\mathsf{D}}} = 0 \ . \tag{3.12}$$

Conditions (3.12) imply that $(\,\cdot\,)^*_{\mathsf{id}}$-type quantities cannot be a function of ρ^*_{D}, so that all dislocation properties must be incorporated into $(\,\cdot\,)^*_{\mathsf{D}}$. These conclusions motivate the equations of state presented below.

According to the elementary theory of dislocation energetics (Suzuki *et al.* 1991; Weertman & Weertman 1992; Humphreys & Hatherly 2004), the elastic energy stored in a unit length of dislocation can be estimated by $\bar{c}\,Gb^2$, where $\bar{c} \sim 0.7$ is a fitting constant and $G(T)$ is the *shear modulus* of ice (see e.g. Frost & Ashby 1982). Likewise, the entropy in a unit length of dislocation is roughly evaluated by $b^{-1} k_{\mathsf{B}} \ln 5$ (Weertman & Weertman 1992), where $k_{\mathsf{B}} \approx 1.38 \times 10^{-23}$ J K^{-1} is the Boltzmann constant. Consequently, the densities of internal energy and entropy stored in dislocations can be estimated by the expressions

$$\varrho^* e^*_{\mathsf{D}} = \bar{c}\,\rho^*_{\mathsf{D}} G b^2 \qquad \text{and} \qquad \varrho^* \eta^*_{\mathsf{D}} = \frac{\rho^*_{\mathsf{D}}}{b}\, k_{\mathsf{B}} \ln 5 \ , \tag{3.13}$$

where the stored energy e^*_{D} is in some cases called the specific *lattice distortion energy* (e.g. Montagnat *et al.* 2003). Equations $(3.1)_{1-5}$ and (3.13) imply the following form for the specific Helmholtz free energy

$$\Psi^* = \Psi^*_{\mathsf{id}} + \left(\bar{c}\,Gb^2 - \frac{k_{\mathsf{B}} T}{b} \ln 5 \right) c^*_{\mathsf{D}} \ , \qquad \text{with} \qquad \Psi^*_{\mathsf{id}} = \psi^*_{\mathsf{id}} = \psi^*_{\mathsf{id}}(\varrho^*, T) \ . \tag{3.14}$$

Thus, from $(3.1)_8$ and (3.14) we derive the dislocation potential

$$\mu^*_{\mathsf{D}} = \Psi^*_{\mathsf{D}} = \left(\bar{c}\,Gb^2 - \frac{k_{\mathsf{B}} T}{b} \ln 5 \right) c^*_{\mathsf{D}} \ . \tag{3.15}$$

Evidently, the linear expressions proposed above for the dislocation energetics are rather modest, being justified by the small energies involved in grain boundary migration and recrystallization. Following these arguments, we are motivated to describe the arrangement of dislocations within the polycrystal in the simplest possible way as well, observing however the consistency with the fundamental properties of the dislocation parameter γ^* (cf. §3a of Part II). Briefly, γ^* must be a non-dimensional field, which depends on integrals over $\mathcal{S}^2$ involving ρ_{D}^* and occasionally also ϱ^*; further, it must obey the condition $\gamma^*|_{\mathrm{E}} = 0$ (see remark 3.4 of Part II). One of the simplest definitions of this kind is†

$$\gamma^* = \frac{c_{\mathrm{D}}^* - c_{\mathrm{D}}}{c_{\mathrm{D}}^{\mathrm{R}}} \,, \qquad \text{with} \qquad c_{\mathrm{D}} = \int_{\mathcal{S}^2} f^* c_{\mathrm{D}}^* \, \mathrm{d}^2 n \,, \tag{3.16}$$

where $c_{\mathrm{D}}(x_i, t)$ denotes the *average concentration of dislocations in the polycrystal* (cf. $(3.27)^{\mathrm{I}}$ and $(3.29)^{\mathrm{I}}$) and $c_{\mathrm{D}}^{\mathrm{R}}$ is simply an arbitrary dimensional constant, called the *reference concentration of dislocations*, used to adjust the order of magnitude of γ^*. Finally, from (3.15) and (3.16) we find

$$\gamma^* = \frac{\mu_{\mathrm{D}}^* - \mu_{\mathrm{D}}}{\mu_{\mathrm{D}}^{\mathrm{R}}} \,, \qquad \text{with} \qquad \mu_{\mathrm{D}} = \int_{\mathcal{S}^2} f^* \mu_{\mathrm{D}}^* \, \mathrm{d}^2 n \qquad \text{and} \qquad \mu_{\mathrm{D}}^{\mathrm{R}} := \mu_{\mathrm{D}}^* \Big|_{c_{\mathrm{D}}^* = c_{\mathrm{D}}^{\mathrm{R}}} \,, \tag{3.17}$$

where $\mu_{\mathrm{D}}(x_i, t)$ is the *average dislocation potential of the polycrystal* and $\mu_{\mathrm{D}}^{\mathrm{R}}(T)$ is the *reference dislocation potential* computed by setting $c_{\mathrm{D}}^* = c_{\mathrm{D}}^{\mathrm{R}}$ in (3.15).

