

Max-Planck-Institut
für Mathematik
in den Naturwissenschaften
Leipzig

Creep and recrystallization of large
polycrystalline masses Part I: General continuum
theory

by

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Preprint no.: 71

2004



Creep and recrystallization of large polycrystalline masses

Part I: general continuum theory

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This is the first of a series of works on the continuum mechanics and thermodynamics of creep and recrystallization of large polycrystalline masses. The general continuum theory presented here is suited to mono- and multi-mineral rocks. It encompasses several symmetry groups (e.g. orthotropic and transversely isotropic) and diverse crystal classes of triclinic, monoclinic, and rhombic systems, among others. The cornerstone of the current approach is the theory of mixtures with continuous diversity, which allows one to regard the polycrystal as a ‘mixture of lattice orientations’. Following this picture, balance equations of mass, linear momentum, lattice spin, energy, dislocations, and entropy are set forth to describe the response of the polycrystal (i.e. the ‘mixture’), as well as of a group of crystallites sharing the same lattice orientation (viz. a ‘species’). The connection between the balance equations for a ‘species’ and those for the ‘mixture’ is established by homogenization rules, formulated for every field of the theory.

Keywords: continuous diversity; thermodynamics; mechanics; polycrystal; plasticity; anisotropy; fabric; texture; ice; olivine; rock-salt

1. Introduction

Geomorphological processes often involve the deformation of large masses of rock, flowing in a slow and continuous viscoplastic regime named *creep*. In nature, creeping rocks are seldom monomineral —like ice in glaciers and ice sheets, or pure halite (rock-salt) in salt domes and beds (Handin *et al.* 1986; Paterson 1994)— but sometimes one mineral may be predominant, constituting what is called the *primary* or *connected phase*: e.g. olivine in the upper mantle, or anhydrite-rich halite in large salt deposits in the crust (Hobbs *et al.* 1976; Chopra 1986). The corroboration of such a prevailing, connected phase is essential for regarding the medium (in a good approximation) as a monomineral rock. Nevertheless, in most common situations the material is indeed multi-mineral, and requires therefore a multiphase description. In this work, both cases (single- and multiphase modelling) will be addressed.

Independently of the mono- or multi-mineral character of the rock, its structure is typically *crystalline*. This means that minerals and rocks are generally composed of *crystallites* (also called *grains*) possessing a highly-ordered atomic structure: the *lattice*. The peculiar symmetry of the lattice, geometrically represented by *crystallographic axes* (Kocks *et al.* 1998), causes crystallites to be remarkably anisotropic. As a consequence, the orientational distribution of crystallographic

axes —called *texture*, or *fabric*†— is of prime importance for the mechanics of the rock. On the other hand, during deformation, the lattice of some crystallites may bend, twist, break, and rotate, changing so the original fabric. The latter may also be modified by the growth and shrink of grains, as well as by *dynamic recrystallization*, which involves the *nucleation* of new grains and the irregular *migration* of their boundaries (Poirier 1985; Humphreys & Hatherly 2004).

Besides all issues mentioned so far, the deformation of large rock masses is also complicated by its experimental unattainability: usual geomorphological processes last for millennia, reaching remarkably large strains in such a slow pace, that it is impossible to reproduce analogous conditions in laboratory. Further, field observations are often hindered by the environment, either because of inhospitality (e.g. ice sheets) or due to natural barriers (e.g. Earth’s mantle). Hence, to proceed on the subject, we are forced to rely on good hypotheses and theories.

This series is an attempt in that direction. Its objective is to present a general continuum theory for the mechanics and thermodynamics of large polycrystalline masses,† including fabric (i.e. texture) evolution, anisotropic response and recrystallization. The theory is intended for mono- and multi-mineral rocks and encompasses several symmetry groups, including transversely isotropic and orthotropic, as well as any crystal class whose symmetry is susceptible of being described in terms of three orthogonal axes. In this Part I, general balance equations and homogenization rules are presented. The ensuing Part II (Faria *et al.* 2005) deals with the construction of a thermodynamically consistent constitutive theory for a whole class of polycrystalline media. Finally, Part III (Faria 2005) illustrates the usefulness of the theory for the particular case of anisotropic ice sheets.

The structure of this article is as follows: §2 introduces the general formalism of mixtures with continuous diversity, which represents the cornerstone of the present theory, and shows how to incorporate polycrystals into this scheme. In §3, balance equations and homogenization rules are derived for monomineral rocks. Finally, §4 ends the article with remarks on the extension of the theory to multi-mineral rocks. Important information about *notation* is provided in Appendix A.

2. Polycrystals as mixtures with continuous diversity

At first sight, we could naively conjecture that polycrystalline minerals are simply dull gatherings of single crystals. However, the truth is much more complex than that: polycrystals are made of grains that interact continually through exchanges of mass, energy, momenta, and entropy. Thus, from a thermodynamic point of view, we may say that crystallites are *mutually-interacting open systems*.

(a) *Mixtures of crystallites*

Examples of interacting open systems are abundant in nature: granules with different sizes in a polydisperse granular medium, distinct phases of a material undergoing phase changes, incompatible populations disputing a common territory, chemical substances reacting in a mixture, just to mention some. All these examples

† In order to avoid the vocabulary conflict between geology and materials science, the terms ‘texture’ and ‘fabric’ are used here as synonyms to the preferred orientations of the lattice. No particular word is employed in reference to grain sizes and shapes.

† Here, ‘large’ means ‘big enough to allow the description of fabric through a continuous function’. In practice, we can bluntly estimate it as ‘ 10^{10^n} crystallites, with $n \geq 1$ ’ (cf. Part III).

have in common the fact that their dynamics is described by the same set of fundamental laws, which form the basis of the *standard theory of mixtures*. Of course, the word ‘mixture’ is used here in its broadest sense, as a ‘mixture of grain sizes’, a ‘mixture of phases’, a ‘mixture of populations’, or a ‘mixture of chemical substances’. It should be noticed that the identification of the constituents (or *species*) in these examples also differs from mixture to mixture. For instance, in mixtures of populations we can use either taxonomic or physiological attributes to identify the members of a species, whereas in a chemical mixture the species are distinguished by chemical composition. For polycrystals, there are many crystallite properties which can be used to identify a species, like grain size and shape, orientation of crystallographic axes, etc., depending on the characteristics of the material and the problem. Experience shows, however, that crystallographic orientation is frequently the most significant distinctive property. Hence, by adhering to such a characterization we may portray the polycrystal as a *mixture of orientations*, in the sense that grains with similar lattice orientations within the same aggregate should behave alike.‡

At this moment we face a technical problem: an appropriate mixture theory for polycrystals should be able to cope with all possible species, viz. an infinite number of them, for the lattice orientation may vary continuously in space. Standard mixture theory is not suitable for this case, since it can deal solely with a limited number of constituents. Hence, we are forced to resort to a different kind of theory, apt to model less orthodox types of mixtures possessing a *continuous diversity* of species.

(b) *Résumé of the theory of mixtures with continuous diversity*

Succinctly, a mixture with continuous diversity can be regarded as a multi-component medium made up of an infinite number of mutually-interacting species whose distinctive properties vary smoothly from one to another. As a matter of fact, the intuitive notion of continuous diversity is remarkably old (see Asimov 1979), and also its mathematical modelling is long-established, being formally rooted in Euler’s (1767) pioneering work on the demography of structured populations. Since then indeed, the same concept has been improved and/or independently rediscovered in diverse contexts, ranging from chemical mixtures (de Donder 1931; Aris & Gavalas 1966) and gas dynamics (Curtiss 1956; Dahler 1959) to anisotropic fluids (Condiff & Brenner 1969) and sea ice (Coon *et al.* 1974). Eventually, the term ‘mixture with continuous diversity’ has been coined (Faria 2001) in an effort to incorporate all those formerly unrelated approaches into a unified thermodynamic theory.

Mathematically, the idea of continuous diversity can be readily grasped by considering the example of an ordinary chemical mixture of N components. In this simple case, the mass density field of the α -th species at position x_i and time instant t is denoted by $\varrho^\alpha(x_i, t)$, with $\alpha = 1, 2, \dots, N$. Notice that the species label α is not just a counter: the mixture can only have a physical meaning if there exists a one-to-one relation between α and the distinctive properties of the constituents, e.g. $\alpha = 1 \mapsto$ liquid, $\alpha = 2 \mapsto$ solid, etc. Now, to derive the respective mass density

‡ The notion of a ‘mixture of orientations’ is well-established in the literature. In rheology, for instance, it has been invoked by Prager (1955), Curtiss (1956), Dahler (1959) and many others (see references in Faria 2001 and Faria & Hutter 2002). Within the context of crystal mechanics, models based on the concept of ‘orientational distribution function’ bear a noticeable resemblance to the present approach (cf. Zhang & Jenkins 1993; Kumar & Dawson 1996; Raabe & Roters 2004), although the analogy between polycrystals and ‘mixtures of orientations’ seems to have been first explicitly exploited by Faria *et al.* (2003).

field in a mixture with continuous diversity we must simply allow the species label α to be a real variable, defined in a compact interval $[\alpha_{\min}, \alpha_{\max}] = \mathcal{A} \subset \mathbb{R}$ called *species assemblage*. The end points α_{\min} and α_{\max} are generally chosen so that \mathcal{A} has *complete diversity*, i.e. it accounts for all possible species in the medium.

