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## Multiscale modeling of ice deformation behavior

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### Abstract

Understanding the flow of ice in glaciers and polar ice sheets is of increasing relevance in a time of potentially significant climate change. The flow of ice has hitherto received relatively little attention from the structural geological community. This paper aims to provide an overview of methods and results of ice deformation modeling from the single crystal to the polycrystal scale, and beyond to the scale of polar ice sheets. All through these scales, various models have been developed to understand, describe and predict the processes that operate during deformation of ice, with the aim to correctly represent ice rheology and self-induced anisotropy. Most of the modeling

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tools presented in this paper originate from the material science community, and are currently used and further developed for other materials and environments. We will show that this community has deeply integrated ice as a very useful "model" material to develop and validate approaches in conditions of a highly anisotropic behavior. This review, by no means exhaustive, aims at providing an overview of methods at different scales and levels of complexity.

*Keywords:* ice mechanical behavior, multiscale modeling, viscoplastic anisotropy, fabric development

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41 **1. Introduction**

42 Ice is a common mineral on the Earth's surface, where it occurs as ice  
43 Ih. As ice is relatively close to its melting temperature, glaciers and polar  
44 ice sheets deform by ductile dislocation creep at strain rates in the order  
45 of  $10^{-12}$  to  $10^{-6}$  s<sup>-1</sup>. Research on the flow of ice is of direct importance  
46 to society as it is needed to understand and predict the effects that global  
47 warming could have on sea level rise, glacier retreat, etc. There is also an  
48 increasing awareness that ice is a valuable analogue for other minerals and  
49 crystalline materials, as it is the only common mineral where this creep can  
50 be readily observed in nature and in the laboratory. Numerical modeling  
51 has become a key method to link the mechanics of ice from the dislocation  
52 scale to that of flowing ice masses.

53 Most of the efforts made to simulate the ductile mechanical behavior of  
54 polycrystalline ice are related to the modeling of ice flow and fabric evolution  
55 in the conditions of polar ice sheets or glaciers. Ice is increasingly considered  
56 a model material to validate micro-macro mechanical approaches for mate-  
57 rials with a high viscoplastic anisotropy. Most of the modeling techniques  
58 presented in this paper are currently used or further developed for other  
59 materials. For geological applications, one main limitation could be related  
60 to the "one phase" approach for most of these techniques, well adapted to  
61 ice. The reader will find, at the end of the paper, a table summarizing the  
62 main aspects of each techniques, with application ranges and limitations.

63 *1.1. Mechanical properties of ductile ice*

64 Ice Ih has an hexagonal crystal structure with a  $c/a$  ratio of 1.628. This  
65  $c/a$  ratio is very close to the 1.633 value for a closely packed structure, but  
66 ice is not closely packed (see Schulson and Duval (2009) for a recent review).  
67 The elastic anisotropy of ice single crystals is small. The Young modulus  $E$   
68 only varies by about 30%, depending on the direction of the loading axis with  
69 respect to the  $c$ -axis. The highest value is along the  $c$ -axis with  $E = 11.8$   
70 GPa at  $-16^\circ\text{C}$  (Gammon et al., 1983).

71 Single crystals deform plastically essentially by glide of dislocations on  
72 the basal plane. There are three equivalent  $\langle 1\bar{2}10 \rangle$  directions for the  
73 Burgers vector, but slip on the basal plane is almost isotropic. In conditions  
74 where basal slip is favored, the stress-strain rate relationship after a strain of  
75 about 5% can be expressed by a power law with a stress exponent  $n = 2 \pm 0.3$   
76 (Higashi et al., 1965; Jones and Glen, 1969; Mellor and Testa, 1969). At  
77 similar strain rates, the equivalent stress requested for non-basal slip is about  
78 60 times larger than for basal slip (Duval et al., 1983).

79 For ice polycrystals deformed under the laboratory conditions (strain rate  
80 between about  $10^{-8} \text{ s}^{-1}$  and  $10^{-6} \text{ s}^{-1}$  and temperature generally higher  
81 than  $-30^\circ\text{C}$ ), strain is essentially due to intracrystalline dislocation glide.  
82 The transient creep regime is characterized by a strong directional hardening  
83 until the strain-rate minimum is reached for an overall strain of 1% (Duval  
84 et al., 1983). This strain-rate decrease can reach three orders of magnitude.  
85 It is associated to the development of a strong internal stress field due to  
86 plastic incompatibility between grains (Ashby and Duval, 1985; Duval et al.,  
87 1983; Castelnau et al., 2008b). A significant part of the transient creep is  
88 recoverable, i.e., on unloading a creep specimen, a reverse creep is observed,  
89 with reverse strain which can be more than ten times the initial elastic strain

90 (Duval, 1976; Duval et al., 1983). In the secondary creep regime, isotropic  
 91 polycrystals deform (at similar stress levels) a 100 times slower than a single  
 92 crystal optimally oriented for basal slip. In this regime, the minimum strain  
 93 rate and the stress are linked by a power law, referred to as Glen’s law in  
 94 glaciology (Glen, 1955), expressed through a relationship of the form (1) for  
 95 temperatures lower than  $-10^{\circ}\text{C}$ .

$$\dot{\epsilon}_{min} = A\bar{\sigma}^n \exp(-E_p/k_B T) \quad (1)$$

96 with  $\bar{\sigma}$  the applied stress,  $E_p = 0.72$  eV and the stress exponent  $n = 3$   
 97 (Barnes et al., 1971; Budd and Jacka, 1989).  $A$  is a constant,  $k_B$  the Boltz-  
 98 mann constant and  $T$  the temperature. Above  $-10^{\circ}\text{C}$ ,  $\dot{\epsilon}_{min}$  rises more rapidly  
 99 with increasing temperature and cannot be described by this equation (Mor-  
 100 gan, 1991). No grain-size effect is expected for power-law secondary creep  
 101 at laboratory conditions (see Duval and Le Gac (1980); Jacka (1994) for  
 102 instance). But a grain size effect was, however, measured during transient  
 103 creep (Duval and Le Gac, 1980).

104 At strains larger than 1 to 2% (tertiary creep regime), dynamic recrystalliza-  
 105 tion is predominant, and new grain microstructures and crystal orientations  
 106 are generated (Jacka and Maccagnan, 1984; Duval et al., 2000).

107 At stresses lower than 0.1 MPa, relevant to deformation conditions in glaciers,  
 108 ice sheets or planetary bodies, there is a clear indication of a creep regime  
 109 with a stress exponent lower than two. This indication results from both  
 110 the analysis of field data and laboratory tests, although the difficulty of  
 111 obtaining reliable data at strain rates lower than  $10^{-10}\text{s}^{-1}$  is at the ori-  
 112 gin of contradictory results (Mellor and Testa, 1969; Barnes et al., 1971;  
 113 Dahl-Jensen and Gundestrup, 1987; Pimienta et al., 1987; Lipenkov et al.,  
 114 1997; Goldsby and Kohlstedt, 1997). In particular, Goldsby and Kohlstedt

115 (1997) suggest a grain-size dependence of the ice viscosity associated with  
116 this low stress regime, based on laboratory experiments performed on very  
117 small grain-size samples. This grain-size effect would be associated with  
118 a grain boundary-sliding dominated creep. Its extrapolation to polar ice-  
119 core deformation conditions remains controversial (Duval and Montagnat,  
120 2002). Diffusional creep, commonly associated with such conditions in many  
121 materials yields a viscosity much higher than that deduced from field data  
122 (Lliboutry and Duval, 1985). For a review on ice behavior, see (Duval et al.,  
123 2010).

124 Ice as a model material exhibits a challenging viscoplastic anisotropy ow-  
125 ing to the presence of only two independent easy slip systems for the dis-  
126 locations (basal plane). While five independent systems are required to  
127 accommodate an arbitrary deformation in a single crystal (Taylor, 1938),  
128 Hutchinson (1977) showed that four systems are required for allowing an  
129 hexagonal polycrystal such as ice to deform. Being able to represent and to  
130 take into account this anisotropy in micro-macro models which aim at link-  
131 ing the single crystal scale to the polycrystal scale, is of primary interest to  
132 the material science community. This anisotropy needs to be accounted for  
133 at the dislocation scale in order to build physically-based model for the acti-  
134 vation of (poorly known) secondary slip systems. The impact of dislocation  
135 induced internal stress fields, but also the characterization and development  
136 of highly heterogeneous strain and stress fields within polycrystals, and their  
137 impact on fabric development turn out to be of strong importance (Castel-  
138 nau et al., 1996a; de la Chapelle et al., 1998).

139 During gravity-driven flow of glaciers and ice sheets, the macroscopic  
140 behavior of ice becomes progressively anisotropic with the development of  
141 fabrics (or textures, c-axis preferred orientations). This anisotropy and its



142 development depends on the flow conditions, but strongly influences the re-  
143 sponse of ice layers to imposed stress (see Gundestrup and Hansen (1984);  
144 Van der Veen and Whillans (1990); Mangeney et al. (1997) for pioneer field  
145 work and modeling on the subject). Indeed, a polycrystal of ice with most  
146 of its c-axes oriented in the same direction deforms at least ten times faster  
147 than an isotropic polycrystal, when sheared parallel to the basal planes.  
148 Fabrics basically develop as the result of lattice rotation by intracrystalline  
149 slip (Azuma and Higashi, 1985; Alley, 1988, 1992). Dynamic recrystalliza-  
150 tion can have a major impact on fabric development, especially at temper-  
151 atures above  $-10^{\circ}\text{C}$  close to bedrocks or within temperate glaciers (Alley,  
152 1992; Duval and Castelnau, 1995; de la Chapelle et al., 1998; Montagnat  
153 et al., 2009), see Section 5. Questions, however, remain to what extent dif-  
154 ferent recrystallization processes operate as a function of depth in polar ice  
155 sheets (Kipfstuhl et al., 2006, 2009; Weikusat et al., 2009).