Intuitively, we may expect from (3.17) and remark 3.4 of Part II that the dislocation parameter γ^* and the recrystallization rate Γ^* should be related somehow.† In order to find such a relation, we notice that, according to current theories of recrystallization (cf. Humphreys & Hatherly 2004), the average driving pressure for recrystallization should be tantamount to the difference of the dislocation potentials (i.e., the Gibbs free energies due to dislocations) in a given crystallite and in its surroundings. Motivated by this interpretation, we postulate

$$P^* := \varrho^* \left(\mu_{\mathrm{D}} - \mu_{\mathrm{D}}^* \right) \,. \tag{3.18}$$

Hence, comparison of (3.2) and (3.10) with (3.17) and (3.18) yields

$$\gamma^* = -(f^*)^{\frac{1}{3}} \frac{Nb}{3\varrho^* M^* \mu_{\mathrm{D}}^{\mathrm{R}}} \, \Gamma^* \,. \tag{3.19}$$

Relations (3.1)–(3.19) comprise the sought-after constitutive theory for polycrystalline ice sheets, including induced anisotropy and recrystallization in the 5-dimensional space of positions and lattice orientations $\mathbb{R}^3 \times \mathcal{S}^2$. Once appropriate forms for the $\widetilde{\varkappa}$ species fabric parameters $\beta_{\varkappa}^*$ are chosen (see Appendix C), and the equations of state for ideal crystallites $e_{\mathrm{id}}^*(\varrho^*, T)$ and $\eta_{\mathrm{id}}^*(\varrho^*, T)$ (or $\psi_{\mathrm{id}}^*(\varrho^*, T)$) are

† As discussed in Parts I and II, the integral $(3.16)_2$ is intended to cover all possible c-axis orientations, with $\mathrm{d}^2 n$ denoting the *infinitesimal normalized solid angle*, which is so defined as to yield unity when integrated over the whole $\mathcal{S}^2$. Hence, by letting θ and φ denote the polar and azimuthal angles of a spherical coordinate system, we have $\mathrm{d}^2 n = \sin\theta \, \mathrm{d}\varphi \, \mathrm{d}\theta / 4\pi$.

† Recall from §3c of Part II that Γ^* replaced γ^* as independent variable, under the supposition that Γ^* is invertible with respect to γ^*, and vice versa (cf. (3.2)).

known, then there remain only eighteen scalar coefficients (viz. $\theta^{*(\zeta)}$, $k^{*(\zeta)}$, $\nu^{*(1,\zeta)}$, $\sigma^{*(\tau)}$, $N^{*(\xi)}$, $\varepsilon^*_{\mathrm{NL}}$, $\Pi^*_{\mathrm{D\,NL}}$ and M^*, with $\zeta = 1, 2$, $\tau = 1, \ldots, 6$ and $\xi = 1, 2, 3$) to be determined either pragmatically (through experiments and field measurements) or by other means (e.g., statistical theories and numerical simulations). Thus, after insertion of (3.1)–(3.19) into $(2.2)^{\mathrm{II}}$–$(2.6)^{\mathrm{II}}$ of Part II, there arises a set of nine field equations which can be used to determine the basic fields (2.1), while the recrystallization rate Γ^* is calculated through (3.10) and (3.18).

(*c*) *Homogenization*

As commented in §3d of Part I (Faria 2006), the basic strategy of the theory of mixtures with continuous diversity applied to polycrystals is to solve the coupled problem of creep, evolving fabric and recrystallization on the species level, viz. the 5-dimensional space of positions and lattice orientations $\mathbb{R}^3 \times \mathcal{S}^2$. Then, once all species fields are determined, the behaviour of the polycrystal in the usual Euclidean space $\mathbb{R}^3$ can be derived by accounting for the responses of all lattice orientations, via the *homogenization rules* presented in Part I.

Of particular interest are the results that we can infer from $(3.27)^{\mathrm{I}}$, $(3.31)^{\mathrm{I}}$, $(3.33)^{\mathrm{I}}$ and $(3.34)^{\mathrm{I}}$. Firstly, from $(3.27)^{\mathrm{I}}$ and (3.16)–(3.18) we obtain

$$\int_{\mathcal{S}^2} \varrho^* \gamma^* \, \mathrm{d}^2 n = 0 \,, \qquad \int_{\mathcal{S}^2} P^* \, \mathrm{d}^2 n = 0 \,. \tag{3.20}$$

Secondly, by invoking $(3.3)_{4-6}$ and the assumptions $I = 0$ and $C^*_i := v^*_i - v_i = 0$ (cf. remark 2.1 and §2b), we conclude from $(3.33)^{\mathrm{I}}$ and $(3.34)^{\mathrm{I}}_1$ that

$$\phi_i = \frac{q_i}{T} \quad \text{and} \quad q_i = k_{ij} \frac{\partial T}{\partial x_j} \,, \quad \text{with} \quad k_{ij} = \int_{\mathcal{S}^2} k^*_{ij} \, \mathrm{d}^2 n \,, \tag{3.21}$$

whereas from (3.1), $(3.33)^{\mathrm{I}}$ and the fact that $t^*_{ij}|_{\mathrm{E}} = p^* \delta_{ij}$ we derive

$$p = \int_{\mathcal{S}^2} p^* \, \mathrm{d}^2 n \,, \quad \Longrightarrow \quad \varrho \, h = \int_{\mathcal{S}^2} \varrho^* h^* \, \mathrm{d}^2 n \,, \quad \varrho \, g = \int_{\mathcal{S}^2} \varrho^* g^* \, \mathrm{d}^2 n \,. \tag{3.22}$$

Finally, from (3.3), $(3.22)_1$, the assumptions $I = 0$, $c^*_i = 0$, $C^*_i := v^*_i - v_i = 0$ (cf. remark 2.1 and §2b), and the rules $(3.27)^{\mathrm{I}}$, $(3.31)^{\mathrm{I}}$ and $(3.33)^{\mathrm{I}}$, we can integrate the balance equation of spin $(2.4)^{\mathrm{II}}$ over $\mathcal{S}^2$ and deduce

$$\int_{\mathcal{S}^2} t^*_{[ij]} \, \mathrm{d}^2 n = 0 \,, \qquad t_{ij} = -p \, \delta_{ij} + \mu_{ijkl} D_{\langle kl \rangle} \,, \qquad \mu_{ijkl} = \int_{\mathcal{S}^2} \mu^*_{ijkl} \, \mathrm{d}^2 n \,. \tag{3.23}$$

As a result of (3.20)–(3.23), it follows that the homogenized balance equations for ice sheets correspond to balance equations for *ordinary* (*non-polar*) *continua*, viz. $(3.11)^{\mathrm{I}}$–$(3.16)^{\mathrm{I}}$. In other words, even though individual ice grains do behave as polar media, the intercrystalline interactions are such that all couples and stress asymmetries vanish on average, resulting in no net outcome.