A result of the procedure outlined above is that $\alpha \in \mathcal{A}$ has acquired the status of a new variable, in addition to x_i and t , in such a manner that the mass density field of the α -th species[†] is given by $\varrho^*(x_i, t, \alpha)$ and should be interpreted as a density on $\mathbb{R}^3 \times \mathcal{A}$. The superscript ‘*’ indicates that the respective field is a function not only of x_i and t , but also of α . Of course, the same procedure can be extended to all other physical quantities of interest, enabling so the definition of the species fields of stress $t_{ij}^*(x_k, t, \alpha)$, internal energy $e^*(x_i, t, \alpha)$, velocity $v_i^*(x_j, t, \alpha)$, etc.

(c) *Definition of a crystalline species*

On many occasions it may happen that the specification of a species requires more than one distinctive property, in such a manner that multiple labels $\alpha_\gamma \in \mathcal{A}^\nu$ ($\gamma = 1, \dots, \nu$) must be introduced (Faria 2001). This is for instance the case of polycrystals modelled as ‘mixtures of crystallographic orientations’, for which we generally need $\nu = 3$, as explained below (see also Fig. 1).

We all know that lattice orientations can be represented in a number of ways, e.g. through *Euler angles*, *quaternions*, *Cayley–Klein parameters*, *Rodrigues vectors*, etc. (Synge 1960; Bunge 1993; Sutton & Balluffi 1995; Goldstein *et al.* 2002). Suppose we decide to use Euler angles, viz. φ , θ and ψ , which are the standard choice for the analytical treatment of fabrics. Thus, we could in principle set $\alpha_1 = \varphi$, $\alpha_2 = \theta$ and $\alpha_3 = \psi$, but this choice of labels turns calculations rather cumbersome. Instead, we follow the standpoint of Liu (1982, 2002) that constitutive relations for anisotropic media—including crystalline matter—are best expressed in terms of *anisotropic invariants*. In diverse situations these invariants account for anisotropy by means of an *orthogonal triad of unit vectors* $\{n_i^1, n_j^2, n_k^3\}$, which determines the axes of symmetry of the lattice. This is the case of transversely isotropic and orthotropic symmetries, as well as diverse crystal classes of triclinic, monoclinic and rhombic systems, among others (for a comprehensive list see Liu 1982).

Equivalence between the nine components of the triad $\{n_i^1, n_j^2, n_k^3\}$ and the three Euler angles φ , θ and ψ is established through the orthonormality conditions[‡]

$$n_k^1 n_k^1 = n_i^2 n_i^2 = 1, \quad n_k^1 n_k^2 = 0 \quad \text{and} \quad n_i^3 = \pm \epsilon_{ijk} n_j^1 n_k^2, \quad (2.1)$$

(cf. Appendix A), which imply that only three components of the triad are in fact independent: n_1^1 , n_2^1 and n_1^2 , say. As illustrated in figure 1b, we can easily identify these three key components with the labels α_1 , α_2 and α_3 which specify a species:

$$\begin{aligned} \alpha_1 &= n_1^1 = \sin \theta \cos \varphi, & \alpha_2 &= n_2^1 = \sin \theta \sin \varphi, \\ \alpha_3 &= n_1^2 = \cos \theta \cos \varphi \cos \psi - \sin \varphi \sin \psi. \end{aligned} \quad (2.2)$$

[†] As a matter of fact, the continuity of α renders the precise determination of a single, definite species impossible: only references to an ‘infinitesimal range of species’ $d\alpha$ (which includes α itself) have strict meaning. Notwithstanding, we adhere here, for simplicity, to the common shorthand ‘the species α ’ when referring to such a ‘species range’ (cf. Aris & Gavalas 1966; Faria *et al.* 2005).

[‡] The \pm sign in (2.1)₃ stands for +1 for a right-handed triad and –1 for a left-handed one. Of course, both triads are related by an inversion transformation. In this sense, the symbol \pm can be interpreted as an axial unit scalar, which ensures that n_i^3 is an absolute vector.

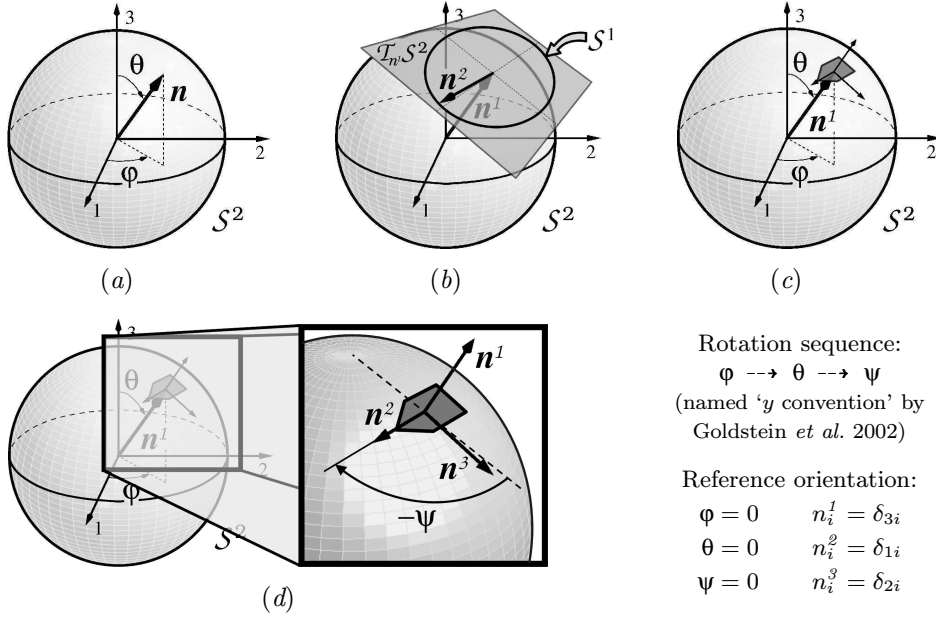


Figure 1. Description of lattice orientations in terms of Euler angles. For the particular case of transverse isotropy (a) just two Euler angles (φ, θ) suffice. In more general situations (b) all three Euler angles (φ, θ, ψ) are needed. The meanings of these angles are best illustrated through the 'drifting boat' metaphor (c) and (d), as explained in the text.

An instructive interpretation of (2.1) and (2.2) is provided by the *drifting boat metaphor* (figures 1c and 1d; see also Kocks *et al.* 1998). The first two Euler angles φ and θ specify, respectively, the longitude and colatitude of a 'fictitious boat' drifting on the surface of the unit sphere $\mathcal{S}^2 \subset \mathbb{R}^3$. Clearly, these two angles establish the orientation of the unit radius vector n_i^1 of \mathcal{S}^2 . On the other hand, rotations about n_i^1 are described by the third Euler angle ψ , which defines the instantaneous direction of the 'bow of the boat' with respect to the *local southward direction*. In other words, the angle ψ determines the orientation of the unit vector n_i^2 , which specifies a point in the unit circle $\mathcal{S}^1 \subset \mathcal{T}_n \mathcal{S}^2$, where $\mathcal{T}_n \mathcal{S}^2$ is the tangent space of \mathcal{S}^2 at n_i^1 (Appendix A; Abraham *et al.* 1988). Of course, any orthonormal triad is completely determined through the knowledge of n_i^1 and n_i^2 , seeing that n_i^3 is given by (2.1)₃.

To sum up, any species in a polycrystal modelled as a 'mixture of orientations' is uniquely determined by three species labels, which can be related to two mutually-orthogonal unit vectors $n_i^1 \in \mathcal{S}^2 \subset \mathbb{R}^3$ and $n_i^2 \in \mathcal{S}^1 \subset \mathcal{T}_n \mathcal{S}^2$. The appropriate species assemblage for the kind of polycrystals considered here is therefore $\mathcal{A}^3 := \mathcal{S}^2 \times \mathcal{S}^1$, also called *orientation space*, since it comprises all possible orientations of the lattice. Accordingly, the vectors n_i^1 , n_i^2 and n_i^3 are also named *orientation vectors*. Hence, by using just two of such vectors n_i^A ($A = 1, 2$) we can introduce, in conformity with §2b, thermodynamic fields that are *orientation dependent*: the species mass density $\varrho^*(x_i, t, n_j^A)$, the species Cauchy stress $t_{ij}^*(x_k, t, n_l^A)$, etc.