## 156 *1.2. Main objectives*

157 Accurate modeling of ice flow under natural conditions is relevant for  
158 many scientific objectives, such as the response of ice sheet to climate  
159 changes (Seddik et al., 2012), the interpretation of climate signals extracted  
160 from ice cores (Faria et al., 2010), the energy balance in extraterrestrial  
161 satellites (Sotin et al., 2009), and since a few years, the accurate prediction  
162 of sea-level rise that is linked to the behavior of fast-moving coastal glaciers  
163 (Gillet and Durand, 2010). In this context, challenges are mainly (i) to  
164 establish an ice flow law adapted to low stress conditions, changes in tem-  
165 peratures and impurity content, (ii) to consider the macroscopic anisotropy  
166 due to fabric development at the given conditions, (iii) to be able to inte-  
167 grate processes such as dynamic recrystallization that can strongly influence

168 fabric development and the flow law.

169

170 The aim of this paper is to present a general overview of the main mod-  
171 eling techniques adapted to ice, and the main modeling results obtained  
172 from the single crystal scale to the large scale that is relevant to ice sheet  
173 flow modeling. Techniques are highly diverse, from dislocation dynamics  
174 (micron scale) to Finite Element methods that are adapted to the whole ice  
175 sheet (km scale), via mean-field and full-field micro-macro approaches and  
176 coupling with a microstructure evolution models (cm to m scale, limited to  
177 a 2D configuration, see 5.2). We will mostly focus on recent advances and  
178 topics that are still under development.

179

## 180 **2. Modeling ice single crystal behavior**

181 Owing to its high viscoplastic anisotropy, with dislocations gliding mostly  
182 on the basal plane, studying and modeling ice single crystal behavior is a  
183 challenge for regular approaches.

184 Recent efforts focused on three main objectives; (i) understanding, repre-  
185 senting and taking into account the dislocation dynamics, (ii) improving our  
186 knowledge about secondary slip systems in ice, (iii) providing an accurate  
187 crystal plasticity constitutive law that can be implemented in mean-field and  
188 full-field approaches for micro-macro polycrystal models. For the two first  
189 objectives, Dislocation Dynamic models (DD) were used at the scale of the  
190 interaction between dislocation populations (Section 2.1). At a larger scale,  
191 the Field Dislocation Mechanic modeling approach (FDM) was applied to  
192 ice to evaluate the role of internal stresses associated with dislocation fields

193 and arrangements (Section 2.2). Section 2.3 presents a crystal-plasticity  
194 model adapted to the transient creep behavior of ice single crystals.

### 195 *2.1. Dislocation Dynamics modeling*

196 Dislocation dynamics in ice was shown to be scale free and intermit-  
197 tent, thanks to dislocation avalanche measurements via acoustic emissions  
198 (Weiss and Grasso, 1997; Weiss et al., 2001; Weiss and Marsan, 2003; Weiss  
199 and Montagnat, 2007). Ice was used as a model material for the following  
200 reasons: (i) transparency allows direct verification that acoustic emission  
201 activity is not related to microcracking, (ii) with the range of stress and  
202 temperature considered, diffusion creep is not a significant mechanism, and  
203 deformation occurs by dislocation glide only. DD modeling tools were used  
204 to better understand and characterize this scale free and intermittent be-  
205 havior (for example Miguel et al. (2001); Weiss and Miguel (2004)).

206 Miguel et al. (2001) made use of a discrete dislocation dynamics model with  
207 a two-dimensional cross-section of the crystal. This 2D space is randomly  
208 filled with edge dislocations gliding along a single slip direction parallel to  
209 their respective Burgers vector. This simplification is an effective way to  
210 describe materials like ice crystals owing to their strong plastic anisotropy  
211 with a single slip system dominating. A basic feature common to most DD  
212 models is that dislocations interact with each other through the long-range  
213 elastic stress field they produce in the host material. In (Miguel et al.,  
214 2001), dislocation velocity depends linearly on this effective stress, and the  
215 Peierls stress is set to zero. Mechanisms for dislocation annihilation and  
216 multiplication are classically taken into account.

217 Within this simplified scheme the authors found that dislocations gener-  
218 ate a slowly evolving configuration landscape which coexists with rapid col-

219 lective rearrangements. These arrangements involve a comparatively small  
220 fraction of dislocations and lead to an intermittent behavior of the net plastic  
221 response. The model was therefore able to reproduce the fact that disloca-  
222 tions themselves, through the various structures such as dipoles and walls,  
223 generate a pinning force landscape that is virtually frozen into a slow state.  
224 Creation and annihilation mechanisms allow the system to jump between  
225 slow dynamics states through bursts of activity.

226 More recently, Chevy et al. (2007, 2012) used DD simulations to analyze  
227 torsion tests performed on ice single crystals. The tests were performed  
228 with the ice-crystal *c*-axis oriented parallel to the torsion axis so that basal  
229 screw dislocations were mainly activated. With synchrotron topography  
230 analyses of the deformed samples, it was possible to show that dislocation  
231 arrangements were highly heterogeneous, with a scale-invariant character  
232 and long-range correlations (Montagnat et al., 2006; Weiss and Montagnat,  
233 2007; Chevy et al., 2010). Although these tests were performed in a way that  
234 highly favored basal glide, the double-cross slip mechanisms was invoked to  
235 explain this scale invariant dislocation arrangement.

236 Three-dimensional DD simulations, based on the TRIDIS code (Verdier  
237 et al., 1998), were adapted to these torsion tests on ice and the hexago-  
238 nal structure. Screw dislocation sources were positioned within one slip  
239 plane at the periphery of a cylinder submitted to a constant torque. Cross-  
240 slip on prismatic planes was made possible thanks to the internal stress  
241 induced by the pile-up of basal dislocations in the center of the cylinder  
242 (where  $\sigma_{app} = 0$ ), which produces the out-of-plane component needed (see  
243 Fig. 1). Simulation results allowed to test this hypothesis, and explain the  
244 power law relationship between stress and strain rate (Chevy et al., 2012).

245 *2.2. Field Dislocation Mechanics (FDM)*

246 Field dislocation theory is a mesoscale approach, which aims at tak-  
247 ing into account the inhomogeneous distribution of dislocations in plasticity  
248 modeling. Therefore, FDM modeling makes it possible to represent and con-  
249 sider the internal stress field created by the dislocation arrangements within  
250 the crystal. FDM is a continuous approach able to deal simultaneously with  
251 long-range correlations associated with distortion fields, internal stresses due  
252 to dislocation arrangements, and short-range correlations (Acharya, 2001).  
253 The reader is referred to (Acharya and Roy, 2006; Varadhan et al., 2006;  
254 Fressengeas, 2010) for details.

255 The first application to ice samples was performed in the configuration of  
256 the torsion test presented in part 2.1 (Taupin et al., 2007). This test is  
257 by itself highly heterogeneous, and this heterogeneity was shown to induce  
258 unexpected non-basal slip. Taking into account the coupled dynamics of  
259 geometrically necessary screw dislocations gliding in the basal plane (also  
260 called "excess" dislocations) and statistical dislocations developed through  
261 cross slip in prismatic planes, the model was able to reproduce the creep  
262 curves during torsion, and the size effect measured experimentally (see Fig.  
263 2). More recently, the model was used to reproduce the complex scale-  
264 invariant character of dislocation arrangements forming during torsion tests  
265 on ice single crystals (Chevy et al., 2010). In particular, the fact that the  
266 model takes into account both the long-range elastic interactions due to  
267 the presence of dislocations and the short-range interactions inherent to the  
268 transport of dislocations (obstacles, cross-slip, etc.) allowed to reproduce  
269 the shift in control of the dislocation distribution by long-range correlations  
270 at low strain to a control by short-range correlations at strain as high as  
271 50%. It was shown that non-basal dislocations activated by the internal

272 stress fields induce a screening potential at large strain, through obstacles  
 273 such as twist sub-boundaries. However, this screening was shown to be too  
 274 small to hinder creep acceleration prevailing during torsion creep test on ice  
 275 single crystals (Chevy et al., 2010).

### 276 2.3. Crystal plasticity modeling

277 Constitutive relations to describe the transient creep of ice single crystals  
 278 have been proposed by Castelnau et al. (2008b) and then used in a modified  
 279 version in Suquet et al. (2011). One of the difficulty here is the description  
 280 of the softening of basal slip in the transient regime, as discussed above.  
 281 As is usual in crystal plasticity at infinitesimal strains, the strain tensor is  
 282 decomposed into the sum of an elastic  $\boldsymbol{\varepsilon}^e$  and a viscoplastic  $\boldsymbol{\varepsilon}^{vp}$  part

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^{vp} . \quad (2)$$

283 The elastic strain is related to the local stress tensor  $\boldsymbol{\sigma}$  with the local com-  
 284 pliance tensor  $\mathbf{S}$ , and the viscoplastic strain results from slips on a total of  
 285  $M$  different slip systems:

$$\boldsymbol{\varepsilon}^e = \mathbf{S} : \boldsymbol{\sigma} , \quad \boldsymbol{\varepsilon}^{vp} = \sum_{k=1}^M \gamma^{(k)} \boldsymbol{\mu}^{(k)} . \quad (3)$$

286 Here,  $\boldsymbol{\mu}^{(k)} = \frac{1}{2}(\mathbf{n}^{(k)} \otimes \mathbf{b}^{(k)} + \mathbf{b}^{(k)} \otimes \mathbf{n}^{(k)})$  is the (purely geometric) Schmid  
 287 tensor depending on the orientation of the slip system ( $k$ ),  $\mathbf{n}$  being the slip  
 288 plane normal and  $\mathbf{b}$  the slip direction (parallel to the Burgers vector and  
 289 orthogonal to  $\mathbf{n}$ ) in that plane, with  $\otimes$  the dyadic product.

290 Ice crystals, which have an hexagonal symmetry, deform easily by shear  
 291 on the basal plane, on the three systems  $\{0001\} \langle 11\bar{2}0 \rangle$  which provide only  
 292 two independent systems. The three prismatic systems  $\{1\bar{1}00\} \langle 11\bar{2}0 \rangle$   
 293 provide two more independent systems. An additional independent slip

294 system is thus required to attain any isochoric deformation at the single  
 295 crystal level and this is achieved by adding the six  $\langle c + a \rangle$  pyramidal  
 296 systems  $\{11\bar{2}2\} \langle 11\bar{2}\bar{3} \rangle$ . In total,  $M = 12$  slip systems are taken into  
 297 account in the present analysis.