Equation (3.23) is the starting point for anisotropic generalizations of *Glen's flow law*, which is the archetypal stress–strain-rate relation for isotropic ice (Glen 1953;

Hobbs 1974; Hutter 1983). Such generalizations depend on the explicit form of the shear viscosity tensor μ^*_{ijkl} (or equivalently, of the coefficients $\sigma^{*(\tau)}$ of (3.8), $\tau = 1, \ldots, 6$), while the fabric evolution is strongly affected by the explicit form of the spin viscosity tensor θ^*_{ijkl}, defined in $(3.3)_3$ and $(3.7)_1$. On these grounds, we conclude that a realistic species-stress/flow law for polycrystalline ice sheets should take into account the explicit dependencies of the viscosity tensors μ^*_{ijkl} and θ^*_{ijkl} not only upon temperature T, strain rate D_{ij}, mass density ϱ^* and lattice anisotropy n_i, but also on the dislocation density ρ^*_{D} and the species fabric parameters $\beta^*_{\varkappa}$ ($\varkappa = 1, \ldots, \widetilde{\varkappa}$; cf. remark 3.2 of Part II and Appendix C). The determination of such explicit expressions is nevertheless somewhat lengthy and will therefore be left for later parts of this series.

4. Relation to previous ice-sheet models

The results derived so far conclude the generic constitutive theory for anisotropic ice sheets undergoing recrystallization. In this section, we explore a few elementary forms of the viscosity tensor μ^*_{ijkl} which, although oversimplified, give rise to expressions comparable to known stress/flow laws for ice sheets.

(a) *The Svendsen–Gödert–Hutter stress law*

Consider for instance the simple choices below (cf. (3.8)):

$$\begin{aligned} &\sigma^{*(1)} = \tfrac{4}{3}\,(\mu_\perp - \mu_\parallel)\, f^* D_{\langle kl\rangle} n_{\langle k} n_{l\rangle}\ , && \sigma^{*(4)} = 0\ , \\ &\sigma^{*(2)} = (3\mu_{\mathrm{ax}} + \mu_\perp - 4\mu_\parallel)\, f^* D_{\langle kl\rangle} n_{\langle k} n_{l\rangle}\ , && \sigma^{*(5)} = 4\,(\mu_\parallel - \mu_\perp)\, f^*\ , \\ &\sigma^{*(3)} = 2\mu_\perp f^*\ , && \sigma^{*(6)} = 0\ , \end{aligned} \tag{4.1}$$

where the viscosity coefficients μ_{ax}, $\mu_\perp$ and $\mu_\parallel$ depend on temperature T, as well as on the scalar invariants of strain-rate $D_{\langle ij\rangle}$ and the so-called (irreducible) *structure tensor* A_{ij} (also named *orientation* or *alignment tensor*; see Doi & Edwards 1986; Ehrentraut & Muschik 1998)

$$A_{ij}(x_k, t) := \int\limits_{\mathcal{S}^2} f^* n_{\langle i} n_{j\rangle}\, \mathrm{d}^2 n\ . \tag{4.2}$$

Clearly, (4.1) is equivalent to the following shear viscosity tensor:

$$\begin{aligned} \mu^*_{ijkl} = {} & (3\mu_{\mathrm{ax}} + \mu_\perp - 4\mu_\parallel)\, f^* n_{\langle i} n_{j\rangle} n_{\langle k} n_{l\rangle} + 2\mu_\perp f^* \delta_{ik}\delta_{jl} \\ & + 2\,(\mu_\parallel - \mu_\perp)\, f^* \left(n_{\langle k} n_{(i\rangle} \delta_{j)l} + n_{\langle l} n_{(i\rangle} \delta_{j)k} - \tfrac{2}{3} n_{\langle k} n_{l\rangle} \delta_{ij} \right)\ , \end{aligned} \tag{4.3}$$

that can be readily integrated with the help of $(3.23)_3$ and (A 1) to†

$$\begin{aligned} \mu_{ijkl} = {} & (3\mu_{\mathrm{ax}} + \mu_\perp - 4\mu_\parallel)\, A_{ij} A_{kl} + 2\mu_\perp \delta_{ik}\delta_{jl} \\ & + 2\,(\mu_\parallel - \mu_\perp) \left(A_{k(i}\delta_{j)l} + A_{l(i}\delta_{j)k} - \tfrac{2}{3} A_{kl}\delta_{ij} \right)\ . \end{aligned} \tag{4.4}$$

† Equation (4.4) was derived with aid of the 'decoupling approximation' (Doi & Edwards 1986; Kröger & Sellers 1995): $\int_{\mathcal{S}^2} f^* n_{\langle i} n_{j\rangle} n_{\langle k} n_{l\rangle}\, \mathrm{d}^2 n \approx A_{ij} A_{kl}$. Better approximations (or higher-order tensors) could be used instead, but they would not yield the desired expression for μ_{ijkl}.

Insertion of (4.4) into (3.23) provides then

$$\begin{aligned}\sigma_{ij} = \; & 2\mu_\perp D_{\langle ij\rangle} + (3\mu_{\rm ax} + \mu_\perp - 4\mu_\parallel)\, A_{kl} D_{\langle lk\rangle} A_{ij} \\ & +4\,(\mu_\parallel - \mu_\perp)\left(A_{k(i} D_{\langle j)k\rangle} - \tfrac{1}{3} A_{kl} D_{\langle lk\rangle}\delta_{ij}\right) \;,\end{aligned} \tag{4.5}$$

which is quite similar to the stress laws for anisotropic ice sheets proposed by Svendsen & Hutter (1996) and Gödert & Hutter (1998).