Remark 2.1. The fact that just n_i^1 and n_i^2 suffice to define a lattice orientation does not mean that n_i^3 is dispensable: all three vectors are needed to describe material symmetries in an intelligible manner. Further, n_i^3 is also requisite to distinguish between crystallites with right- and left-handed symmetries, as occurring e.g.

in *deformation twins* (Humphreys & Hatherly 2004). It must be noticed, however, that from the viewpoint of the present theory no continuous process can transform a right-handed lattice into a left-handed one, and vice versa: twinning is a discontinuous transformation. Consequently, crystallites with left- and right-handed symmetries must be treated as distinct materials, requiring so a *multiphase theory*, just like the case of multi-mineral rocks. This topic is examined in §4.

Remark 2.2. In the simple case of a polycrystal made of *transversely isotropic grains*, just one crystallographic axis turns out to be relevant (figure 1a). The angle ψ becomes superfluous, and the triad $\{n_i^1, n_j^2, n_k^3\}$ reduces to a single orientation vector: $n_i^1 = n_i$. Accordingly, the orientation space is restricted to \mathcal{S}^2 and the species fields assume the forms $\varrho^*(x_i, t, n_j)$, $t_{ij}^*(x_k, t, n_l)$, etc. Materials of this sort are examined in Parts II and III (Faria *et al.* 2005; Faria 2005).

3. Balance equations for several crystal classes

Continuous diversity inevitably implies some kind of ‘species hierarchy’, which is intuitively expressed by the notion of *familiarity*: two species are said *familiar* if their distinctive properties—and consequently, their behaviours—are alike, though not identical. The concept of familiarity stems from the existence of a metric in \mathcal{A}^ν , and it is clearly the counterpart in \mathcal{A}^ν of the usual notion of closeness in \mathbb{R}^3 . As discussed below, familiarity plays a key role in the construction of balance equations, owing to its relevance for interactions and mass exchanges between species.

(a) Transition rate, lattice spin velocity and orientational gradient

One of the greatest virtues of familiarity is that it allows us to treat the species labels α_γ and the position vector x_i at the same footing. For instance, we can conceive a situation in which, besides usual mass transfers by transport phenomena, the mass of constituent α_γ varies in time through *inter-species transitions*. From the obvious similarity of these transitions in \mathcal{A}^ν with ordinary motions in \mathbb{R}^3 , we immediately conclude that the rate at which such continuous mutations occur can be described by a kind of ‘velocity’, called *transition rate* and denoted by $u_\beta^*(x_i, t, \alpha_\gamma)$, with $\gamma, \beta = 1, \dots, \nu$. In fact, by considering a unit volume in a medium at rest (viz. $v_i^*(x_j, t, \alpha_\gamma) \equiv 0$), we readily infer that u_β^* determines the rate at which the amount of mass ϱ^* performs a continuous transition from the constituent α_γ to some other *familiar species*, by altering its distinctive properties.

Now, let us apply the concepts of familiarity and transition rate to polycrystals. The starting point is a suitable interpretation of *familiarity in polycrystalline media*: within a given material particle, two crystalline regions made of the same substance and possessing the same symmetry are said to belong to familiar species if their relevant crystallographic axes are closely oriented. Clearly, what is meant by ‘closely oriented’ depends on the medium and the problem under consideration, (familiarity in $\mathcal{S}^2 \times \mathcal{S}^1$, like neighbourhood in \mathbb{R}^3 , is a relative notion). Be that as it may, the formation of subgrain boundaries can be used to establish a natural upper bound for familiarity in polycrystals. Hence, in this work we assume the simple convention that *subgrains of a given crystallite belong to familiar species*, whereas highly misoriented grains ($> 10^\circ$, say) pertain to disparate species.

Turning attention now to transition rates, we conclude from §2b and the discussion above that continuous transitions in $\mathcal{S}^2 \times \mathcal{S}^1$ must correspond to smooth

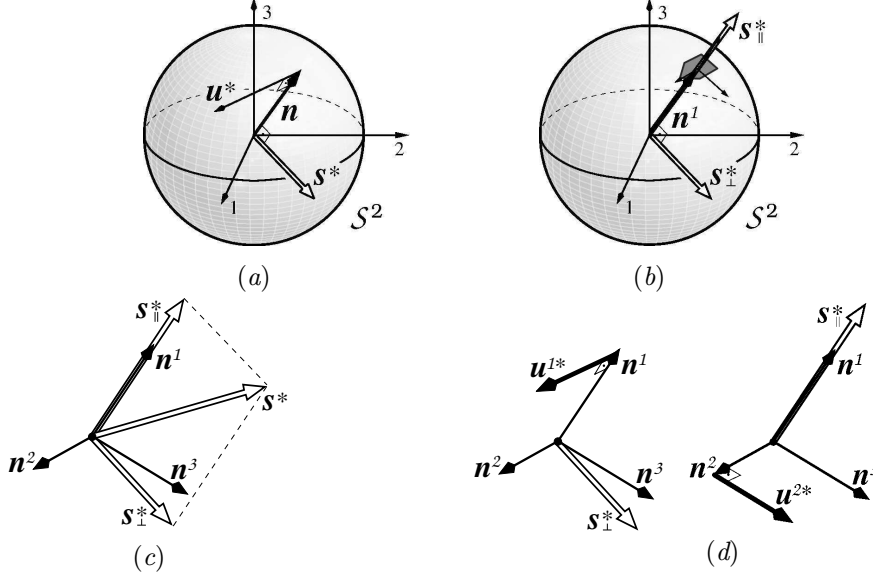


Figure 2. Relation between transition rates and the lattice spin velocity. In the particular case of transverse isotropy (a) the lattice spin velocity s_i^* is always orthogonal to both, the orientation vector n_i and the transition rate u_i^* . Yet, in a general situation (b,c) the lattice spin velocity may have an arbitrary orientation, though it can still be decomposed in two parts: one orthogonal ($s_{i\perp}^*$) and another parallel ($s_{i\parallel}^*$) to n_i^1 , cf. (c) and (3.3). Associated to each of these parts (d) there is a corresponding transition rate, namely u_i^{1*} and u_i^{2*} .

changes of orientation. We may express such changes by two transition rate vectors (cf. Goldstein *et al.* 2002) —viz. $u_i^{A*}(x_j, t, n_k^B)$, with $A, B = 1, 2$ — related to the time rates of the Euler angles φ , θ ($A = 1$), and ψ ($A = 2$). It is evident that only three of the six components of u_i^{A*} are independent: u_1^{1*} , u_2^{2*} and u_1^{2*} , say, while the other three are determined by the conditions (cf. (2.1))

$$n_k^1 u_k^{1*} = n_i^2 u_i^{2*} = 0, \quad \text{and} \quad n_k^1 u_k^{2*} = 0. \quad (3.1)$$

Hence, both transition rate vectors are tangent to the sphere \mathcal{S}^2 , while in addition, u_i^{2*} must also be tangent to the circle \mathcal{S}^1 (cf. figures 1b and 2d). On the other hand, from the notion of familiarity we immediately infer that the continuous transitions expressed by the rates u_i^{A*} must correspond to *rotations* of the crystalline lattice. This conclusion is illuminating, because it implies that u_i^{A*} can be expressed in terms of a more fundamental quantity: the *lattice spin velocity* s_i^* (cf. figure 2)

$$\begin{aligned} u_i^{1*} &:= \epsilon_{ijk} s_{j\perp}^* n_k^1 = \epsilon_{ijk} s_j^* n_k^1 = S_{ik}^* n_k^1, \\ u_i^{2*} &:= \epsilon_{ijk} s_{j\parallel}^* n_k^2 = (s_p^* n_p^1) \epsilon_{ijk} n_j^1 n_k^2 = (n_j^3 S_{jk}^* n_k^2) n_i^3, \end{aligned} \quad (3.2)$$

$$s_{i\parallel}^* := (s_k^* n_k^1) n_i^1, \quad s_{i\perp}^* := s_i^* - s_{i\parallel}^*, \quad S_{ij}^* = -\epsilon_{ijk} s_k^*. \quad (3.3)$$

Of course, in the case of transverse isotropy we have $s_{i\perp}^* = s_i^*$, the vector n_i^2 becomes superfluous, and hence we can set $n_i^1 = n_i$ and $u_i^{1*} = u_i^*$, as it should be.