298 In the constitutive relations originally proposed by Castelnau et al.  
 299 (2008b), the slip rate on the  $k$ -th system is related to the resolved shear  
 300 stress  $\tau^{(k)}$  on that system through:

$$\dot{\gamma}^{(k)} = \dot{\gamma}_0^{(k)} \left( \frac{|\tau^{(k)}|}{\tau_0^{(k)}} \right)^{n^{(k)}} \text{sgn}(\tau^{(k)}), \quad \tau^{(k)} = \boldsymbol{\sigma} : \boldsymbol{\mu}^{(k)}, \quad (4)$$

301 where  $\tau_0^{(k)}$ , the reference resolved shear stress on system  $k$ , depends on the  
 302 activity of the other systems through:

$$\dot{\tau}_0^{(k)} = \sum_{\ell=1}^M H^{(k,\ell)} \left( \frac{\tau_{sta}^{(\ell)} - \tau_0^{(\ell)}}{\tau_{sta}^{(\ell)} - \tau_{ini}^{(\ell)}} \right) |\dot{\gamma}^{(\ell)}|. \quad (5)$$

303 The two material parameters  $\tau_{ini}^{(\ell)}$  and  $\tau_{sta}^{(\ell)}$  refer, respectively, to the initial  
 304 value of  $\tau_0^{(\ell)}$  at the onset of plasticity (when the  $\gamma^{(k)}$ 's are small ) and to the  
 305 stationary value of  $\tau_0^{(\ell)}$  at saturation when the plasticity is fully developed  
 306 (*i.e.* when the  $\gamma^{(k)}$ 's are large). Therefore the contribution of system  $\ell$  in  
 307 the hardening (or softening) of system  $k$  vanishes when  $\tau_0^{(\ell)}$  is close to  $\tau_{sta}^{(\ell)}$ .  
 308 The hardening matrix  $H^{(k,\ell)}$  expresses the influence of the plastic activity  
 309 of system  $\ell$  on the hardening of system  $k$  and is taken to be symmetric.  
 310 Material data for this model are given in Castelnau et al. (2008b).

311 In (Suquet et al., 2011), Eqs (4) and (5) are improved in two ways:

312 1. Kinematic hardening is introduced in (4) through a back stress  $X^{(k)}$ :

$$\dot{\gamma}^{(k)} = \dot{\gamma}_0^{(k)} \left( \frac{|\tau^{(k)} - X^{(k)}|}{\tau_0^{(k)}} \right)^{n^{(k)}} \text{sgn}(\tau^{(k)} - X^{(k)}), \quad (6)$$

313 where the back stress evolves with the plastic activity according to an  
 314 Armstrong-Frederick type law (Chaboche, 2008):

$$\dot{X}^{(k)} = c^{(k)}\dot{\gamma}^{(k)} - d^{(k)}X^{(k)} \left| \dot{\gamma}^{(k)} \right| - e^{(k)}X^{(k)}, \quad (7)$$

315 including static recovery through coefficient  $e^{(k)}$ . The introduction  
 316 of a back stress on each slip system is motivated by the experimen-  
 317 tal observation of recovery strain developing in single crystals when  
 318 specimens are subjected to recovery tests (see Section 2.3.2 and Fig.  
 319 4).

320 2. The equation governing the reference resolved shear stress  $\tau_0^{(k)}$  is mod-  
 321 ified into

$$\dot{\tau}_0^{(k)} = \left( \tau_{sta}^{(k)} - \tau_0^{(k)} \right) \dot{p}^{(k)}, \quad \dot{p}^{(k)} = \sum_{\ell=1}^M H^{(k,\ell)} \left| \dot{\gamma}^{(\ell)} \right|. \quad (8)$$

322 The motivation for the change in the evolution rule for the reference  
 323 resolved shear stresses  $\tau_0^{(k)}$  is that with the original rule (5) they never  
 324 reach their stationary value, unless all systems do so at the same time,  
 325 a condition which cannot be met in a polycrystal (see details in (Su-  
 326 quet et al., 2011)). By contrast, the law (8) ensures convergence of  
 327  $\tau_0^{(k)}$  towards its stationary value, provided all coefficients  $H^{(k,\ell)}$  are  
 328 positive. Indeed, in this case,  $\dot{p}^{(k)}$  is always positive and  $p^{(k)}$  is in-  
 329 creasing with time, acting on system  $k$  in a similar way as the classical  
 330 cumulated plastic strain of von Mises plasticity. The differential Eq.  
 331 (8) can be integrated into

$$\tau_0^{(k)}(p^{(k)}) = \tau_{sta}^{(k)} + (\tau_{ini}^{(k)} - \tau_{sta}^{(k)}) \exp(-p^{(k)}), \quad (9)$$

332 which shows that  $\tau_0^{(k)} - \tau_{sta}^{(k)}$  has the same sign as  $\tau_{ini}^{(k)} - \tau_{sta}^{(k)}$ . Further-  
 333 more  $\tau_0^{(k)}$  tends to  $\tau_{sta}^{(k)}$  when  $p^{(k)}$  becomes large.



334 *2.3.1. Data for elasticity*

335 As mentioned in Section 1, ice crystals exhibit a low elastic anisotropy,  
 336 the largest stiffness ( $E \sim 11.8\text{GPa}$ ) being along the  $c$ -axis (Fig. 3). The  
 337 tensor of elastic moduli (in Kelvin’s notations) at  $-16^\circ\text{C}$  is given by (10)  
 338 (Gammon et al., 1983),

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sqrt{2}\sigma_{23} \\ \sqrt{2}\sigma_{13} \\ \sqrt{2}\sigma_{12} \end{pmatrix} = \begin{pmatrix} 13930. & 7082. & 5765. & 0. & 0. & 0. \\ 7082. & 13930. & 5765. & 0. & 0. & 0. \\ 5765. & 5765. & 15010. & 0. & 0. & 0. \\ 0. & 0. & 0. & 6028. & 0. & 0. \\ 0. & 0. & 0. & 0. & 6028. & 0. \\ 0. & 0. & 0. & 0. & 0. & 6848. \end{pmatrix} \begin{pmatrix} \varepsilon_{11}^e \\ \varepsilon_{22}^e \\ \varepsilon_{33}^e \\ \sqrt{2}\varepsilon_{23}^e \\ \sqrt{2}\varepsilon_{13}^e \\ \sqrt{2}\varepsilon_{12}^e \end{pmatrix}, \quad (10)$$

339 where all entries are in MPa and 3 is the axis of transverse isotropy ( $c$ -axis of  
 340 the hexagonal crystalline structure). For conditions prevailing in ice sheets  
 341 and glaciers, elastic constants vary little with temperature: a temperature  
 342 change of  $5^\circ\text{C}$  only modifies the elastic constants by about 1.5%.

343 *2.3.2. Data for basal slip*

344 The literature provides a number of experimental data for the behavior  
 345 of ice crystals deformed in such a way that only basal slip is activated. Due  
 346 to the very large viscoplastic anisotropy of ice single crystals, it is stressed  
 347 that mechanical tests have to be carried out very carefully to avoid any  
 348 heterogeneity of the stress field within the specimen (Boehler et al., 1987).

349 Mechanical tests on single crystals where solely non-basal systems are  
 350 activated have not been reported so far. This would require straining the  
 351 crystal along or perpendicular to the  $c$ -axis, but unfortunately any unavoi-  
 352 dable deviation from perfect alignment activates basal slip. Duval et al. (1983)  
 353 has given upper bounds for the flow stress on non-basal systems.

354       Consequently, only the material parameters of Eq. (6) relevant for basal  
355 slip can be identified with confidence from experimental data on single crys-  
356 tals :

- 357       • First, data compiled by Duval et al. (1983) were used to determine the  
358 stationary flow stress and the stress-sensitivity exponent  $n^{(k)}$  of basal  
359 slip. There is quite a large spread in these experimental results from  
360 different authors. Despite these uncertainties, the stress-sensitivity  
361 exponent for basal slip can be directly identified from these experi-  
362 mental data (numerical values are reported in Table 1), whereas the  
363 stationary flow stress depends on both the stationary reference stress  
364  $\tau_{sta}^{(k)}$  and the stationary backstress  $X^{(k)}$ .
  
- 365       • Next, data from Weertman (1973) were used for the identification of  
366 the transient creep regime of basal systems. Single crystals were de-  
367 formed under uniaxial compression at different strain rates, with  $c$ -axis  
368 oriented at  $45^\circ$  from the loading direction (Fig. 4). The observed stress  
369 peak is associated with the increase in density of mobile dislocations  
370 (Duval et al., 1983), a behavior typical for material with very low ini-  
371 tial dislocation density (see Sauter and Leclercq (2003); Cochard et al.  
372 (2010)). These tests shed light on the softening of basal slip in the  
373 transient regime. The static recovery term  $e^{(k)}$  in the constitutive law  
374 (7) helps achieving the correct stationary stress at very small strain  
375 rates (since  $X^{(k)}$  tends to a constant value  $c^{(k)}/d^{(k)}$  at large shear  $\gamma^{(k)}$   
376 if static recovery is not introduced).
  
- 377       • Finally, the recovery test of Taupin et al. (2008) performed on sin-  
378 gle crystals under uniaxial compression was considered. Here the  $c$ -  
379 axis orientation was not precisely defined experimentally, but it made

380 an angle “less than  $10^\circ$ ” with the compression direction. The sin-  
381 gle crystal was submitted to four creep loadings for 30 minutes sepa-  
382 rated by unloading stages for respectively 1 minute, 10 minutes, and  
383 100 minutes (Fig. 4). Upon reloading, the strain rate is larger than  
384 just before the last unloading, indicating that dislocations are rear-  
385 ranging during the time intervals where the specimen is unloaded.  
386 This is accounted for in the model by the back stress  $X^{(k)}$ , and by  
387  $e^{(k)}$ .

388 Fig. 4 shows the good match between the model (constitutive Eq. (6)) with  
389 the set of parameters given in Table 1 and these experimental results.