Remark 4.1. In the derivation of (4.5) by Gödert & Hutter (1998) it was assumed that stress should be the same *in every grain* ('Sachs hypothesis'). In contrast, the current derivation does not impose any constraint upon the strain/stress on the grain scale (see remark 2.1). Further, the definition of structure tensor used by Svendsen & Hutter (1996) and Gödert & Hutter (1998) is not identical to (4.2), since the referred authors adopted a particular definition of orientational distribution function that accounts only for the *number* of grains with a given c-axis orientation, in contrast to the species mass fraction f^* used here, which accounts also for the volume fraction of each species (cf. §2b of Part II).

(*b*) *The Azuma–Goto-Azuma flow law*

Instead of (4.1), we could also make another simple choice for (3.8):

$$\begin{aligned} \sigma^{*(1)} &= -\tfrac{4}{3}\,\mu^* D_{\langle kl\rangle} n_{\langle k} n_{l\rangle} \;, & \sigma^{*(4)} &= 0 \;, \\ \sigma^{*(2)} &= -4\,\mu^* D_{\langle kl\rangle} n_{\langle k} n_{l\rangle} \;, & \sigma^{*(5)} &= 4\,\mu^* \;, \\ \sigma^{*(3)} &= \tfrac{4}{3}\,\mu^* \;, & \sigma^{*(6)} &= 0 \;, \end{aligned} \tag{4.6}$$

which is equivalent to the shear viscosity tensor

$$\mu^*_{ijkl} = 2\,\mu^*\big[n_i n_l\,(\delta_{jk} - n_j n_k) + n_j n_l\,(\delta_{ik} - n_i n_k)\big] \;, \tag{4.7}$$

where the scalar coefficient μ^* is a function of ϱ^*, $\rho^*_{\rm D}$, $\beta^*_\varkappa$, T, $D_{\langle ij\rangle}$, and the dyadic $n_i n_j$. Insertion of (4.7) into $(3.3)_2$ leads to

$$\sigma^*_{ij} = 2\,\mu^*\big[n_i\,(\delta_{jk} - n_j n_k) + n_j\,(\delta_{ik} - n_i n_k)\big] D_{\langle kl\rangle} n_l \;, \tag{4.8}$$

and consequently

$$\begin{aligned}\sigma^*_{ij} n_j &= 2\,\mu^*(\delta_{ik} - n_i n_k)\, D_{\langle kl\rangle} n_l \\ &= (\delta_{ik} - n_i n_k)\, \sigma^*_{kl} n_l \;.\end{aligned} \tag{4.9}$$

Hence, if we introduce the shorthands

$$t^*_i := (\delta_{ik} - n_i n_k)\, \sigma^*_{kl} n_l \qquad \text{and} \qquad d^*_i := (\delta_{ik} - n_i n_k)\, D_{\langle kl\rangle} n_l \;, \tag{4.10}$$

we can rewrite (4.9) as

$$t^*_i = 2\,\mu^*\, d^*_i \;. \tag{4.11}$$

The physics behind (4.6) is revealed by (4.10): the tensors $\sigma^{*\,\rm eff}_{ij} := (\delta_{ik} - n_i n_k)\, \sigma^*_{kj}$ and $D^{*\,\rm eff}_{ij} := (\delta_{ik} - n_i n_k)\, D_{\langle kj\rangle}$ represent the *effective stress and strain rate* in the crystallites with c-axes parallel to n_i. Thus, neither stress nor strain rate is the same for all species. Accordingly, the vectors t^*_i and d^*_i denote the *resolved stress*

and strain rate on the basal planes of the grains with c-axes parallel to n_i. In this sense, (4.11) describes an *average* viscous response by basal slip.

Now, if we set

$$\mu^* = \left(\tfrac{8}{5}A^* d_k^* d_k^*\right)^{-\frac{1}{3}} \ , \qquad \text{with} \qquad A^* = A^*\left(\varrho^*, \rho_{\mathrm{D}}^*, \beta_{\varkappa}^*, T\right) \ , \tag{4.12}$$

then we can perform the straightforward inversion

$$t_i^* = \left(\tfrac{1}{5}A^* d_k^* d_k^*\right)^{-\frac{1}{3}} d_i^* \qquad \Longleftrightarrow \qquad d_i^* = \tfrac{1}{5}A^*\left(t_k^* t_k^*\right) t_i^* \ . \tag{4.13}$$

On the other hand, by introducing the *Schmid tensor*

$$M_{ij}^* := \frac{t_i^* \, n_j}{\sqrt{t_k^* t_k^*}} \tag{4.14}$$

we find

$$\begin{aligned} t_k^* t_k^* = t_k^* \sigma_{kl}^* n_l &= \left(\sigma_{kl}^* M_{\langle kl\rangle}^*\right)\left(t_k^* t_k^*\right)^{\frac{1}{2}} \\ &= \left(\sigma_{kl}^* M_{\langle kl\rangle}^*\right)\frac{t_k^* t_k^*}{\sqrt{t_k^* t_k^*}} = \left(\sigma_{kl}^* M_{\langle kl\rangle}^*\right)^2 \ , \end{aligned} \tag{4.15}$$

so that

$$d_i^* n_j = \tfrac{1}{5}A^*\left(\sigma_{kl}^* M_{\langle kl\rangle}^*\right)^3 M_{ij}^* \ . \tag{4.16}$$