From a different perspective, we may interpret the introduction of transition rates as a direct generalization of the notion of velocity, by replacing v_i with $\{v_i^*, u_j^{1*}, u_k^{2*}\}$. Evidently, such a generalization stems from a related extension of

the concept of position, from x_i to $\{x_i, n_j^1, n_k^2\}$. Now, it is obvious that any change in the description of position entails upon a corresponding extension of the spatial gradient operator $\partial/\partial x_i$, which becomes $\{\partial/\partial x_i, \partial_j^1, \partial_k^2\}$, where ∂_i^A (with $A = 1, 2$) denote the *orientational differential operators* in \mathcal{S}^2 and \mathcal{S}^1 , respectively:

$$\begin{aligned}\partial_i^1 &:= \frac{\partial}{\partial n_i^1} - n_i^1 n_k^1 \frac{\partial}{\partial n_k^1}, \\ \partial_i^2 &:= \frac{\partial}{\partial n_i^2} - n_i^2 n_k^2 \frac{\partial}{\partial n_k^2} - n_i^1 n_k^1 \frac{\partial}{\partial n_k^2} = n_i^3 n_k^3 \frac{\partial}{\partial n_k^2}.\end{aligned}\quad (3.4)$$

The first term on the right-hand side of (3.4)₁ represents the usual directional derivative along n_i^1 , while the second term arises from the normalization condition (2.1)₁, which implies that ∂_i^1 cannot have a component in the n_i^1 direction. Likewise, it follows from (2.1)_{1,2} that ∂_i^2 cannot have components in the directions given either by n_i^1 or by n_i^2 —there remains just the n_i^3 direction available— as expressed by (3.4)₂. Of course, in the simple instance of transversely isotropic crystallites we have $n_i^1 = n_i$ and consequently $\partial_i^1 = \partial_i$, since ∂_i^2 is not defined in this case.

(b) *Balance equations for polycrystals*

Within the framework of continuum theories, crystals and polycrystals have sometimes been modelled as *polar media*† (e.g. Forrest *et al.* 2000), a supposition which dates back to Voigt (1887) and the Cosserat brothers (1909). Presently, the equations of polar theory are well-known (Dahler & Scriven 1963; Truesdell & Noll 1965; Capriz 1989; Svendsen 2001) and consist of the balance equations of mass, linear momentum, angular momentum (spin) and internal energy, respectively:

$$\frac{\partial \varrho}{\partial t} + \frac{\partial}{\partial x_i} (\varrho v_i) = 0, \quad (3.5)$$

$$\frac{\partial \varrho v_i}{\partial t} + \frac{\partial}{\partial x_j} (\varrho v_i v_j - t_{ij}) = \varrho g_i, \quad (3.6)$$

$$\frac{\partial \varrho I s_i}{\partial t} + \frac{\partial}{\partial x_j} (\varrho I s_i v_j - m_{ij}) + \epsilon_{ijk} t_{jk} = \varrho c_i, \quad (3.7)$$

$$\frac{\partial \varrho e}{\partial t} + \frac{\partial}{\partial x_j} (\varrho e v_i + q_i) - t_{ij} \frac{\partial v_i}{\partial x_j} - m_{ij} \frac{\partial s_i}{\partial x_j} - \epsilon_{ijk} s_i t_{jk} = \varrho r, \quad (3.8)$$

where ϱ , ϱv_i , $\varrho I s_i$ and ϱe denote the densities of mass, linear momentum, spin momentum and internal energy, respectively. For brevity, other fields occurring in (3.5)–(3.8) are defined in Appendix A. In some situations it may be advantageous to replace (3.8) by the more fundamental balance equation of total energy

$$\frac{\partial \varrho E}{\partial t} + \frac{\partial}{\partial x_i} (\varrho E v_i + Q_i) = \varrho R, \quad (3.9)$$

$$E = e + \frac{1}{2} v^2 + \frac{1}{2} I s^2, \quad Q_i = q_i - t_{ki} v_k - m_{ki} s_k, \quad R = r + g_k v_k + c_k s_k, \quad (3.10)$$

from which (3.8) can be derived with the help of (3.6) and (3.7).

† Roughly, polar media are microstructured continua characterized by couple stresses, body couples, and additional degrees of freedom subsumed in an intrinsic angular momentum called *spin* (Dahler & Scriven 1963; Truesdell & Noll 1965; Capriz 1989; Svendsen 2001).

In practice, however, the classification of polycrystals as polar media is often unnecessary. Experience shows that in many situations $m_{ij} = I = c_i = 0$ and $s_i = w_i$ (where $w_i := \frac{1}{2}\epsilon_{ijk}\partial v_k/\partial x_j$ denotes the local angular velocity of the continuum, i.e. one half of vorticity) may be good assumptions, in such a manner that (3.5)–(3.8) reduce to the balance equations of ordinary (non-polar) continua:

$$\frac{\partial \varrho}{\partial t} + \frac{\partial}{\partial x_i}(\varrho v_i) = 0, \quad (3.11)$$

$$\frac{\partial \varrho v_i}{\partial t} + \frac{\partial}{\partial x_j}(\varrho v_i v_j - t_{ij}) = \varrho g_i, \quad (3.12)$$

$$\epsilon_{ijk} t_{jk} = 0, \quad (3.13)$$

$$\frac{\partial \varrho e}{\partial t} + \frac{\partial}{\partial x_j}(\varrho e v_j + q_i) - t_{ij} \frac{\partial v_i}{\partial x_j} = \varrho r. \quad (3.14)$$

Consequently, (3.9) and (3.10) simplify to

$$\frac{\partial \varrho E}{\partial t} + \frac{\partial}{\partial x_i}(\varrho E v_i + Q_i) = \varrho R, \quad (3.15)$$

$$E = e + \frac{1}{2}v^2, \quad Q_i = q_i - t_{ki}v_k, \quad R = r + g_k v_k. \quad (3.16)$$

Equations (3.11)–(3.13), (3.15) are also known as the *continuity equation*, *Euler's first and second laws of motion*, and the *first law of thermodynamics*, respectively.

The set of balance equations (3.11)–(3.16) has since long been used in many theories for polycrystals as a rule of thumb. Notwithstanding, in the current approach we do not need to *postulate* the validity of (3.11)–(3.16); rather, we may adopt, a priori, the more general equations (3.5)–(3.10) and then, through an appropriate constitutive theory, it is possible to *prove* that (3.11)–(3.16) are valid for some particular problem (see Part III, Faria 2005).

That grains in a polycrystal should generally be modelled as polar media is justified by the micromechanics of crystals (see e.g. Asaro 1983; Forrest *et al.* 2000): torsion/bending of grains and the rotation of crystallographic axes relative to the matrix are clear indications of couples and asymmetric stresses acting on the grains. In this sense, polycrystals can also be seen as ‘mixtures of polar media’. What remains questionable is if such ‘mixtures of polar media’ do behave themselves as polar media, or if the couples and asymmetric stresses acting on distinct species cancel each other on average, resulting in no net outcome.

In ordinary mixture theory (e.g. Faria & Hutter 2002), species balance equations are obtained from (3.5)–(3.10) in two simple steps. First, every field in (3.5)–(3.10) is replaced by its respective species field, characterized by the label $\alpha = 1, \dots, N$, viz.: $\varrho(x_i, t)$ becomes $\varrho^\alpha(x_i, t)$, and $s_i(x_j, t)$ becomes $s_i^\alpha(x_j, t)$, etc. Second, a production/exchange term describing *inter-species interactions* is added to every balance equation, since mixed species are in fact interacting open systems (cf. §2a).

In contrast, polycrystals modelled as mixtures with continuous diversity need slightly more complex species balance equations, in view of the generalizations discussed in §3a. Hence, we must convert the two steps mentioned above into four:

1. Every field in (3.5)–(3.10) is replaced by its respective species field, viz.: $\varrho(x_i, t)$ becomes $\varrho^*(x_i, t, n_j^A)$, and $s_i(x_j, t)$ becomes $s_i^*(x_j, t, n_k^A)$, etc.

2. A production/exchange term describing interspecies interactions is added to every balance equation, since mixed species are in fact interacting open systems.

3. As explained in §3a, the velocity v_i is replaced by $\{v_i^*, u_j^{1*}, u_k^{2*}\}$, with u_i^{A*} given by (3.2), while the gradient operator $\partial/\partial x_i$ is replaced by $\{\partial/\partial x_i, \partial_j^1, \partial_j^2\}$, with ∂_j^A defined in (3.4).

4. Following the same reasoning of the last item, also fluxes and stresses must be extended to have their counterparts in the species assemblage $\mathcal{S}^2 \times \mathcal{S}^1$. These extensions are the *interspecies stresses and fluxes* τ_{ij}^{A*} , ϖ_{ij}^{A*} and ξ_i^{A*} , with $A = 1, 2$ (see Appendix A for the definitions of these fields).