### 390 **3. Mean field approaches for the mechanical response of ice poly-** 391 **crystals**

#### 392 *3.1. Microstructure characterization*

393 From the mechanical point of view, polycrystalline materials have to be  
394 considered as a specific class of composites. They are composed of many  
395 grains, with grain size in the range of mm to cm for natural ice. Grains are  
396 assembled in a random way, *i.e.* their size, shape, and lattice orientation do  
397 generally not depend on the size, shape, and orientation of the surrounding  
398 grains (Fig. 5). Therefore, the microstructure of ice polycrystals can hardly  
399 be described exactly in 3-D, unless one makes use of tomography techniques  
400 (Rolland du Roscoat et al., 2011). From (2-D) thin sections, one can at best  
401 access a statistical characterization of the 3-D grain arrangement *e.g.* with  
402 the help of cross-correlation functions, although the description is generally  
403 limited to a few parameters, such as the average grain size and grain shape  
404 (aspect ratio). In the Euler orientation space, microstructure description is

405 based on the distribution of crystal lattice orientations (Orientation Distri-  
406 bution Function, ODF, or crystallographic texture, often denoted "fabric"  
407 in the geophysical community). The complex behavior of polycrystalline  
408 materials comes from the anisotropic behavior at the grain scale, closely re-  
409 lated to the symmetry of the crystal lattice. This is true for all quantities of  
410 interest here, such as elasticity, viscoplasticity and thermal dilation. Grains  
411 with different lattice orientations react differently to a given stress level.  
412 As far as grain boundaries maintain the cohesion of the material, the *local*  
413 stress (*i.e.* inside a grain) differs from the *overall* one (the applied stress),  
414 leading to a heterogeneous distribution of stress and strain fields within the  
415 polycrystal.

416 Most research efforts in the past years have focussed on the understand-  
417 ing of the build-up of these heterogeneities, in relation with the microstruc-  
418 ture and local (grain) behavior, since they greatly influence the overall be-  
419 havior (for ice, see Grennerat et al. (2012) for instance). For instance, plas-  
420 ticity in a polycrystal can start far below the macroscopic yield stress, as it  
421 is sufficient that the local stress reaches the local yield stress somewhere in  
422 the structure where stress concentration is large enough, such as along grain  
423 boundaries (Brenner et al., 2009).

424 There are basically two strategies to get the mechanical response: mean-  
425 field (this section) and full-field (next section) approaches. For both of  
426 them, the key issue is the estimation of the stress or strain localization  
427 (or heterogeneities), in relation to the microstructure and local behavior of  
428 grains. Basically, the problem to be solved is to find an equilibrated stress  
429 field, related to a compatible strain field with the local constitutive relation,  
430 both fields fulfilling the applied boundary conditions. In the following, we  
431 review (not in an exhaustive way) some homogenization techniques used for

432 the investigation of the mechanical behavior of ice polycrystals.

### 433 3.2. Linear thermo-elasticity

434 For reasons that will become evident below, let us consider the case of  
 435 thermo-elastic ice polycrystals. The local constitutive relation at point  $(\mathbf{x})$   
 436 reads

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \mathbf{S}(\mathbf{x}) : \boldsymbol{\sigma}(\mathbf{x}) + \boldsymbol{\varepsilon}_0(\mathbf{x}), \quad (11)$$

437 with  $\boldsymbol{\varepsilon}_0$  a stress-free thermal strain (*e.g.* a dilation), due to temperature  
 438 changes. The local stress  $\boldsymbol{\sigma}(\mathbf{x})$  can be related to the overall stress (applied  
 439 at the polycrystal scale) by means of the stress-concentration tensor  $\mathbf{B}(\mathbf{x})$   
 440 for the purely elastic problem

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{B}(\mathbf{x}) : \bar{\boldsymbol{\sigma}} + \boldsymbol{\sigma}_{\text{res}}(\mathbf{x}), \quad (12)$$

441 with  $\boldsymbol{\sigma}_{\text{res}}$  the residual stress, *i.e.* the stress field remaining locally when  
 442 the overall load is suppressed ( $\bar{\boldsymbol{\sigma}} = \mathbf{0}$ ). It can be shown that the overall  
 443 polycrystal behavior takes a similar form as Eq. (11)

$$\bar{\boldsymbol{\varepsilon}} = \tilde{\mathbf{S}} : \bar{\boldsymbol{\sigma}} + \tilde{\boldsymbol{\varepsilon}}_0, \quad (13)$$

444 with symbols  $\tilde{\cdot}$  and  $\bar{\cdot}$  denoting the homogenized (or effective) property and  
 445 the volume average over the whole polycrystal volume (also denoted  $\langle \cdot \rangle$ ),  
 446 respectively. Therefore, one has  $\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma}(\mathbf{x}) \rangle$  and  $\bar{\boldsymbol{\varepsilon}} = \langle \boldsymbol{\varepsilon}(\mathbf{x}) \rangle$ , and it can be  
 447 shown that the effective compliance  $\tilde{\mathbf{S}}$  and the effective thermal strain  $\tilde{\boldsymbol{\varepsilon}}_0$   
 448 are given by (Laws, 1973)

$$\tilde{\mathbf{S}} = \langle \mathbf{S}(\mathbf{x}) : \mathbf{B}(\mathbf{x}) \rangle, \quad \tilde{\boldsymbol{\varepsilon}}_0 = \langle \boldsymbol{\varepsilon}_0(\mathbf{x}) : \mathbf{B}(\mathbf{x}) \rangle. \quad (14)$$

449 Since, for thermo-elastic polycrystals, the elastic compliance and the  
 450 thermal dilation coefficients are uniform properties inside grains, the quan-  
 451 tities  $\mathbf{S}(\mathbf{x})$  and  $\boldsymbol{\varepsilon}_0(\mathbf{x})$  in Eq. (11) can be replaced by the corresponding

452 homogeneous values  $\mathbf{S}^{(r)}$  and  $\boldsymbol{\varepsilon}_0^{(r)}$  of the considered phase ( $r$ ). A similar  
 453 substitution can be made in Eq. (14), leading to

$$\tilde{\mathbf{S}} = \sum_r c^{(r)} \mathbf{S}^{(r)} : \bar{\mathbf{B}}^{(r)}, \quad \tilde{\boldsymbol{\varepsilon}}_0 = \sum_r c^{(r)} \boldsymbol{\varepsilon}_0^{(r)} : \bar{\mathbf{B}}^{(r)} \quad (15)$$

454 with  $\bar{\cdot}^{(r)}$  indicating the average over the volume of phase ( $r$ ), *e.g.*  $\bar{\mathbf{B}}^{(r)} =$   
 455  $\langle \mathbf{B}(\mathbf{x}) \rangle^{(r)}$ , and  $c^{(r)}$  the volume fraction of phase ( $r$ ). Here, a *mechanical*  
 456 *phase* ( $r$ ) denotes the set of all grains of the polycrystal having the same  
 457 crystal orientation; those grains have different shape and environment but  
 458 their elastic and thermal properties are identical. From (15), it can be  
 459 observed that the sole knowledge of the mean (phase average) values  $\bar{\mathbf{B}}^{(r)}$  is  
 460 sufficient to estimate the overall polycrystal behavior. It can be anticipated  
 461 that, if the quantities  $\bar{\mathbf{B}}^{(r)}$  can be calculated without having to know the  
 462 complete field of  $\mathbf{B}(\mathbf{x})$ , computation will be way faster. Hence the name of  
 463 "mean-field" approaches presented here.

464 With the effective behavior (Eq. 14) in hand, statistical averages over  
 465 crystal orientations ( $r$ ) can be estimated. Basically, two quantities can be  
 466 obtained from mean-field approaches:

- 467 1. The phase average stress (or first moment)  $\bar{\boldsymbol{\sigma}}^{(r)} = \langle \boldsymbol{\sigma}(\mathbf{x}) \rangle^{(r)}$

$$\bar{\boldsymbol{\sigma}}^{(r)} = \bar{\mathbf{B}}^{(r)} : \bar{\boldsymbol{\sigma}} + \bar{\boldsymbol{\sigma}}_{\text{res}}^{(r)}, \quad (16)$$

468 with  $\bar{\boldsymbol{\sigma}}_{\text{res}}^{(r)}$  the average residual stress of phase ( $r$ ). The knowledge  
 469 of  $\bar{\boldsymbol{\sigma}}^{(r)}$  for all phases ( $r$ ) allows investigating the so-called *interphase*  
 470 heterogeneities, *i.e.* the variation of the phase average stress with  
 471 respect to the crystal orientation.

- 472 2. Deeper insight into the stress distribution can be obtained from the  
 473 second moment  $\langle \boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \rangle^{(r)}$  of the stress. This second moment can be

474 obtained by a derivation of the effective energy with respect to lo-  
 475 cal compliances, see (Bobeth and Diener, 1987; Kreher, 1990; Ponte-  
 476 Castañeda and Suquet, 1998; Brenner et al., 2004).

477 The standard deviation of the stress distribution within a given crystal ori-  
 478 entation ( $r$ ) can be estimated from these two moments as the square root  
 479 of  $\langle \boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \rangle^{(r)} - \langle \boldsymbol{\sigma} \rangle^{(r)} \otimes \langle \boldsymbol{\sigma} \rangle^{(r)}$  (*i.e.* the mean of the square of  
 480 the stress minus the square of the mean); it is related to the width of the  
 481 stress distribution in crystal orientation ( $r$ ), and accounts for both the het-  
 482 erogeneity of stress distribution *inside* grains but also for the heterogeneity  
 483 *between* grains of identical orientation but exhibiting different shapes and  
 484 having different neighborhood. Similar relations can be derived for the strain  
 485 statistics.

### 486 3.3. Reuss and Voigt approximations

487 First, two very basic models can be derived, namely *Reuss* (also called  
 488 *static* in the viscoplastic context) and *Voigt* (or *Taylor*) models. The Reuss  
 489 model is constructed by considering a uniform stress throughout the poly-  
 490 crystal, *i.e.*  $\boldsymbol{\sigma}(\mathbf{x}) = \bar{\boldsymbol{\sigma}} \quad \forall \mathbf{x}$ , or equivalently  $\mathbf{B}(\mathbf{x}) = \mathbf{I}$  (with  $\mathbf{I}$  the identity ten-  
 491 sor), and leads to vanishing intra- and inter-granular stress heterogeneities,  
 492 and uniform strain within grains. The Voigt model considers uniform strain,  
 493 *i.e.*  $\boldsymbol{\varepsilon}(\mathbf{x}) = \bar{\boldsymbol{\varepsilon}} \quad \forall \mathbf{x}$ , *i.e.* no intra- and inter-granular strain heterogeneities,  
 494 and uniform stress within grains. These models violate strain compatibility  
 495 and stress equilibrium, respectively, and are of limited accuracy when the  
 496 local behavior is highly nonlinear and/or highly anisotropic, as will be il-  
 497 lustrated in the next section. Besides simplicity, the main interest of Reuss  
 498 and Voigt models is based on their bounding character, since they provide,  
 499 respectively, a lower and an upper bound for the effective stress potential.