Finally, with the aid of (A 5), we compute the integral

$$\int\limits_{\mathcal{S}^2} d_i^* n_j \, \mathrm{d}^2 n = \int\limits_{\mathcal{S}^2} \left(\delta_{ik} - n_i n_k\right) D_{\langle kl\rangle} n_l n_j \, \mathrm{d}^2 n = \tfrac{1}{5} D_{\langle ij\rangle} \ , \tag{4.17}$$

which implies

$$D_{\langle ij\rangle} = \int\limits_{\mathcal{S}^2} A^*\left(\sigma_{kl}^* M_{\langle kl\rangle}^*\right)^3 M_{\langle ij\rangle}^* \, \mathrm{d}^2 n \ . \tag{4.18}$$

This last equation is of particular importance: it resembles somewhat the flow law proposed by Azuma & Goto-Azuma (1996), viz.

$$D_{\langle ij\rangle} = A \exp\left(-\frac{Q}{k_{\mathrm{B}} T}\right)\left(\sigma_{kl} M_{\langle kl\rangle}\right)^3 M_{\langle ij\rangle} \ , \tag{4.19}$$

$$\text{with} \qquad M_{ij} = \int\limits_{\mathcal{S}^2} M_{ij}^* \, \mathrm{d}^2 n \ , \tag{4.20}$$

where A is a material parameter and Q is an activation energy. Evidently, the flow laws (4.18) and (4.19) are not identical in general. Nevertheless, it is possible to derive (4.19) from (4.18) if we impose some additional conditions:

1. set $A^* = A \exp\left(-Q/k_{\mathrm{B}} T\right)$;

2. take for granted the 'Sachs hypothesis' $\sigma_{ij}^*(x_i, t, n_j) \equiv \sigma_{ij}(x_i, t)$;

3. adopt the following approximation (Thorsteinsson *et al.* 1999):

$$\int\limits_{\mathcal{S}^2}\left(M_{\langle ij\rangle}^* M_{\langle kl\rangle}^* M_{\langle pq\rangle}^* M_{\langle rs\rangle}^*\right) \mathrm{d}^2 n \approx M_{\langle ij\rangle} M_{\langle kl\rangle} M_{\langle pq\rangle} M_{\langle rs\rangle} \ .$$

Remark 4.2. It must be emphasized that the additional conditions listed above were originally not invoked by Azuma & Goto-Azuma (1996). Indeed, although the mentioned conditions are tolerable, it is evident that (4.18) may be equivalent to (4.19) only under very restricted circumstances.

5. Conclusion

Large-scale continuum theories for polycrystals are essential in geophysical applications, and in particular for the modelling of ice sheets. However, incorporation of recrystallization into continuum approaches has been a problematic task for ice sheet modellers. In the present work, a set of constitutive relations has been established for the thermomechanics of cold ice sheets, with consideration of strain-induced anisotropy and recrystallization. These constitutive relations should be combined with the balance equations put forward in Part II in order to give rise to a thermomechanical field theory for polycrystalline ice sheets. The cornerstone of this theory is the characterization of the polycrystal as a *mixture with continuous diversity* —more precisely a *mixture of lattice orientations*— in the manner explained in Parts I and II (Faria 2006; Faria *et al.* 2006).

In contrast to former attempts to model recrystallization through artificial assumptions (e.g., Van der Veen & Whillans 1994; Staroszczyk & Morland 2001), the current approach incorporates polygonization, recovery and recrystallization in a consequent and natural way, through the introduction of the c-axis spin velocity s_i^*, the polygonization tensor ϖ_{ij}^*, the production rate of dislocations Π_{D}^*, the recrystallization pressure P^*, the dislocation potential μ_{D}^* and the recrystallization rate Γ^*, among other quantities (see (3.1)–(3.4)). Fabric (texture) is described by the species mass density $\varrho^*(x_i, t, n_j)$, or alternatively the species mass fraction $f^*(x_i, t, n_j) := \varrho^*/\varrho$, which stands for the mass/volume fraction of grains with c-axes oriented in the n_i-direction. This description of fabric represents a great advantage in comparison to former ice-sheet models based on a simplified definition of orientational distribution function that reckons simply the number of grains in each orientation, regardless of their sizes (Meyssonnier & Philip 1996; Svendsen & Hutter 1996; Gödert & Hutter 1998).

Furthermore, the current theory imposes no constraint at all upon the strain or stress of individual crystallites (see remark 2.1), in contrast to most ice-sheet models based on restrictive assumptions like Voigt–Taylor and Sachs–Reuss upper and lower bounds (Lliboutry 1993; Van der Veen & Whillans 1994; Castelnau *et al.* 1996; Gödert & Hutter 1998; Thorsteinsson *et al.* 1999). Indeed, the theory presented here comes from the line of large-scale ('macroscopic') continuum approaches that ignore inhomogeneities on the grain scale, by regarding ice-sheet particles big enough to encompass myriads of grains (Hutter 1983; Morland 1984; Greve 1997; Morland & Staroszczyk 1998). Nevertheless, in contrast to the continuum approach by Morland & Staroszczyk (1998) (the so-called 'orthotropic ice model', see also Staroszczyk & Morland 2001), which is based on the simplistic hypothesis that fabric and deformation are directly correlated,† the effects of fabric and recrystallization are incorporated in the present theory by regarding the ice sheet as a

† As pointed out by Placidi *et al.* (2003), one of the greatest shortcomings of this hypothesis is that it implies a 'reversible fabric', i.e. the fabric returns to its initial configuration when the deformation is reversed.

mixture with continuous diversity. This scheme enables us to obtain a precise description of microstructure evolution without giving up the large-scale character, i.e. without the need to refer to the micromechanics of individual crystallites.