Through these four steps, we derive from (3.5)–(3.10) the species balance equations for polycrystals modelled as mixtures with continuous diversity (summation convention applied to lowercase *and* capital repeated indices, cf. Appendix A)

- mass

$$\frac{\partial \varrho^*}{\partial t} + \frac{\partial}{\partial x_i} (\varrho^* v_i^*) + \partial_i^A (\varrho^* u_i^{A*}) = \varrho^* \Gamma^* , \quad (3.17)$$

- linear momentum

$$\frac{\partial \varrho^* v_i^*}{\partial t} + \frac{\partial}{\partial x_j} (\varrho^* v_i^* v_j^* - t_{ij}^*) + \partial_j^A (\varrho^* v_i^* u_j^{A*} - \tau_{ij}^{A*}) = \varrho^* g_i^* + \varrho^* \kappa_i^* , \quad (3.18)$$

- lattice spin momentum

$$\frac{\partial \varrho^* I s_i^*}{\partial t} + \frac{\partial}{\partial x_j} (\varrho^* I s_i^* v_j^* - m_{ij}^*) + \partial_j^A (\varrho^* I s_i^* u_j^{A*} - \varpi_{ij}^{A*}) + \epsilon_{ijk} t_{jk}^* = \varrho^* c_i^* + \varrho^* \nu_i^* , \quad (3.19)$$

- internal energy

$$\begin{aligned} \frac{\partial \varrho^* e^*}{\partial t} + \frac{\partial}{\partial x_j} (\varrho^* e^* v_j^* + q_j^*) + \partial_i^A (\varrho^* e^* u_i^{A*} + \xi_i^{A*}) \\ - \epsilon_{ijk} s_i^* t_{jk}^* - t_{ij}^* \frac{\partial v_i^*}{\partial x_j} - m_{ij}^* \frac{\partial s_i^*}{\partial x_j} - \tau_{ij}^{A*} \partial_j^A v_i^* - \varpi_{ij}^{A*} \partial_j^A s_i^* = \varrho^* r^* + \varrho^* \varepsilon^* . \end{aligned} \quad (3.20)$$

It must be noticed that (3.20) is not derived directly from (3.8), but rather from (3.9) and (3.10) through the species balance equation of total energy

$$\frac{\partial \varrho^* E^*}{\partial t} + \frac{\partial}{\partial x_i} (\varrho^* E^* v_i^* + Q_i^*) + \partial_i^A (\varrho^* E^* u_i^{A*} + \Xi_i^{A*}) = \varrho^* R^* + \varrho^* L^* , \quad (3.21)$$

$$\begin{aligned} E^* &= e^* + \frac{1}{2} v^{*2} + \frac{1}{2} I s^{*2} , \\ Q_i^* &= q_i^* - t_{ki}^* v_k^* - m_{ki}^* s_k^* , \quad \Xi_i^{A*} = \xi_i^{A*} - \tau_{ki}^{A*} v_k^* - \varpi_{ki}^{A*} s_k^* , \\ L^* &= \varepsilon^* + \kappa_i^* v_i^* + \nu_i^* s_i^* , \quad R^* = r^* + g_k^* v_k^* + c_k^* s_k^* . \end{aligned} \quad (3.22)$$

Again, all fields in (3.17)–(3.22) are defined in Appendix A. Details of the derivation of (3.20) from (3.9), (3.10), (3.21) and (3.22) are given in Faria & Hutter (2002).[†]

Remark 3.1. Two points are worthy of notice concerning (3.17)–(3.21): first, no balance equation is proposed for u_i^{A*} , since these fields can be derived from s_i^* via (3.2). Second, the corresponding balance equations for transversely isotropic crystal-lites are much simpler, seeing that in this case we can drop the superscripts ‘A’ out of all equations (e.g. ξ_i^{A*} becomes ξ_i^* , etc.; see also remark 2.2 and Faria *et al.* 2005).

[†] The cited authors considered only the particular case of transverse isotropy, but the procedure is exactly the same for more complex symmetries considered here.

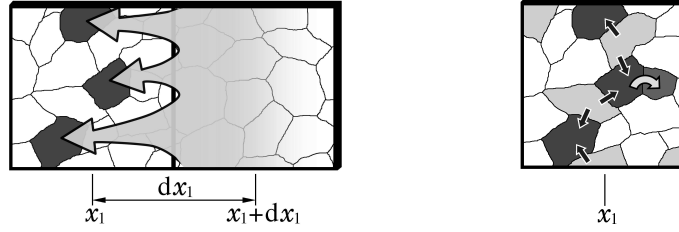


Figure 3. Distinction between spatial fluxes, conductive fluxes, and production rates. *Left:* a material particle at x_1 (x_2 and x_3 are irrelevant here) contains some grains with the lattice orientation n_i^A , identified by dark grey. Spatial fluxes/stresses to this species (e.g. q_1^* , t_{i1}^* , etc.) represent conductive transfers from *all crystallites in the neighbourhood* to the dark-grey grains at x_1 . *Right:* the same polycrystalline particle at x_1 , but now under the action of production/exchange rates and interspecies fluxes/stresses. In this case *all interactions occur within the same material particle*. For simplicity, only three disparate lattice orientations are considered: white, light grey and dark grey. The effect of a familiar species is illustrated by an additional grain in a slightly lighter dark grey, representing a crystallite closely oriented to n_i^A . Dark arrows stand for production/exchange rates (ϵ^* , κ_i^* , etc.), viz. high-angle interactions between light- and dark-grey grains. Interspecies fluxes/stresses (ξ_i^{A*} , τ_{jk}^{A*} , etc.) are represented by the curved, light-grey arrow, which symbolizes the low-angle interaction between the two familiar dark-grey grains.

At first sight, (3.17)–(3.22) may look somewhat formidable in comparison to (3.5)–(3.10). However, a careful analysis shows that the differences are actually not so striking. There is even an interpretation of (3.17)–(3.22), without direct reference to $\mathcal{S}^2 \times \mathcal{S}^1$, that can be valuable in certain situations. Consider for instance the species balance equation of linear momentum (3.18). We can readily rearrange it as

$$\frac{\partial \varrho^* v_i^*}{\partial t} + \frac{\partial}{\partial x_j} (\varrho^* v_i^* v_j^* - t_{ij}^*) - \varrho^* g_i^* = \varrho^* \kappa_i^* + \partial_j^A \tau_{ij}^{A*} - \partial_j^B (\varrho^* v_i^* u_j^{B*}) . \quad (3.23)$$

The left-hand side of (3.23) has exactly the form of the usual balance equation of linear momentum (3.6) or (3.12). Now, the right-hand side of (3.23) can, as a whole, be interpreted as an *effective production/exchange rate* of linear momentum within a polycrystalline particle (cf. figure 3): the first term describes interactions between highly misoriented crystallites, i.e. *interactions across high-angle grain boundaries*; on the other hand, the term $\partial_j^A \tau_{ij}^{A*}$ can be interpreted as a specialized production/exchange rate in \mathbb{R}^3 that describes *interactions across low-angle grain boundaries* (i.e. *subgrain boundaries*). Finally, the last term on the right-hand side of (3.23) does not represent a production/exchange by interactions, but rather by mass transfer: when the lattice of a grain rotates, its mass is in effect transferred from one orientation to another, and consequently its inherent properties (e.g. stored energy, etc.) are carried with it through a kind of ‘rotational convection’.

(c) *On the irreversibility of recrystallization:*

the balance equation of dislocations and the second law of thermodynamics

Mass, momenta and energy are clearly not enough to model the thermodynamics of creep and recrystallization. Indeed, the basic fields ϱ^* , v_i^* , s_i^* and e^* , that are solutions of the system (3.17)–(3.20), do suffice to describe fabric, motion, lattice spin and temperature, respectively, but they fail to define uniquely a recrystallization

process. The cause of this failure lies in the fact that the driving force for recrystallization is closely related to a particular part of the internal energy, which is stored during deformation in linear lattice defects called *dislocations*. Consequently, what we need is a balance equation of dislocations.

Kröner (2001) has shown that the notion of dislocation density as a scalar internal variable can be illuminatingly introduced in continuum mechanics by means of statistical arguments. Using a similar approach, Faria *et al.* (2003) proposed a species balance equation of dislocations for ice sheets. Here, based on the results derived so far, such an equation can be generalized for diverse classes of polycrystals, by proposing the following *species balance equation of dislocations*

$$\frac{\partial \rho_{\text{D}}^*}{\partial t} + \frac{\partial}{\partial x_i} (\rho_{\text{D}}^* v_i^*) + \partial_i^A (\rho_{\text{D}}^* u_i^{A*} + j_{\text{D}i}^{A*}) = \Pi_{\text{D}}^* , \quad (3.24)$$

Succinctly, the species dislocation density ρ_{D}^* is an internal variable representing the total length of dislocations in crystallites with crystallographic axes directed towards n_i^A and enclosed in a unit volume of the polycrystal. Hence, its dimension is length/volume, i.e. length⁻². The dislocation production rate Π_{D}^* represents the production/consumption of dislocations by Frank–Read sources, dipole annihilation, etc., (Asaro 1983; Poirier 1985). Finally, the interspecies dislocation fluxes $j_{\text{D}i}^{A*}$ portray the dislocation exchange between subgrains. Clearly, such interspecies fluxes are relevant only in specialized models of dislocation–subgrain-boundary interactions, so that $j_{\text{D}i}^{A*}$ may be neglected in most common applications.

Comparison of (3.24) with (3.17)–(3.21) reveals that there are two terms absent in (3.24), namely the (spatial) divergence of a conductive flux and an external supply. The absence of the latter is obvious: dislocations cannot be supplied from external sources to the bulk of the polycrystal. In contrast, the absence of a conductive flux of dislocations is less obvious and was discussed in detail by Faria *et al.* (2003). Succinctly, it is a particularity of the theory of mixtures with continuous diversity applied to *large polycrystalline masses* (see footnote in §1): in this case the mean free path of mobile dislocations turns out to be many orders of magnitude smaller than the size of a single material particle, in such a manner that —on a large-scale perspective— all dislocations seem to be ‘tied’ to the material.