500 *3.4. The Self-Consistent (SC) scheme*

501 Unlike full-field approaches detailed in the Section 4, mean-field methods  
502 are based on a statistical description of the microstructure, *e.g.* based on  
503 few  $n$ -points correlation functions, so that the exact position and shape of  
504 a specific grain with respect to its neighbors is not known. However, as al-  
505 ready introduced, all grains exhibiting the same crystallographic orientation  
506 are treated as a single mechanical phase. Owing to the random character  
507 of the microstructure with all grains playing geometrically similar roles, the  
508 Self-Consistent (SC) scheme (Hershey, 1954; Kröner, 1958; Willis, 1981) is  
509 especially well suited for polycrystals. This model, which provides a rela-  
510 tively simple expression for  $\bar{\mathbf{B}}^{(r)}$ , relies on specific microstructures exhibiting  
511 perfect disorder and infinite size graduation (Kröner, 1978). The SC scheme  
512 has often been described as if the interaction between each grain and its sur-  
513 rounding could be approximated by the interaction between one ellipsoidal  
514 grain with the same lattice orientation as the original grain and a homoge-  
515 neous equivalent medium whose behavior represents that of the polycrystal,  
516 taking thus advantage of the analytical solution of Eshelby (1957) for the in-  
517 clusion/matrix interaction. This reasoning led to the conclusion that the SC  
518 scheme implicitly considers uniform stress and strain rate inside grains. This  
519 interpretation turns out to be incorrect, since intraphase stress and strain  
520 heterogeneities do not vanish as explained above, see Ponte-Castañeda and  
521 Suquet (1998) for a review.

522 The ability of the SC scheme to estimate polycrystal behavior is shown  
523 in Fig. 6. Numerical reference solutions from the full-field FFT method  
524 (see Section 4) have been generated for many randomly generated Voronoi  
525 microstructures, and ensemble average over these random microstructures  
526 has been calculated in order to attain results that are representative for



527 a Representative Volume Element, *i.e.* a volume sufficiently large to be  
 528 statistically representative of the material (Kanit et al., 2003; Lebensohn  
 529 et al., 2004b). In Fig. 6, we provide results for the effective behavior, that  
 530 is entirely defined by the effective reference stress  $\tilde{\sigma}_0$  which enters in the  
 531 effective constitutive relation

$$\frac{\dot{\tilde{\epsilon}}_{eq}}{\dot{\tilde{\epsilon}}_0} = \frac{\bar{\sigma}'_{eq}}{\bar{\sigma}_0} \quad (17)$$

532 with  $\dot{\tilde{\epsilon}}_0$  a reference strain rate (taken here equal to  $\dot{\gamma}_0$ ), and  $\bar{\sigma}'_{eq}$  and  $\dot{\tilde{\epsilon}}_{eq}$  the ef-  
 533 fective equivalent stress and strain rate respectively ( $\bar{\sigma}'_{eq} = \sqrt{3\bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\sigma}}/2}$ ,  $\dot{\tilde{\epsilon}}_{eq} =$   
 534  $\sqrt{2\dot{\tilde{\boldsymbol{\epsilon}}} : \dot{\tilde{\boldsymbol{\epsilon}}}/3}$ ). Calculations are performed for various viscoplastic anisotropy  
 535 contrasts (or slip system contrasts) at the grain level, defined by the ratio  
 536 between non-basal and basal reference shear stresses, *i.e.*  $\tau_0^{(Pr)}/\tau_0^{(Ba)}$  for  
 537  $\tau_0^{(Pr)} = \tau_0^{(Pr)}$ . It can be observed that the SC model perfectly reproduces  
 538 the reference full-field (FFT) results. Note also that the Reuss bound, of-  
 539 ten used for highly anisotropic materials like ice, predicts a much too soft  
 540 overall behavior. This simple approach does not allow to make a realis-  
 541 tic link between local and overall rheologies. We also report in this figure  
 542 the standard deviations (or overall heterogeneities) of equivalent stress and  
 543 strain rate. These standard deviations have been calculated over the whole  
 544 polycrystal. Recall that they account for both intra- and inter-granular field  
 545 heterogeneities for both SC and FFT approaches. It can be observed that  
 546 the increase of standard deviation with the slip system contrast is well re-  
 547 produced by the SC scheme, although some discrepancies with FFT results  
 548 arise at very large contrasts (mostly for the strain-rate fluctuation). Note  
 549 again that Reuss and Voigt bound do not reproduce these results, even in  
 550 a qualitative way, since they predict, by construction, vanishing fluctuation  
 551 of stress and strain rate, respectively. Unlike these simple approaches, the

552 SC scheme not only predicts the correct effective stress, but also accurately  
 553 captures the field heterogeneities within the polycrystal. Similar agreement  
 554 have been obtained for Voronoi and EBSD 2-D microstructures under an-  
 555 tiplane shear by Lebensohn et al. (2005).

### 556 3.5. Nonlinear viscoplasticity

557 The mean-field estimate of *nonlinear materials* is significantly more com-  
 558 plex than the thermo-elastic case treated above. We consider the case of a  
 559 viscoplastic polycrystal of ice in which grains are deforming by glide of dis-  
 560 locations on specific slip planes, as discussed above, with slip rates given by  
 561 Eq. (4), so that the local strain rate reads, since elastic deformations are  
 562 neglected:

$$\dot{\boldsymbol{\epsilon}}(\mathbf{x}) = \sum_k \boldsymbol{\mu}_{(k)}^{(r)} \dot{\gamma}_{(k)}(\mathbf{x}) . \quad (18)$$

563 Here, reference stresses  $\tau_0$  and stress sensitivities  $n$  are supposed to be con-  
 564 stant. The constitutive Eq. (18) can also be written

$$\dot{\boldsymbol{\epsilon}}(\mathbf{x}) = \mathbf{M}(\mathbf{x}) : \boldsymbol{\sigma}(\mathbf{x}) \quad (19)$$

565 with

$$\mathbf{M}(\mathbf{x}) = \sum_k \frac{\dot{\gamma}_0^{(k)}}{\tau_0^{(k)}} \left| \frac{\boldsymbol{\mu}^{(k)}(\mathbf{x}) : \boldsymbol{\sigma}(\mathbf{x})}{\tau_0^{(k)}} \right|^{n^{(k)}-1} \boldsymbol{\mu}^{(k)}(\mathbf{x}) \otimes \boldsymbol{\mu}^{(k)}(\mathbf{x}) . \quad (20)$$

566 Obviously, the viscous compliance  $\mathbf{M}$  relating  $\dot{\boldsymbol{\epsilon}}(\mathbf{x})$  and  $\boldsymbol{\sigma}(\mathbf{x})$  – which plays  
 567 a similar role as  $\mathbf{S}$  in Eq. (11) – is not uniform within a phase, owing to the  
 568 stress sensitivities  $n \neq 1$  and the heterogeneity of  $\boldsymbol{\sigma}$  in the phases. Conse-  
 569 quently, (14) cannot be replaced by (15) for nonlinear behavior. The basic  
 570 method to deal with such nonlinear behavior is to define a *Linear Compari-*  
 571 *son Polycrystal* (LCP) having the same microstructure as the real nonlinear

572 polycrystal, and to which the linear homogenization scheme applies (Ponte-  
573 Castañeda and Suquet, 1998). Of course, the effective behavior estimated  
574 this way remains nonlinear, since the definition of the LCP depends on the  
575 applied macroscopic stress. The difficult part of the problem consists of  
576 finding the best *linearization* procedure leading to the optimal selection of  
577 the LCP. Since decades, there has been quite a number of propositions in  
578 the literature dealing with this issue, leading to a *generalization* of the SC  
579 scheme for nonlinear behavior. The local constitutive relation given by Eqs  
580 (18-20) has to be linearized in a suitable way to obtain a form similar to  
581 (11), with  $\mathbf{S}$  and  $\dot{\boldsymbol{\varepsilon}}_0$  uniform per phase (and where  $\boldsymbol{\varepsilon}$  is replaced everywhere  
582 by  $\dot{\boldsymbol{\varepsilon}}$ ). Generally speaking, the linearization can be expressed in the form  
583 depicted in Fig. 7, (Liu and Ponte Castañeda, 2004).

$$\dot{\gamma}_{(k)}(\mathbf{x}) = \alpha_{(k)}^{(r)} \tau_{(k)}(\mathbf{x}) + \dot{\varepsilon}_{(k)}^{(r)}, \quad (21)$$

584 thus leading to the following expressions for  $\mathbf{S}^{(r)}$  and  $\dot{\boldsymbol{\varepsilon}}_0^{(r)}$

$$\mathbf{S}^{(r)} = \sum_k \alpha_{(k)}^{(r)} \boldsymbol{\mu}_{(k)}^{(r)} \otimes \boldsymbol{\mu}_{(k)}^{(r)}, \quad \dot{\boldsymbol{\varepsilon}}_0^{(r)} = \sum_k \dot{\varepsilon}_{(k)}^{(r)} \boldsymbol{\mu}_{(k)}^{(r)}, \quad (22)$$

585 where the shear compliance  $\alpha_{(k)}^{(r)}$  and stress-free slip-rate  $\dot{\varepsilon}_{(k)}^{(r)}$  can be easily  
586 expressed with respect to two reference shear stresses  $\check{\tau}_{(k)}^{(r)}$  and  $\hat{\tau}_{(k)}^{(r)}$ , see Fig.  
587 7. The optimal choice (from the point of view of the variational mechanical  
588 problem) of those reference stresses is not straightforward; this is the main  
589 reason why several extensions of the SC scheme have been proposed in the  
590 literature. Obviously, all of them reduce to the same SC model in the linear  
591 case  $n = 1$ .