Among the most relevant results of the constitutive theory, we found that the ice sheet behaves as an ordinary (i.e., non-polar) material, since the species Voigt couple stress m^*_{ij} vanishes identically (see $(3.3)_4$) and the Cauchy stress t_{ij} of the 'mixture' is symmetric (cf. (3.23)). Notice however that couples may exist on the grain scale, owing to the asymmetry of the species Cauchy stress t^*_{ij} (see $(3.3)_{1-3}$). Additionally, bending and twisting couples associated to polygonization —modelled by the tensor ϖ^*_{ij} (cf. $(2.4)^{\text{II}}$ and §4 of Part II)— are generated by directional inhomogeneities in the species pressure p^*, see $(3.3)_7$. Another conclusion is that the species fields of Cauchy stress t^*_{ij} and heat flux q^*_i do not depend *directly* on the recrystallization rate Γ^*. However, they depend upon the *current fabric* outlined by the species mass density ϱ^*, the species fabric parameters $\beta^*_\varkappa$ (with $\varkappa = 1, \ldots, \widetilde{\varkappa}$), and the c-axis orientation n_i. Moreover, according to (3.13) and (3.14) the species densities of internal energy, entropy, and Helmholtz free energy are all linearly proportional to the dislocation density ρ^*_{D}, implying via $(3.1)_8$ and (3.15) that the dislocation potential μ^*_{D} is equal to the Helmholtz free energy of dislocations Ψ^*_{D}. Thus, from $(3.1)_{9,10}$, (3.12), and the discussion in §3b, we conclude that the species enthalpy of dislocations h^*_{D} is identical to the stored energy e^*_{D}, defined in (3.13). Finally, from (3.18) we have that the recrystallization pressure P^* is linearly proportional to the dislocation parameter γ^*, defined as the dimensionless difference of the dislocation potentials, i.e. the Gibbs free energies due to dislocations, of crystallites with distinct c-axis orientations (cf. (3.17)).

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Appendix A. Useful integrals

Homogenization of species fields often involves integrals of the orientation vector n_i and the species mass fraction $f^* := \varrho^*/\varrho$. Therefore, it is helpful to have a list of the most frequent integrals of this kind, for further reference. We start with four elementary integrals (cf. $(3.27)^{\text{I}}_1$ and $(3.29)^{\text{I}}$ of Part I):

$$\int_{\mathcal{S}^2} \mathrm{d}^2 n = 1 \,, \qquad \int_{\mathcal{S}^2} f^* \,\mathrm{d}^2 n = 1 \,, \qquad \int_{\mathcal{S}^2} n_i \,\mathrm{d}^2 n = 0 \qquad \int_{\mathcal{S}^2} f^* n_i \,\mathrm{d}^2 n = 0 \,, \tag{A 1}$$

where $(\mathrm{A}\,1)_1$ follows from the normalization of the infinitesimal solid angle $\mathrm{d}^2 n$. Equation $(\mathrm{A}\,1)_4$ vanishes because of the fore–aft symmetry of the c-axis (see hypothesis 3.1 of Part II), which implies that f^* is an even function of the orientation

vector n_i. Using the same argument, we immediately conclude that

$$\int_{\mathcal{S}^2} n_i n_j n_k \, \mathrm{d}^2 n = \int_{\mathcal{S}^2} n_i n_{\langle j} n_{k\rangle} \, \mathrm{d}^2 n = \int_{\mathcal{S}^2} n_{\langle i} n_j n_{k\rangle} \, \mathrm{d}^2 n = 0 \, , \tag{A 2}$$

$$\int_{\mathcal{S}^2} f^* n_i n_j n_k \, \mathrm{d}^2 n = \int_{\mathcal{S}^2} f^* n_i n_{\langle j} n_{k\rangle} \, \mathrm{d}^2 n = \int_{\mathcal{S}^2} f^* n_{\langle i} n_j n_{k\rangle} \, \mathrm{d}^2 n = 0 \, . \tag{A 3}$$

Notice that the tensor $n_{\langle i} n_j n_{k\rangle}$ is symmetric and traceless with respect to all indices within the angular brackets, viz. (cf. Appendix A of Part I)

$$n_{\langle i} n_j n_{k\rangle} = n_i n_j n_k - \tfrac{1}{5} \left(n_i \delta_{jk} + n_j \delta_{ik} + n_k \delta_{ij} \right) \, . \tag{A 4}$$

Evidently, $(\mathrm{A}\,1)_4$ and (A 3) remain valid when f^* is replaced by any other even function of n_i.

In contrast, two useful non-vanishing integrals are

$$\int_{\mathcal{S}^2} n_i n_j \, \mathrm{d}^2 n = \tfrac{1}{3} \delta_{ij} \quad \text{and} \quad \int_{\mathcal{S}^2} n_i n_j n_k n_l \, \mathrm{d}^2 n = \tfrac{1}{15} \left(\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \, , \tag{A 5}$$

which can be straightforwardly computed with the help of the spherical coordinates $0 \leqslant \theta < \pi$ and $0 \leqslant \varphi < 2\pi$, since we have in this case

$$n_1 = \sin\theta \, \cos\varphi \, , \quad n_2 = \sin\theta \, \sin\varphi \, , \quad n_3 = \cos\theta \, , \quad \mathrm{d}^2 n = \frac{\sin\theta}{4\pi} \, \mathrm{d}\theta \, \mathrm{d}\varphi \, . \tag{A 6}$$

The computation of more complex integrals can be found, e.g., in the works by Hess & Köhler (1980) and Ehrentraut & Muschik (1998).

Appendix B. Grain boundary mobility

The mobility of a grain boundary can be generically defined as the ratio between its normal speed of migration and the driving pressure acting on it (Humphreys & Hatherly 2004). In the present theory, however, this definition must be adapted somehow, since every material point of the continuum is supposed to contain a huge number of crystallites, and consequently also grain boundaries. In other words, we do not have the resolution to identify single grain boundaries. Rather, we can only describe their average behaviour (cf. remark 2.1).