The last but not least fundamental quantity to be introduced in this theory is the *entropy*, which expresses the irreversibility of natural processes. Its species balance equation arises as part of the so-called *entropy principle*, which sets up the *second law of thermodynamics* in a suitable mathematical form for continuum theories:

Axiom 3.1 (Entropy Principle). *There exists for every species in a mixture with continuous diversity a scalar quantity called entropy, such that:*

1. *it is additive and evolves according to the species balance equation of entropy*

$$\frac{\partial \varrho^* \eta^*}{\partial t} + \frac{\partial}{\partial x_i} (\varrho^* \eta^* v_i^* + \phi_i^*) + \partial_i^A (\varrho^* \eta^* u_i^{A*} + \varphi_i^{A*}) = \varrho^* s^* + \varrho^* \zeta^* ; \quad (3.25)$$

2. *for every species of the mixture, the specific entropy η^* , its fluxes ϕ_i^* and φ_i^{A*} , as well as its specific production rate ζ^* are all given by constitutive relations;*

3. *the net entropy production rate density of the mixture is non-negative for all thermodynamic processes.*

As regards the last item, it should be emphasized that the entropy production rates of some species can be *negative* —provided that any such losses are compensated for with simultaneous positive productions by other species— so that ζ^* may have a non-vanishing lower bound. The crucial question is thus whether such a lower bound can be mathematically expressed in a tractable form, viz. by a *conventional* constitutive equation.† The answer is fortunately affirmative:‡

Proposition 3.1. *There exists for every species in a mixture with continuous diversity a scalar quantity δ^* , called specific entropy deviation rate, such that:*

1. *it is given by a conventional constitutive equation;*
2. *the inequality $\delta^* \leq \zeta^*$ holds for all thermodynamic processes.*

The proposition above offers an interpretation of the second law of thermodynamics that is as general as —and is much simpler to be exploited on the species level than— the one presented in item 3 of axiom 3.1 (see Part II, Faria *et al.* 2005). A formal proof of it can be found in (Faria 2001). The fact that the lower bound for ζ^* can indeed be expressed by a conventional constitutive equation is only possible because the species entropy production rate can always be written, without loss of generality, as $\zeta^* = \delta^* + \zeta^{*P}$, where $\zeta^{*P} \geq 0$ denotes the specific entropy production rate of the *pure species*, i.e. in the limiting case when all other species are absent. For polycrystals modelled as mixtures with continuous diversity, such a pure species is evidently a *single crystal* (with crystallographic axes parallel to n_i^A).

(d) *Homogenization rules*

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 first on the species level, where a solution is easier to be found. Then, once all species fields are determined, the behaviour of the polycrystal (i.e., of the ‘mixture’) can be derived by accounting for the response of all species. The connection between species and mixture responses is set out by certain averaging relations, called *homogenization rules*. Such rules can be derived in a similar manner as done for ordinary chemical mixtures, namely by exploring the additivity of density fields, combined with the expected forms of the mixture balance equations. For polycrystals, such equations are (3.5)–(3.9), together with the mixture balance equations of dislocations and entropy (cf. Groma 1997; Acharya & Beaudoin 2000; Liu 2002)

$$\frac{\partial \rho_D}{\partial t} + \frac{\partial}{\partial x_i} (\rho_D v_i) = \Pi_D, \quad \frac{\partial \varrho \eta}{\partial t} + \frac{\partial}{\partial x_i} (\varrho \eta v_i + \phi_i) = \varrho s + \varrho \zeta, \quad (3.26)$$

where all quantities are defined, as usual, in Appendix A.

Homogenization rules appropriate for polycrystals made of transversely isotropic grains have been discussed by Faria & Hutter (2002). Here, we extend those rules to more general crystal symmetries. First, we notice that all species density fields have been defined with respect to a common volume, viz. a unit volume of the *mixture*.

† Here, ‘conventional constitutive equation’ means a non-linear, constitutive function (or functional) of the same general type supposed to hold for ζ^* , η^* , e^* , etc. (cf. Faria *et al.* 2005).

‡ This result is trivial for ordinary mixtures, but not for mixtures with continuous diversity, since in the latter case the entropy production rate of the mixture is given by a non-conventional, integral relation (see (3.27)) that can hardly be exploited on the species level.

Consequently, all such fields are additive, in the sense that mixture densities result from the combination of the densities of all species. From this reasoning we obtain the first three series of homogenization rules, valid for the fundamental density fields (D_μ) and their respective production/exchange rate densities (P_λ and C_ζ)

$$\begin{pmatrix} D_\mu \\ P_\lambda \end{pmatrix} = \int_{\mathcal{A}^\nu} \begin{pmatrix} D_\mu^* \\ P_\lambda^* \end{pmatrix} d^\nu\alpha, \quad \int_{\mathcal{A}^\nu} C_\zeta^* d^\nu\alpha = 0, \quad \begin{aligned} D_\mu &= \{\varrho, \varrho v_i, \varrho I s_j, \varrho E, \rho_D, \varrho \eta\}, \\ P_\lambda &= \{II_D, \varrho \zeta\}, \\ C_\zeta &= \{\varrho \Gamma, \varrho \kappa_i, \varrho \nu_j, \varrho L\}. \end{aligned} \quad (3.27)$$

The last integral in (3.27) vanishes because of the *conservation* of mass, momenta and total energy of the mixture. The explicit forms of the integrals (3.27) depend on the domains of their respective integrands: for polycrystals in general, we have†

$$\int_{\mathcal{A}^\nu} (\cdot)^* d^\nu\alpha = \int_{\mathcal{S}^2 \times \mathcal{S}^1} (\cdot)^* d^3n = \frac{1}{8\pi^2} \int_0^\pi \int_0^{2\pi} \int_0^{2\pi} (\cdot)^* \sin\theta \, d\psi \, d\phi \, d\theta, \quad (3.28)$$

whereas for the particular case of polycrystals made of transversely isotropic grains:

$$\int_{\mathcal{A}^\nu} (\cdot)^* d^\nu\alpha = \int_{\mathcal{S}^2} (\cdot)^* d^2n = \frac{1}{4\pi} \int_0^\pi \int_0^{2\pi} (\cdot)^* \sin\theta \, d\phi \, d\theta. \quad (3.29)$$

Notice that in both instances the integrals are normalized, so that they yield unity when the integrand is just a unit constant.

Now, to derive further homogenization rules we will need the the following result:

Proposition 3.2. *Let \mathcal{A}^ν be a compact manifold and $Q_\gamma^* : \mathcal{A}^\nu \mapsto \mathcal{TA}^\nu$ a vector field of class $C_c^k(\text{int } \mathcal{A}^\nu)$, with $\alpha_\gamma \in \mathcal{A}^\nu$, $k \geq 1$, and $\gamma = 1, \dots, \nu$. Then*

$$\int_{\mathcal{A}^\nu} \sum_{\gamma=1}^{\nu} \frac{\partial Q_\gamma^*}{\partial \alpha_\gamma} d^\nu\alpha = 0. \quad (3.30)$$

This proposition is a direct specialization of the divergence theorem in ν dimensions (Abraham *et al.* 1988). In order to apply it to polycrystals, we observe first that the diversity completeness of the orientation space $\mathcal{A}^3 := \mathcal{S}^2 \times \mathcal{S}^1$ implies the *tangentiality* of interspecies fluxes, i.e. $J_{\beta_j}^{A^*} : \mathcal{S}^2 \times \mathcal{S}^1 \mapsto \mathcal{T}(\mathcal{S}^2 \times \mathcal{S}^1)$ —otherwise the interspecies fluxes $J_{\beta_j}^{A^*}$ could reach extraneous species outside $\mathcal{S}^2 \times \mathcal{S}^1$ — so that

$$\int_{\mathcal{A}^\nu} \partial_j^A J_{\beta_j}^{A^*} d^\nu\alpha = 0, \quad J_{\beta_j}^{A^*} = \{D_\mu^* u_j^{A^*}, \kappa_{ij}^{A^*}, \varpi_{kj}^{A^*}, \Xi_j^{A^*}, \xi_j^{A^*}, j_{D_j}^{A^*}, \varphi_j^{A^*}\}, \quad (3.31)$$

where D_μ is defined in (3.27) and the explicit form of the integral above is given by (3.28) or (3.29). Hence, integration of the balance equations (3.17)–(3.21), (3.24), (3.25) over the whole orientation space $\mathcal{S}^2 \times \mathcal{S}^1$, combined with (3.27) and (3.31), with subsequent subtraction of the resulting expressions from (3.5)–(3.9), (3.26),

† Application of (3.28) to (3.27) implies $\varrho = \int_{\mathcal{S}^2 \times \mathcal{S}^1} \varrho^* d^3n$, $\int_{\mathcal{S}^2 \times \mathcal{S}^1} \varrho^* \kappa_i^* d^3n = 0$, etc.