592 Following Ponte Castañeda (1996), Masson et al. (2000) proposed the  
593 so-called “affine” (AFF) linearization scheme which is based on the simple

594 idea of a linear behavior (21) tangent to the nonlinear one (4) at the mean  
 595 shear stress, leading to

$$\tilde{\tau}_{(k)}^{(r)} = \hat{\tau}_{(k)}^{(r)} = \langle \tau_{(k)} \rangle^{(r)}, \quad \alpha_{(k)}^{(r)} = \left. \frac{\partial \dot{\gamma}}{\partial \tau} \right|_{\tau = \tilde{\tau}_{(k)}^{(r)}}. \quad (23)$$

596 The main limitations of this procedure are discussed in detail in Masson  
 597 et al. (2000) and Bornert and Ponte Castañeda (1998). One of them is the  
 598 violation of rigorous upper bounds for the effective behavior. More generally,  
 599 the affine extension is known to overestimate the overall viscosity, *i.e.* to  
 600 predict an effective behavior that is too stiff. This negative feature can be  
 601 alleviated by means of the energy formulation originally proposed by Ponte  
 602 Castañeda (1996) (see Bornert et al. (2001)).

603 Alternative, more sophisticated ways to generalize the SC scheme have  
 604 been proposed by Ponte Castañeda and co-workers during the last decades.  
 605 The basic idea of these methods is to guide the choice of the properties of the  
 606 LCP by a suitably designed variational principle. An “optimal” solution has  
 607 been obtained in the context of the so-called “variational” procedure (VAR)  
 608 (Ponte Castañeda, 1991), which was extended to polycrystals by De Botton  
 609 and Ponte Castañeda (1995), leading to the choice

$$\tilde{\tau}_{(k)}^{(r)} = 0, \quad \hat{\tau}_{(k)}^{(r)} = \left[ \langle \tau_{(k)}^2 \rangle^{(r)} \right]^{1/2}. \quad (24)$$

610 The main advantage of this procedure is to provide a rigorous bound, sharper  
 611 than the Voigt bound, for the effective potential. More recently, the “second-  
 612 order” (SO) method of Ponte Castañeda (2002), extended to polycrystals in  
 613 (Liu and Ponte Castañeda, 2004) has been proposed. It leads to reference  
 614 shear stresses reading

$$\tilde{\tau}_{(k)}^{(r)} = \langle \tau_{(k)} \rangle^{(r)}, \quad \hat{\tau}_{(k)}^{(r)} = \tilde{\tau}_{(k)}^{(r)} \pm \left[ \langle (\tau_{(k)} - \tilde{\tau}_{(k)}^{(r)})^2 \rangle^{(r)} \right]^{1/2}. \quad (25)$$

615 The main differences between AFF, VAR, and SO models may be sum-  
 616 marized as follows. The AFF estimate can be regarded as a relatively simple  
 617 model, allowing rapid computations which can even be rather accurate for  
 618 polycrystals with weak grain anisotropy and small stress sensitivity. How-  
 619 ever, its predictions can become unrealistic (*e.g.* bound violation) at a strong  
 620 anisotropy or nonlinearity. Contrary to AFF, for which linearization only  
 621 accounts for the phase average stress, VAR accounts for the second moments  
 622 of the stress, whereas the SO procedure accounts for both the phase aver-  
 623 age stress *and* intraphase standard deviation (first and second moments)  
 624 to build the LCP. They can therefore provide better estimates in cases of  
 625 highly heterogeneous stress distributions, such as for strongly nonlinear or  
 626 anisotropic polycrystals. Applications of the VAR procedure to polycrystals  
 627 with grains having cubic or hexagonal crystallographic structures can be  
 628 found in (Nebozhyn et al., 2001; Liu et al., 2003).

629 Finally, the “tangent” (TGT) extension of the SC scheme (Molinari  
 630 et al., 1987; Lebensohn and Tomé, 1993), often referred to as the “VPSC  
 631 model” in the literature, is based on the same tangent linearization (23) as  
 632 the AFF method. However, unlike the AFF extension, this procedure takes  
 633 advantage of the fact that, for power-law polycrystals with a single stress  
 634 exponent  $n$  for all slip systems, the tangent behavior (21) can be replaced  
 635 by a secant-like relation, with  $\dot{\epsilon}_{(k)}^{(r)} = 0$  and  $\alpha_{(k)}^{(r)}$  replaced by  $\alpha_{(k)}^{(r)}/n$ . The  
 636 same procedure is further applied at the macroscopic level, leading to an  
 637 inconsistent definition for the stress localization tensor  $\mathbf{B}^{(r)}$  that combines a  
 638 secant description for the local and global behaviors but a tangent analysis  
 639 for the inclusion/matrix interaction (Masson et al., 2000). When expressed  
 640 in the form of tangent expressions, it can be shown that  $\dot{\epsilon}_0$  differs from the  
 641 exact relation given in (15).

642 3.5.1. Application to natural ices: effective behavior

643 Application of homogenization techniques to natural ices aims at un-  
644 derstanding (and predicting) the anisotropic behavior of strongly textured  
645 specimens, as encountered at depth in natural ice sheets. As will be seen in  
646 section 6, the viscoplastic anisotropy of polycrystals significantly influences  
647 ice flow at large scales (Mangeny et al., 1996; Gillet-Chaulet et al., 2006;  
648 Pettit et al., 2007; Martín et al., 2009). Castelnau et al. (1998) reported  
649 mechanical tests performed on specimens from the GRIP ice core (Central  
650 Greenland). Along the ice core, the ice microstructure, and in particular  
651 the crystallographic fabric, is evolving; with increasing depth, randomly ori-  
652 ented  $c$ -axis at the surface of the ice sheet tend to concentrate towards the  
653 *in situ* vertical direction down to a depth of  $\sim 2600$  m. Beneath this depth,  
654 less pronounced textures are observed due to the initiation of migration re-  
655 crystallization (Thorsteinsson et al., 1997). In (Castelnau et al., 1998), the  
656 experimental stationary creep behavior of those ices have been obtained for  
657 two loading conditions (Fig. 8). The first one corresponds to an *in situ* ver-  
658 tical compression, showing an increasing flow stress (decreasing strain rate  
659 for a constant applied stress) with increasing depth, since the activation of  
660 non-basal slip systems is necessary for pronounced fabrics. The second load-  
661 ing condition corresponds to *in situ* horizontal shear, promoting basal slip  
662 and resulting in a softening of the ice with increasing fabric strength. It can  
663 be seen that for a given applied stress, strain rates can vary by more than  
664 two orders of magnitude depending on the orientation of the applied stress  
665 with respect to the specimen fabric, reflecting the very strong viscoplastic  
666 anisotropic of ice specimens.

667 The effective behavior predicted by the affine (AFF) SC model is com-

668 pared to the experimental data in Fig. 8. It can be observed that the agree-  
 669 ment is excellent, meaning that the relation between fabric and effective rhe-  
 670 ology is very well captured by the model. The model captures correctly the  
 671 increasing anisotropy from the surface down to  $\sim 2600$  m depth, and the de-  
 672 crease below. The difference by more than two orders of magnitude between  
 673 the vertical and shear strain-rates at  $\sim 2600$  m is also well reproduced, al-  
 674 though this was a challenging feature for the model. To get these results, the  
 675 reference shear stress  $\tau_0^{(k)}$  entering the local constitutive relation, and also  
 676 the stress sensitivity  $n^{(k)}$ , for each slip system ( $k$ ), had to be identified from  
 677 comparison with a database that included single-crystal experimental tests,  
 678 and polycrystal ones on many different crystallographic textures (Castelnau  
 679 et al., 2008b). The resulting single-crystal rheology, used as input in the SC  
 680 model to get the effective behavior described above, is shown in Fig. 9. For  
 681 basal slip, agreement with experimental data from the literature is almost  
 682 perfect. Non-basal systems are much stiffer than the basal systems, and  
 683 pyramidal slip is found to be much more difficult than prismatic slip. These  
 684 results are in good agreement with the available data on single crystals, and  
 685 in qualitative agreement with the known dislocation structure in ice. There-  
 686 fore, it can be anticipated that the affine SC model does a good job in making  
 687 the link between the grain and the polycrystal scales, and provides an ac-  
 688 curate estimate of the mechanical interaction between deforming grains. In  
 689 other words, one can anticipate that results shown in Fig. 8 are based on a  
 690 realistic description of the mechanical interaction between grains and phys-  
 691 ical deformation processes (dislocation glide) at the (sub)grain level. It can  
 692 also be seen on Fig. 9 that this identification procedure leads to different  
 693 stress sensitivities for the different slip system families. A value  $n^{(k)} = 2$  was  
 694 imposed for basal slip in accordance with experimental data, but values for

695 prismatic and pyramidal systems were considered as adjustable parameters.  
 696 It is also worth noting that the affine model perfectly reproduces an effective  
 697 stress sensitivity (i.e. at the polycrystal scale)  $\tilde{n} = 3$  in agreement with ex-  
 698 perimental data, although the two major slip systems, basal and prismatic  
 699 slip, have stress sensitivities smaller than 3 ( $n^{(bas)} = 2.0$ ,  $n^{(pr)} = 2.85$ ). A  
 700 larger value was considered only for pyramidal slip ( $n^{(py)} = 4.0$ ), but it is  
 701 worth mentioning that the contribution of pyramidal slip is only very mi-  
 702 nor (<2%). It can be concluded that, in ice, although basal slip is by far  
 703 the most active deformation mechanism, secondary slip systems are of great  
 704 importance for explaining the polycrystal behavior. Basal slip alone does  
 705 not allow for plastic deformation of ice polycrystals, since it only provides  
 706 two independent slip systems. Secondary slip systems, here prismatic and  
 707 pyramidal slip, *must* therefore be activated to add two more independent  
 708 slip systems. The strength of these stiffer mechanisms determines the vis-  
 709 coplastic anisotropy at the grain scale, and therefore they also control the  
 710 level of inter- and intra-granular heterogeneities of stress and strain(-rate),  
 711 and therefore the effective polycrystal rheology. Similar conclusions have  
 712 been drawn for olivine, a mineral with only three independent slip systems  
 713 (Castelnau et al., 2008a, 2009, 2010a,b). We therefore anticipate that the  
 714 strong effect of secondary deformation mechanisms observed here might be  
 715 a general feature for all polycrystalline materials with less than four inde-  
 716 pendent slip systems. The corollary of these results is that simple or *ad hoc*  
 717 polycrystal models, such as the Reuss (uniform stress) model, in which ice  
 718 polycrystals can deform with only basal slip, cannot be accurate. This has  
 719 been shown for example in (Castelnau et al., 1997): whatever the strength  
 720 used for prismatic and pyramidal systems, the Reuss model is not able to  
 721 reproduce the very large anisotropy of GRIP specimens shown in Fig. 8.