We start by recalling that polar ice is modelled as an incompressible (density-preserving) material, so that the resultant mass of all crystallites that possess c-axes parallel to n_i, within a unit volume, is given by

$$m^* := \varrho^* N^3 b^3 = \varrho \, V^* \, , \tag{B 1}$$

where $\varrho \approx 0.920 \, \mathrm{g\,cm^{-3}}$ is the mass density of polar ice (Thorsteinsson 1996), $b = 0.452 \, \mathrm{nm}$ is the magnitude of the Burgers vector (Hobbs 1974; Hondoh 2000), $N \approx 2.21 \times 10^9$ (in SI units) is the number of Burgers vectors necessary to form a unit length, and $V^* := l^{*3}$ is the volume occupied by these particular crystallites. On the other hand, the product of the species mass density ϱ^* with the recrystallization

rate Γ^* and the unit volume N^3b^3 represents just the rate of increase/decrease of the mass m^* by grain boundary migration†, i.e. (cf. (2.2)^{II} of Part II)

$$\varrho^*\Gamma^*N^3b^3 = \dot{m}^* = \varrho\,\dot{V}^* = 3\,\varrho\,\dot{l}^*\,l^{*2}\ . \tag{B 2}$$

Hence, division of (B 2) by (B 1) results in

$$\Gamma^* = \frac{3\,\dot{l}^*}{l^*} = \frac{3\,\dot{l}^*\,(f^*)^{-\frac{1}{3}}}{Nb} \qquad \Longrightarrow \qquad \dot{l}^* = (f^*)^{\frac{1}{3}}\,\frac{Nb}{3}\,\Gamma^*\ . \tag{B 3}$$

Finally, we have by construction that $\dot{l}^*$ is the average *migration velocity* of the boundaries of those grains with c-axes parallel to n_i. Consequently, we can now introduce the definition of *species grain boundary mobility*

$$M^* := \frac{\dot{l}^*}{P^*} \tag{B 4}$$

where P^* denotes the driving pressure for grain boundary migration discussed in §3a and §3b. Hence, combination of (B 3) and (B 4) leads to (3.10),

$$P^* = (f^*)^{\frac{1}{3}}\,\frac{Nb}{3M^*}\,\Gamma^*\ . \tag{B 5}$$

Appendix C. Species fabric parameters

Throughout this work no restriction was imposed on the explicit forms of the $\widetilde{\varkappa}$ species fabric (texture) parameters $\beta^*_{\varkappa}$. The objective of this appendix is to discuss some possible forms of these parameters, for illustration.

Any reference to fabric parameters invariably calls to mind the notion of fabric statistics via eigenvalues of the structure tensor A_{ij} defined in (4.2) (Woodcock 1977; Thorsteinsson 1996; Azuma *et al.* 2000). Let the eigenvalues E^λ ($\lambda = \text{I}, \text{II}, \text{III}$) of A_{ij} be the scalars that satisfy the equation (*no sum over repeated* Greek *indices*)

$$A_{ij}a^\lambda_j = E^\lambda a^\lambda_i\ , \qquad\qquad E^{\text{I}} \geq E^{\text{II}} \geq E^{\text{III}}\ , \tag{C 1}$$

where a^λ_i denote the respective eigenvectors of A_{ij}. The largest eigenvalue, viz. E^{I}, indicates the amount of crystalline mass with c-axes concentrated near the mean direction a^{I}_i, about which the *'moment of inertia' of the fabric*† is minimized. This is easily understood if we observe that the specific 'inertia' tensor of the fabric is given by the integral (cf. (4.2) and (A 1))

$$\int\limits_{\mathcal{S}^2} f^*\,(\delta_{ij} - n_in_j)\ \mathrm{d}^2n \ = \ \tfrac{2}{3}\delta_{ij} - A_{ij}\ . \tag{C 2}$$

† For the current purposes we can neglect the effect of c-axis rotation by setting $u^*_i = 0$.

† By 'moment of inertia of the fabric' it should be understood the *fictitious* moment of inertia of the mass density ϱ^* distributed over $\mathcal{S}^2$, cf. (C 2). Admittedly, the notion of a fictitious 'moment of inertia' fails to hold when the fabric has a symmetry lower than orthorhombic (e.g. monoclinic and triclinic symmetries; Woodcock 1977), but such low-symmetric fabrics are in any case seldom in polar ice (Thorsteinsson 1996; Azuma *et al.* 2000; Wang *et al.* 2003).

Hence, if the c-axes are symmetrically distributed about a_i^{I}, then $E^{\mathrm{I}} > E^{\mathrm{II}} = E^{\mathrm{III}}$ and we have a *unimodal cluster texture*, also named *single maximum fabric*. Conversely, the eigenvector a_i^{III} (associated with the smallest eigenvalue E^{III}) is related to the largest 'moment of inertia' of the fabric. Hence, when $E^{\mathrm{I}} = E^{\mathrm{II}} > E^{\mathrm{III}}$ the c-axes form a *girdle* radially symmetric about the eigenvector a_i^{III} (which defines the pole of the girdle). Of course, an isotropic distribution of c-axes (so that $\varrho^* = \varrho$) implies the equality of all eigenvalues. Finally, it is a trivial exercise to show that, by using the Cayley–Hamilton theorem (see e.g. Liu 2002) and the properties of the tensor A_{ij}, the eigenvalues E^λ can be computed via‡

$$\begin{gathered} E^{\mathrm{I}} + E^{\mathrm{II}} + E^{\mathrm{III}} = 0\,, \qquad E^{\mathrm{I}}E^{\mathrm{II}}E^{\mathrm{III}} = \tfrac{1}{3}A_{ij}A_{jk}A_{ki}\,, \\ E^{\mathrm{I}}E^{\mathrm{II}} + E^{\mathrm{II}}E^{\mathrm{III}} + E^{\mathrm{I}}E^{\mathrm{III}} = -\tfrac{1}{2}A_{ij}A_{ji}\,. \end{gathered} \tag{C 3}$$