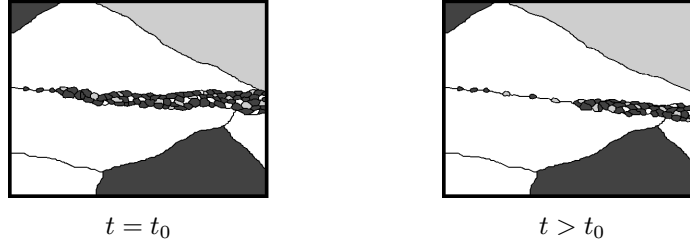


Figure 4. Selective grain shifting (remark 3.2). For simplicity, just three lattice orientations are considered (white, light and dark grey). We suppose that recrystallization occurs at one grain boundary only, and the new grains nucleate with a preferred lattice orientation, viz. dark grey. The aggregate of small crystallites is likely to deform by grain boundary sliding, whereas the large grains deform mainly by dislocation glide and climb. *Left*: initial configuration. *Right*: during deformation, small grains move rightwards by grain boundary sliding. Thus, there is a net shifting of the dark-grey species to the right ($C_i^* \neq 0$).

leads directly to the last homogenization rules of interest. Such a procedure is described in detail in Faria & Hutter (2002) and references therein. In short, its outcome is the set of homogenization rules for external supplies

$$S_\sigma = \int_{A^\nu} S_\sigma^* d^\nu\alpha, \quad S_\sigma = \{\varrho g_i, \varrho c_i, \varrho R, \varrho s\}, \quad (3.32)$$

and for stresses and fluxes

$$F_{\chi j} = \int_{A^\nu} (F_{\chi j}^* - \varrho^* U_\chi^* C_j^*) d^\nu\alpha, \quad \begin{aligned} F_{\chi j} &= \{t_{ij}, m_{kj}, Q_j, \phi_j\}, \\ U_\chi^* &= \{C_i^*, IG_k^*, E^*, \eta^*\}, \end{aligned} \quad (3.33)$$

where the relative velocities $C_i^* := v_i^* - v_i$ and $G_i^* := s_i^* - s_i$ are respectively called *grain shifting velocity* and *lattice deflecting rate*. Finally, from (3.10), (3.22), (3.27), (3.32) and (3.33) we obtain the homogenization rules for the heat flux and for the density, production/exchange and supply of internal energy, respectively

$$\begin{aligned} q_j &= \int_{A^\nu} \left\{ q_j^* + \varrho^* \left(e^* + \frac{1}{2} C^{*2} + \frac{1}{2} IG^{*2} \right) C_j^* - t_{ij}^* C_i^* - m_{ij}^* G_i^* \right\} d^\nu\alpha, \\ \varrho e &= \int_{A^\nu} \varrho^* \left(e^* + \frac{1}{2} C^{*2} + \frac{1}{2} IG^{*2} \right) d^\nu\alpha, \\ \int_{A^\nu} \varrho^* (\varepsilon^* + \kappa_i^* C_i^* + \nu_i^* G_i^*) d^\nu\alpha &= 0, \quad \varrho r = \int_{A^\nu} \varrho^* (r^* + g_i^* C_i^* + c_i^* G_i^*) d^\nu\alpha. \end{aligned} \quad (3.34)$$

Thus, with the help of (3.27), (3.31)–(3.34) we can recover the balance equations (3.5)–(3.9), (3.26), for the polycrystal through integration of the species balance equations (3.17)–(3.21), (3.24), (3.25) over all possible lattice orientations.

Remark 3.2. The homogenization rules presented in this section are very general, occasionally *too* general even, in the sense that $C_i^* = I = 0$ are often reasonable assumptions. Indeed, the velocity C_i^* is only relevant when a pronounced, selective

shifting of grains with some particular lattice orientation takes place (figure 4). This is most likely to occur during *superplastic flow* (Poirier 1985). Nevertheless, superplastic flow with *selective grain shifting* constitutes a very particular situation: in most common cases we may set $v_i^*(x_j, t, n_k^A) \equiv v_i(x_j, t)$ instead, which represents a prodigious simplification to the theory.† In contrast, it is obvious that we cannot expect $s_i^*(x_j, t, n_k^A) \equiv s_i(x_j, t)$ to hold in general, because this would imply a ‘frozen fabric’, i.e. no texture development. Nevertheless, it is evident that the *rotational inertia* of the lattice must be extremely small—the lattice does not continue rotating after cessation of the applied torques—so that $I = 0$ is valid as a rule.

4. Closing remarks

This work presented a general continuum theory for the thermomechanics of large polycrystalline masses, including fabric (i.e. texture) evolution, anisotropic response and recrystallization. It encompasses several symmetry groups, including transversely isotropic and orthotropic, as well as all crystal classes whose symmetries can be described in terms of three orthogonal axes (cf. Liu 1982). The theory is based on the concept of a mixture with continuous diversity (Faria 2001), by regarding the polycrystal as a ‘mixture of lattice orientations’. Its strategy consists in solving the coupled problem of creep, evolving fabric and recrystallization on the species level (i.e. for every ‘component of the mixture’) as described by the system of equations (3.17)–(3.20) and (3.24). Once all species fields are determined, the original initial/boundary-value problem for the polycrystal can thus be solved by application of the homogenization rules (3.27) and (3.31)–(3.34).

It should be observed, however, that the approach studied so far is suitable only to monomineral rocks, in contrast to the assertion in §1 (cf. also remark 2.1). Nevertheless, the extension of the theory for *multi-mineral rocks* is formally direct: it represents what was named by Faria (2001) and Faria & Hutter (2002) a *hybrid mixture with continuous diversity* (viz. involving discrete and continuous species labels). Effectively, the essential difference between mono- and multi-mineral rocks is that in the latter case we must deal with N phases (every rock-forming mineral being regarded as a particular phase), i.e. with N distinct ‘mixtures of orientations’. Thus, in a multiphase polycrystal we need to add a discrete species label $\alpha = 1, \dots, N$ to every field of the theory presented so far. For instance, the species fields of mass density and Cauchy stress in a rock made of N minerals read $\varrho^{*\alpha}(x_i, t, n_j^A)$ and $t_{ij}^{*\alpha}(x_k, t, n_l^A)$, respectively, with $\alpha = 1, 2, \dots, N$ and $A = 1, 2$. The fundamental equations (3.17)–(3.22), (3.24) and (3.25) remain exactly the same as before (except, of course, for the appearance of the superscript α in every field), whereas the homogenization rules (3.27) and (3.31)–(3.34) incorporate now a sum

† The assumption $v_i^* = v_i$ has *no relation at all* to artificial constraints on the strain of individual grains (e.g. Voigt–Taylor/Sachs–Reuss upper/lower bounds, cf. Asaro 1983; Humphreys & Hatherly 2004). In the present theory, all crystallites may undergo arbitrary deformations, since each material particle is large enough to contain a huge number of grains. Thus, stress and strain inhomogeneities on the grain level are already smeared out in the definitions of v_i^* and t_{ij}^* , which describe the average response of the grains belonging to a given species (cf. remark 2.1 of Part III).

over α . For instance, the homogenization rule (3.33) for the Cauchy stress becomes

$$t_{ij} = \int_{\mathcal{A}^\nu} \sum_{\alpha=1}^N (t_{ij}^{*\alpha} - \varrho^{*\alpha} C_i^{*\alpha} C_j^{*\alpha}) \, d\nu_\alpha, \quad \text{where} \quad C_i^{*\alpha} := v_i^{*\alpha} - v_i. \quad (4.1)$$

Further details about balance equations and homogenization rules for hybrid mixtures with continuous diversity are available in Faria & Hutter (2002).

Finally, the construction of constitutive equations is studied in the subsequent parts of this series (Faria *et al.* 2005; Faria 2005).

This work was conceived during the EPICA–DML 2003/04 deep-drilling expedition in Dronning Maud Land, Antarctica. It was resumed in Brazil, and finished in Leipzig. I am grateful to D. Freche, K. Hutter, G. M. Kremer, P. Shipman and E. Zeidler for suggestions and assistance, as well as to I. Hamann, S. Kipfstuhl, H. Miller and the science group of the mentioned expedition for enjoyable discussions in situ. Financial support is acknowledged from the Alfred Wegener Institute for Polar and Marine Research (Bremerhaven) and the Darmstadt University of Technology. This work is a contribution to the ‘European Project for Ice Coring in Antarctica’ (EPICA), a joint ESF (European Science Foundation)/EC scientific programme, funded by the European Commission and by national contributions from Belgium, Denmark, France, Germany, Italy, the Netherlands, Norway, Sweden, Switzerland and the United Kingdom. This is EPICA publication no. xxx.