722 This comes from the fact that internal stresses, that have a large influence  
723 on the material behavior, are ignored.

724 Finally, it is also worth mentioning that the TGT SC approach, used  
725 in earlier studies, *e.g.* (Castelnau et al., 1997), does not provide as good a  
726 match to experimental data as the AFF SC extension. There can be two  
727 reasons for that: (i) first of all, it is now known that the inconsistency in  
728 the formulation of the TGT SC version leads to an underestimation of the  
729 internal stress level, predicting a too soft polycrystal behavior (Gilormini,  
730 1995; Masson et al., 2000); (ii) second, by construction, the TGT model is  
731 limited to grain behavior for which all slip systems exhibit the same stress  
732 sensitivity  $n^{(k)}$ . When applied to ice, one must thus consider  $n^{(k)} = 3.0$  for  
733 all systems, including basal slip, in order to get an effective  $\tilde{n} = 3$ . The fact  
734 that the AFF extension does not have this limitation might also explain a  
735 better consistency with experimental data.

### 736 *3.5.2. Application to natural ices: texture development*

737 Using the Reuss approximation, Van der Veen and Whillans (1994) and  
738 Castelnau and Duval (1994) described the fabric evolution under compres-  
739 sion, tension, simple and pure shear. Van der Veen and Whillans (1994)  
740 needed to impose a kind of "recrystallization" criterion (see Section 5.1) to  
741 be able to correctly represent the single-maximum fabric (with c-axis ori-  
742 ented along one direction) in ice deforming in pure shear. Nevertheless, the  
743 Reuss approximation faces inconsistency to describe the fabric evolution at  
744 the polycrystal scale, as it requires additional kinematical constraints to  
745 link the grain rotation-rate with the polycrystal rotation-rate. In most of  
746 the "Reuss" type models, these two rates are supposed to be equal, although  
747 the velocity field is not continuous.

748 Models that modify this homogeneous stress assumption were proposed  
749 by Azuma (1994) and Thorsteinsson (2002). They introduce some redistri-  
750 bution of stress through neighborhood interaction to define the crystal strain  
751 at a given bulk equivalent strain. In particular, Thorsteinsson (2002) defines  
752 a crystal arrangement on a three-dimensional cubic grid, where each crystal  
753 has six nearest neighbors. The nearest neighbor interaction (NNI) is taken  
754 into account by defining a local softness parameter for each crystal which  
755 modifies the stress acting on the central crystal compared to the macro-  
756 scopic stress. This softness parameter further influences the rotation rate  
757 of the crystal lattice compared to the bulk. For uniaxial compression tests,  
758 the fabrics obtained with the NNI formulation are less concentrated than  
759 the ones where no NNI is considered. The reason for this is that the NNI  
760 formulation allows all crystals to deform to some extent, while only "soft"  
761 crystals would deform in the no-NNI formulation. The fabric obtained after  
762 50% shortening strain compares qualitatively well with the one measured  
763 along the GRIP ice core at a depth where the strain is similar (1293 m)  
764 (Thorsteinsson et al., 1997).

765 The VPSC model in its "tangent" version was applied to simulate the  
766 fabric development along ice cores (Castelnau et al., 1996b,a, 1998). In  
767 (Castelnau et al., 1996a), a comparison was made with bound estimates  
768 (Reuss and Voigt). Fabrics simulated in uniaxial compression and extension  
769 were found to be qualitatively similar for all models. However, large dif-  
770 ferences in the rate of fabric development were found. This was explained  
771 by the different interaction stiffness between grain and matrix for the three  
772 approaches. The fabrics obtained with the VPSC model for uniaxial defor-  
773 mation were in close agreement with the one measured along the ice core  
774 (see Fig. 10). In particular, this model well reproduced the fabric evolution

775 along the GRIP ice core within the upper 650 m where dynamic recrystal-  
776 lization is not supposed to strongly impact this evolution (Castelnau et al.,  
777 1996b). Lower down, the modeled fabric concentration is too high. Al-  
778 though Castelnau et al. (1996b) attributed this discrepancy to the effects  
779 of rotation recrystallization along the core, it was later shown that the tan-  
780 gent approximation overestimates the lattice rotation. In simple shear, the  
781 single-maximum fabric found along the ice cores or experimentally could  
782 not be reproduced with the VPSC scheme. To get close to this fabric, an  
783 extensive (and probably unrealistic) activity of non-basal slip systems was  
784 required. More recently, the "second order" (SO) mean field method of  
785 Ponte Castañeda (2002) was used to simulate the fabric development along  
786 the Talos Dome ice core (Montagnat et al., 2012). Although no recrystalliza-  
787 tion mechanisms were implemented in this version, the fabric development  
788 was astonishingly well reproduced, under the crude assumption of uniaxial  
789 compression with a constant strain rate (see Fig. 11). In particular, a good  
790 match was obtained when the initial fabric is non isotropic and similar to  
791 the one measured in the top firn, at 18 m depth. The cumulated compres-  
792 sive strain along the core was derived from the thinning function provided  
793 by the TALDICE-1 chronology (Buiron et al., 2011). The good prediction  
794 performed by the VP-SO scheme is probably due to the fact that this SO ap-  
795 proach provides a better estimate of the effective behavior than the classical  
796 tangent "VPSC" model does in the case of strongly anisotropic materials  
797 such as ice (see Section 3.5). Nevertheless, the modeled fabric evolution  
798 could not capture the strengthening rate associated with the Glacial to In-  
799 terglacial climatic transition. At these transition, a change in ice viscosity  
800 is expected. It induces an higher sensitivity to the impact of shear stress  
801 increasing with depth, that the modeling approach did not considered.

802 It is also recalled that the heterogeneity of shear on slip systems at the  
803 grain level gives rise to heterogeneities of lattice rotation, and therefore  
804 generates intragranular misorientations that somehow spread crystal orien-  
805 tations. It is however worth mentioning that *all* models presented above  
806 do not consider this strain heterogeneity for estimating fabric evolutions at  
807 finite strain. Even in VAR and SO procedures, intraphase strain hetero-  
808 geneities are considered for defining the LCP, but so far not for estimating  
809 microstructure evolutions. As a consequence, mean-field approaches gener-  
810 ally predict too sharp textures. The same applies to the prediction of strain  
811 hardening, associated with dislocation processes such as storage and an-  
812 nealing. A quantitative study, based on comparisons with reference results  
813 obtained by a FFT full-field approach, can be found in (Castelnau et al.,  
814 2006).

815 Most of the efforts to simulate the fabric development in ice, and espe-  
816 cially along ice cores, had to face the fact that recrystallization mechanisms  
817 could impact this fabric development. This was, most of the time, the anal-  
818 ysis made for the observed discrepancies between simulated and measured  
819 fabrics (Van der Veen and Whillans, 1994; Wenk et al., 1997; Castelnau  
820 et al., 1996b; Thorsteinsson, 2002). Some efforts to implement recrystal-  
821 lization mechanisms in mean-field approaches will be described in Section  
822 5.1.

### 823 *3.6. Modeling the elasto-viscoplastic behavior*

824 Transient creep is typically encountered when ice flow changes direction,  
825 such as in glaciers flowing above irregular bedrock or submitted to tide forc-  
826 ing close to the sea-shore or in icy satellites. During laboratory experiments,  
827 transient creep is characterized by a strain-rate drop of more than two or-

828 ders of magnitude before reaching the secondary creep close to 1% strain,  
829 following Andrade’s law (Duval, 1978). This decrease is associated with the  
830 development of large internal stress fields due to intergranular interactions  
831 and a strong kinematic hardening (Duval et al., 1983; Ashby and Duval,  
832 1985; Castelnau et al., 2008b). To reproduce this transient behavior, one  
833 has to consider the coupling between elasticity and viscoplasticity that gives  
834 rise to the so-called ”long-term memory effect”, as explained below.

835     The application of homogenization schemes to the *elasto-viscoplasticity*  
836 of polycrystals is more complicated than for viscoplasticity, see for instance  
837 (Laws and McLaughlin, 1978). In short, it can be shown that, even in the  
838 simple case of a polycrystal comprising grains whose behavior exhibits a sin-  
839 gle relaxation time (so-called “short-term memory”), the effective behavior  
840 exhibits a continuous spectrum of relaxation time (“long-term memory ef-  
841 fect”) (Sanchez-Hubert and Sanchez-Palencia, 1978; Suquet, 1987). In other  
842 words, the overall behavior of a polycrystal is not of the Maxwell type (par-  
843 allel association of a spring and a dashpot with constant viscosity), even  
844 though the individual grains do exhibit local Maxwell type behavior. The  
845 basic difference between elasto-viscoplasticity and viscoplasticity is that, for  
846 elasto-viscoplasticity, the local strain rate depends on both the stress (vis-  
847 cous part) and the stress-rate (elastic part), whereas it only depends on the  
848 stress for viscoplasticity. Therefore, the local strain rate not only depends  
849 on the actual local stress, but also on the whole stress history from the  
850 initial specimen loading at  $t = 0$  up to the current time. To obtain the  
851 exact effective mechanical response at time  $t$ , it is thus required to keep  
852 track of all information (or internal variables) corresponding to the strains  
853 at all previous times, and therefore the problem is not simple. Within mean-  
854 field approaches, some approximations (with hopefully limited effects on the

855 accuracy of the solution) are thus necessary.