It should be noticed from $(\mathrm{C}\,3)_1$ that only two eigenvalues are independent. Thus, assuming that $\widetilde{\varkappa} = 4$, a first choice of species fabric parameters may be

$$\beta_1^* = (n_i a_i^{\mathrm{I}})^2\,, \quad \beta_2^* = (n_i a_i^{\mathrm{III}})^2\,, \quad \beta_3^* = E^{\mathrm{I}}\,, \quad \beta_4^* = E^{\mathrm{III}}, \tag{C 4}$$

where the first two parameters determine the orientation of the fabric with respect to n_i (i.e., the *relative* orientation of the eigenbasis of A_{ij}) while the last two describe the fabric shape.

There are, however, alternative measures of fabric shape in the place of E^{I} and E^{III}. We can employ e.g. the *Woodcock parameters* (Woodcock 1977)

$$K_{\mathrm{w}} := \frac{\ln(E^{\mathrm{I}}/E^{\mathrm{II}})}{\ln(E^{\mathrm{II}}/E^{\mathrm{III}})} \qquad \text{and} \qquad C_{\mathrm{w}} := \ln(E^{\mathrm{I}}/E^{\mathrm{III}})\,, \tag{C 5}$$

which measure girdle ($K_{\mathrm{w}} \to 0$) and cluster ($K_{\mathrm{w}} \to \infty$) shape tendencies, as well as the fabric strength ($C_{\mathrm{w}} = 0$ for isotropic fabric). Thus, a second choice of species fabric parameters could be

$$\beta_1^* = (n_i a_i^{\mathrm{I}})^2\,, \quad \beta_2^* = (n_i a_i^{\mathrm{III}})^2\,, \quad \beta_3^* = K_{\mathrm{w}}\,, \quad \beta_4^* = C_{\mathrm{w}}\,. \tag{C 6}$$

In some simple situations, in which it suffices to adopt just a coarse characterization of the fabric as an axisymmetric, unimodal c-axis distribution, it turns out that two of the eigenvalues E^λ coincide and only one eigenvector, a_i, is enough for defining the orientation of the fabric relative to the n_i direction. Under such particular conditions it might be appropriate to replace eigenvalues and Woodcock parameters by a more straightforward description of fabric, based solely on the relative orientation of the vectors a_i and n_i. Two common choices are the *degree of orientation* R_{g}, and the *spherical aperture* α_{s} (Thorsteinsson 1996; Wang *et al.* 2003), which can be defined in a continuum context by

$$R_{\mathrm{g}} := \int_{\mathcal{S}^2} \left\{ 2f^*(n_i n_j a_i a_j)^{\frac{1}{2}} - 1 \right\} \mathrm{d}^2 n \qquad \text{and} \qquad \alpha_{\mathrm{s}} := \arcsin\left(\sqrt{1 - R_{\mathrm{g}}}\right)\,. \tag{C 7}$$

‡ In the literature on structural analysis and petrography, the structure (or orientation) tensor is often defined with normalized trace (Woodcock 1977; Thorsteinsson 1996) instead of the traceless tensor A_{ij} introduced in (4.2). The use of a normalized structure (orientation) tensor would modify slightly certain relations, e.g. the right-hand side of (C 2) and (C 3), but it would not affect the physics. Notwithstanding, the adoption in this work of the traceless structure tensor A_{ij} is justified by its mathematical advantages, since it is irreducible.

Hence, two species fabric parameters are enough in this simplistic situation (i.e. $\widetilde{\varkappa} = 2$), and we can choose between the options (among others)

$$\beta_1^* = (n_i a_i)^2 \,, \quad \beta_2^* = R_{\mathrm{g}} \,, \qquad \text{or} \qquad \beta_1^* = (n_i a_i)^2 \,, \quad \beta_2^* = \alpha_{\mathrm{s}} \,. \tag{C 8}$$

Finally, we may also attack the problem of fabric parameters from a completely different viewpoint, by reckoning *intergranular interactions*. This kind of approach, often used in polymer science to describe excluded volume effects (Doi & Edwards 1986; Faria 2001), has the advantage of subsuming into itself a rough estimate of the energy and structure of the grain boundaries. In the simplest case, we may choose $\widetilde{\varkappa} = 1$ and propose the general expression

$$\begin{aligned} \beta^*(x_i, t, n_j) \;&=\; W_{\mathrm{iso}}^{-1} \int\limits_{\mathcal{S}^2} f^*(x_i, t, p_l)\, W^*(n_k p_k)\, \mathrm{d}^2 p \,, \\ \text{with} \qquad W_{\mathrm{iso}} \;&:=\; \int\limits_{\mathcal{S}^2} W^*(n_k p_k)\, \mathrm{d}^2 p \;=\; \text{const.} \,, \end{aligned} \tag{C 9}$$

where $p_i \in \mathcal{S}^2$ is an arbitrary orientation vector, $\mathrm{d}^2 p$ is its respective infinitesimal normalized solid angle, and $f^*(x_i, t, p_l)$ denotes the species mass fraction of crystallites with c-axes directed towards p_i. The species field $W^*(n_i p_i)$ stands for the *misorientation grain boundary energy*, while W_{iso} denotes the total grain boundary energy in an *isotropic polycrystal* such that $f^* = \beta^* = 1$ holds.

Evidently, the greatest disadvantage of (C 9) is that there is currently not enough data for conjecturing an explicit form for $W^*(n_i p_i)$.

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