Appendix A. Notation

The notation described here holds also for Parts II and III (Faria *et al.* 2005; Faria 2005).

All fields are assumed continuously differentiable, except when mentioned otherwise. Vectors and tensors are always expressed in terms of their three-dimensional Cartesian components (e.g. v_i , t_{ij} , etc., with $i, j = 1, 2, 3$). Einstein’s summation convention (see e.g. Chadwick 1999) is adopted for *repeated lowercase Latin indices* (i , j , etc.). For convenience, a similar summation convention is also applied to *repeated capital Latin indices* (A , B , etc.) written as superscripts and ranging from 1 to 2, in a context explained in the text. In contrast, *any other kind of repeated indices should not be summed*, except when explicitly indicated.

German letters (\mathfrak{F} , \mathfrak{G} , etc.) represent functions and functionals, while sans serif Latin letters (\mathbf{A} , \mathbf{B} , etc.) refer to generic fields. As usual, \mathbb{R}^n stands for the n -dimensional Euclidean space. Manifolds in \mathbb{R}^n are indicated by calligraphic Latin letters (\mathcal{A} , \mathcal{B} , etc.). Two manifolds of special interest are the 2-sphere \mathcal{S}^2 , conceived as a closed spherical surface of unit radius in \mathbb{R}^3 , and the 1-sphere \mathcal{S}^1 , which is, likewise, thought of as a closed unit circle in \mathbb{R}^2 (Abraham *et al.* 1988; figure 1). In this context, $\mathcal{T}_N \mathcal{S}^2$ denotes the tangent space of \mathcal{S}^2 at the point $N_i \in \mathcal{S}^2$.

Several mathematical expressions are for convenience written in condensed form. In particular, $N_i \in \mathcal{S}^2$ (or alternatively $N_i \in \mathcal{S}^2 \subset \mathbb{R}^3$) is used as a shorthand for ‘the vector that specifies a point in \mathcal{S}^2 and whose Cartesian components in \mathbb{R}^3 are N_i ’. As a rule, mathematical operations involving vectors and tensors are performed in \mathbb{R}^3 ; it is in this context that products like $N_i G_i$ or $\epsilon_{ijk} N_j G_k$ (with $N_i \in \mathcal{S}^2 \subset \mathbb{R}^3$ and $G_i \in \mathcal{S}^1 \subset \mathcal{T}_N \mathcal{S}^2 \subset \mathbb{R}^3$) should make sense.

Finally, $G^2 := G_i G_i$ represents the scalar self-product of the vector G_i , while the symmetric, skew-symmetric, and deviatoric parts of a tensor G_{ij} are denoted respectively by $G_{(ij)} := \frac{1}{2}(G_{ij} + G_{ji})$, $G_{[ij]} := \frac{1}{2}(G_{ij} - G_{ji})$, $G_{\langle ij \rangle} := G_{(ij)} - \frac{1}{3} G_{kk} \delta_{ij}$.

Further symbols frequently used in all three parts of this series are listed below.

Conventions: G = generic quantity; \mathcal{G} = generic set; $G^- = G^*, G$.

References: [1] Abraham *et al.* 1988; [2] Faria *et al.* 2005; [3] Chadwick 1999.

..... Miscellany	
$G^- _E$... Equilibrium part of G^- .	b ... Burgers vector (material constant).
$G^- _E$... Non-equilibrium part of G^- .	\bar{c} ... Fitting constant of the stored energy ($\bar{c} \sim 0.7$).
G_D^- ... Part of G^- due to dislocations.	I ... Material constant of spin inertia (specific lattice spin inertia).
G_{id}^- ... Dislocation-free part of G^- ($G_{id}^- := G^- - G_D^-$).	k_B ... Boltzmann constant.
G_{NL}^- ... Part of G^- with strictly non-linear dependence on dissipative variables.	n_i^A, n_i ... Orientation vector.
$\partial\mathcal{G}$... Boundary of \mathcal{G} .	t ... Time instant.
int \mathcal{G} ... Interior of \mathcal{G} (int $\mathcal{G} := \mathcal{G} \setminus \partial\mathcal{G}$).	x_i ... Position vector.
$T\mathcal{G}$... Tangent bundle of \mathcal{G} . ^[1]	α_γ, α ... Generic species label ($\gamma = 1, \dots, \nu$).
$C_c^k(\mathcal{G})$... Set of all continuous functions on \mathcal{G} with compact support and continuous derivatives up to order k .	$\delta(\cdot)$... Dirac delta 'function'. ^[1]
\dot{G}^- ... Material time derivative of G^- . ^[2,3]	δ_{ij} ... Identity tensor (Kronecker delta). ^[3]
∂_i^A, ∂_i ... Orientational differential operator (orientational gradient).	ϵ_{ijk} ... Permutation tensor (Levi-Civita symbol). ^[3]
$\hat{\partial}_i^A, \hat{\partial}_i$... Constrained orientational gradient. ^[2]	(φ, θ, ψ) Euler angles.
	$\left. \begin{array}{l} A_i^*, A_D^*, \\ \Lambda^*, \lambda_i^*, \lambda^* \end{array} \right\}$ Lagrange multipliers. ^[2]
..... Fields	
A_{ij} ... Structure tensor.	m_{ij}^- ... Voigt couple stress.
C_i^* ... Grain shifting velocity ($C_i^* := v_i^* - v_i$).	P^* ... Driving pressure for grain boundary migration (recrystallization pressure).
c_D^- ... Concentration of dislocations per unit mass ($c_D^- := \rho_D^- / \varrho^-$).	p^- ... Thermodynamic pressure.
c_i^- ... Specific external supply of lattice spin (body couple).	Q_i^- ... Total energy flux density.
D_{ij}^- ... Strain rate.	q_i^- ... Heat flux density.
E^- ... Specific total energy.	R^- ... Specific external supply of total energy.
e^- ... Specific internal energy.	r^- ... Specific external supply of internal energy (radiation supply).
f^* ... Species mass fraction ($f^* := \varrho^* / \varrho$).	S_{ij}^- ... Lattice spin velocity tensor ($S_{ij}^- = \epsilon_{jik} s_k^-$).
G ... Shear modulus.	s^- ... Specific external supply of entropy.
G_i^* ... Lattice deflecting rate ($G_i^* := s_i^* - s_i$).	s_i^- ... Lattice spin velocity.
g^- ... Specific Gibbs free energy ($g^- := h^- - T\eta^-$).	T ... Thermodynamic temperature.
g_i^- ... Specific external supply of linear momentum (body force).	$T_{,i}$... Temperature gradient ($T_{,i} := \partial T / \partial x_i$).
H_{ij}^- ... Relative spin velocity tensor ($H_{ij}^- := S_{ij}^- - W_{ij}^-$).	t_{ij}^- ... Cauchy stress.
h^- ... Specific free enthalpy ($h^- := e^- + p^- / \varrho^-$).	u_i^{A*}, u_i^* Interspecies transition rate.
$j_{D_i}^{A*}, j_{D_i}^*$ Interspecies flux density of dislocations.	v_i^- ... Translational velocity.
k_{ij}^- ... Thermal conductivity tensor.	W_{ij}^- ... Vorticity tensor.
L^- ... Specific production rate of total energy.	β_\varkappa^* ... Fabric parameter ($\varkappa = 1, \dots, \tilde{\varkappa}$).
M^* ... Species grain boundary mobility.	Γ^- ... Specific production rate of mass (recrystallization rate).
M_{ij}^- ... Schmid tensor.	γ^* ... dislocation parameter.
	δ^* ... Specific entropy deviation rate.
	ε^- ... Specific production rate of internal energy.

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η^- Specific entropy.	π_{ij}^* Surplus of the interspecies couple stress.
$\vartheta^* n_i n_j$ Equilibrium anisotropic stress.	$\varpi_{ij}^{A*}, \varpi_{ij}^*$ Interspecies couple stress.
ι_i^* Surplus of the interspecies flux density of entropy.	ϱ^- Mass density.
κ_i^- Specific production rate of linear momentum (high-angle interaction force).	ρ_D^- Dislocation density.
μ_D^- Specific Gibbs free energy of dislocations (dislocation potential).	ζ^- Specific production rate of entropy.
μ_{ijkl}^- Viscosity tensor.	ζ^{*P} Specific production rate of entropy of a ‘pure species’ (e.g. a single crystal).
ν_i^- Specific production rate of lattice spin (high-angle interaction couple).	σ_{ij}^- Dissipative stress.
Ξ_i^{A*}, Ξ_i^* Interspecies flux density of total energy.	$\tau_{ij}^{A*}, \tau_{ij}^*$ Interspecies stress.
ξ_i^{A*}, ξ_i^* . Interspecies heat flux density.	ϕ_i^- Entropy flux density.
Π_D^- Production rate density of dislocations.	$\varphi_i^{A*}, \varphi_i^*$ Interspecies flux density of entropy.
	Ψ^-, ψ^- . . Specific Helmholtz free energy ($\psi^- := e^- - T\eta^-$).

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