856 Basically, two approaches have been proposed to deal with this issue. A  
857 promising method based on an incremental variational procedure has been  
858 proposed by Lahellec and Suquet (2006, 2007). These authors have shown  
859 that the homogenization of a *linear visco-elastic* material (*i.e.* with  $n = 1$ )  
860 can be expressed in terms of a homogenization problem for a linear ther-  
861 moelastic composite with non piecewise uniform eigenstrains. One advantage  
862 of this formulation is that it can make use of the intraphase heterogeneities  
863 of stress and strain (-rate), and it can therefore probably provide accurate  
864 results even at high stress sensitivity and/or local anisotropy. An alternative  
865 approach, which provides a good compromise between accuracy of the solu-  
866 tion and simplicity of the formalism, is the so-called “affine” Self-Consistent  
867 method of Masson and Zaoui (1999). It is based on the correspondence  
868 principle (Mandel, 1966), which states that the elasto-viscoplastic problem  
869 can be reduced to a simpler homogenization problem (in fact similar to a  
870 standard thermo-elastic problem) if solved in Laplace space. One difficulty  
871 of this approach is the calculation of the inverse Laplace transforms, that  
872 has to be carried out numerically. An approximate inversion procedure,  
873 adapted for creep, has been proposed by Brenner et al. (2002b). It has pro-  
874 vided promising results for the creep behavior of Zirconium alloys (Letouzé  
875 et al., 2002; Brenner et al., 2002a), since it retains the long-term memory  
876 effect associated with the elasto-viscoplastic coupling. Recent developments  
877 (Ricaud and Masson, 2009) have shown that an internal variable formulation  
878 arises naturally from this affine method, providing results in perfect match  
879 with reference FFT solutions in the case of linear viscoelasticity (Vu et al.,  
880 2012).

881 To the best of our knowledge, this affine method is the only mean-field

882 approach that has been applied to simulate the transient creep of ice (Castel-  
883 nau et al., 2008b). Applications make use of the crystal plasticity model  
884 for single crystals detailed in Section 2.3. It was shown that the strong  
885 hardening *amplitude* during the transient creep (*i.e.* the decrease of the  
886 overall strain rate by several orders of magnitude) is explained by the stress  
887 redistribution within the specimen: when the overall stress is applied in-  
888 stantaneously, the instantaneous polycrystal response is purely elastic, and  
889 since the elastic anisotropy is small, stress distribution within and between  
890 grains is almost uniform. But plastic deformation comes into play rapidly to  
891 cause a strong redistribution of stress (with large interphase and intraphase  
892 heterogeneities) due to the strong viscoplastic anisotropy at the grain scale.  
893 This significantly reduces the overall strain rate. On the other hand, the  
894 experimental hardening rate (*i.e.* the time necessary to reach the secondary  
895 creep regime) is much too slow to be explained by the same process, and is  
896 attributed to the hardening of hard-glide slip systems (prismatic slip) in the  
897 transient regime, associated with dislocation processes (Fig. 12).

#### 898 **4. Full field approaches for the polycrystal**

899 Mean-field approaches have been extensively used to predict the mechan-  
900 ical behavior of ice polycrystals, and the fabric development as measured  
901 along ice cores. Due to its high viscoplastic anisotropy, deformation in ice is  
902 expected to be strongly heterogeneous, with a strong impact of grain inter-  
903 actions and kinematic hardening (Duval et al., 1983; Hamman et al., 2007;  
904 Montagnat et al., 2011; Grennerat et al., 2012). The mean-field approaches  
905 described above are based on the statistical characterization of the intragran-  
906 ular mechanical fields (in terms of average grain stresses and strain rates,

907 and, in the most advanced formulations, also through the determination of  
908 the intracrystalline average field fluctuations), but the actual micromechan-  
909 ical fields remain inaccessible to these homogenization approaches. Model-  
910 ing the full intracrystalline heterogeneity that develops in ice polycrystals  
911 requires the use of full-field approaches. This part will concentrate on full-  
912 field approaches that are using the Fast Fourier Transform method to solve  
913 the constitutive equations in a discretized polycrystal. It aims at studying  
914 the correlation between the heterogeneous deformation patterns that appear  
915 inside the constituent single-crystal grains of an ice aggregate and their cor-  
916 responding crystallographic orientations, along with the influence of other  
917 factors, such as orientation and size of neighboring grains. Both viscoplastic  
918 and elasto-viscoplastic behavior were investigated, and are presented in the  
919 two following sections.

#### 920 *4.1. Viscoplastic approach - FFT*

##### 921 *4.1.1. Viscoplastic FFT-based formulation*

922 The intracrystalline states that are developed during creep of polycrys-  
923 talline ice can be obtained using an extension of an iterative method based on  
924 FFT, originally proposed by Moulinec and Suquet (1998) and Michel et al.  
925 (2001) for linear and non-linear composites (Lebensohn et al., 2009; Mon-  
926 tagnat et al., 2011). This formulation was later adapted to polycrystals and  
927 applied to the prediction of texture development of fcc materials (Leben-  
928 sohn, 2001), and in turn used for the computation of field statistics and  
929 effective properties of power-law 2D polycrystals (Lebensohn et al., 2004a,  
930 2005) and 3D cubic, hexagonal (Lebensohn et al., 2004b) and orthorhombic  
931 (Castelnau et al., 2008a) materials. The FFT-based formulation was also ap-  
932 plied to compute the development of local misorientations in polycrystalline



933 copper, with direct input from orientation images (Lebensohn et al., 2008).  
 934 As will be detailed in Section 4.2 it was further extended to transient behav-  
 935 ior with an elasto-viscoplastic formulation (Idiart et al., 2006; Suquet et al.,  
 936 2011; Lebensohn et al., 2012). The FFT-based full-field formulation for vis-  
 937 coplastic polycrystals is conceived for a periodic unit cell, provides an exact  
 938 solution of the governing equations, and has better numerical performance  
 939 than a FE calculation for the same purpose and resolution. The viscoplas-  
 940 tic FFT-based formulation consists in finding a strain-rate field, associated  
 941 with a kinematically-admissible velocity field, which minimizes the average  
 942 of local work-rate, under the compatibility and equilibrium constraints. The  
 943 method is based on the fact that the local mechanical response of a periodic  
 944 heterogeneous medium can be calculated as a convolution integral between  
 945 the Green function of a linear reference homogeneous medium and the ac-  
 946 tual heterogeneity field. Such type of integrals reduce to a simple product  
 947 in Fourier space, therefore the FFT algorithm can be used to transform the  
 948 heterogeneity field into Fourier space and, in turn, to get the mechanical  
 949 fields by antitransforming that product back to real space. However, since  
 950 the actual heterogeneity field depends precisely on the a priori unknown me-  
 951 chanical fields, an iterative scheme should be implemented to obtain, upon  
 952 convergence, a compatible strain-rate field and a stress field in equilibrium.

953 The periodic unit cell representing the polycrystal is discretized by means  
 954 of a regular grid  $\{x^d\}$ , which in turn determines a corresponding grid of the  
 955 same dimensions in Fourier space  $\{\xi^d\}$ . Velocities and tractions along the  
 956 boundary of the unit cell are left undetermined under the sole condition of  
 957 periodicity. An average velocity gradient  $V_{i,j}$  is imposed to the unit cell,  
 958 which gives an average strain rate  $\dot{\bar{\epsilon}}_{ij} = \frac{1}{2}(V_{i,j} + V_{j,i})$ . The local strain-rate  
 959 field is a function of the local velocity field, i.e.  $\dot{\epsilon}_{ij}(\mathbf{v}_k(\mathbf{x}))$ , and can be

960 split into its average and a fluctuation term:  $\dot{\epsilon}_{ij}(\mathbf{v}_k(\mathbf{x})) = \dot{\bar{\epsilon}}_{ij} + \tilde{\epsilon}_{ij}(\tilde{\mathbf{v}}_k(\mathbf{x}))$ ,  
 961 where  $\mathbf{v}_i(\mathbf{x}) = \dot{\bar{\epsilon}}_{ij}x_j + \tilde{\mathbf{v}}_i(\mathbf{x})$ . By imposing periodic boundary conditions, the  
 962 velocity fluctuation field  $\tilde{\mathbf{v}}_k(\mathbf{x})$  is assumed to be periodic across the boundary  
 963 of the unit cell, while the traction field is antiperiodic, to meet equilibrium on  
 964 the boundary between contiguous unit cells. The local constitutive equation  
 965 that relates the deviatoric stress  $\boldsymbol{\sigma}'(\mathbf{x})$  and the strain rate  $\dot{\boldsymbol{\epsilon}}(\mathbf{x})$  at point  $\mathbf{x}$   
 966 is obtained from Eqs (18) to (20).

967 If  $p(\mathbf{x})$  is the unknown pressure field introduced by the incompressibility  
 968 constraint, the Cauchy stress field can be written as:

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{L}^0 : \dot{\boldsymbol{\epsilon}}(\mathbf{x}) + \boldsymbol{\varphi}(\mathbf{x}) - p(\mathbf{x})\mathbf{I} \quad (26)$$

969 where the polarization field  $\boldsymbol{\varphi}(\mathbf{x})$  is given by:

$$\boldsymbol{\varphi}(\mathbf{x}) = \boldsymbol{\sigma}'(\mathbf{x}) - \mathbf{L}^0 : \dot{\boldsymbol{\epsilon}}(\mathbf{x}) \quad (27)$$

970 where  $\mathbf{L}^0$  is the stiffness (viscosity) of a linear reference medium. Eqs. (26)  
 971 and (27) amount to transform the actual heterogeneity problem into an  
 972 equivalent one, corresponding to a homogenous medium with eigen-strain-  
 973 rates. Note, however, that the above defined polarization field depends  
 974 on the unknown  $\dot{\boldsymbol{\epsilon}}(\mathbf{x})$ . Combining Eq. (27) with the equilibrium and the  
 975 incompressibility conditions gives:

$$L_{ijkl}^0 v_{k,lj}(\mathbf{x}) + \varphi_{ij,j}(\mathbf{x}) - p_{,i}(\mathbf{x}) = 0, v_{k,k}(\mathbf{x}) = 0 \quad (28)$$

976 Assuming for a moment that the polarization field  $\boldsymbol{\varphi}(\mathbf{x})$  is known, the sys-  
 977 tem of partial differential equations (28), with periodic boundary conditions  
 978 across the unit cell boundary, can be solved by means of the Green function  
 979 method.

980 If  $G_{km}$  and  $H_m$  are the periodic Green functions associated with the velocity

981 and hydrostatic pressure fields, the solutions of system (28) are convolution  
 982 integrals between those Green functions and the actual polarization term.  
 983 The velocity gradient, after some manipulation is given by:

$$\tilde{v}_{i,j}(\mathbf{x}) = \int_{R^3} G_{ik,jl}(\mathbf{x} - \mathbf{x}') \varphi_{kl}(\mathbf{x}') d\mathbf{x}'. \quad (29)$$

984 Convolution integrals in direct space are simply products in Fourier space.  
 985 Hence:

$$\hat{\tilde{\epsilon}}_{ij}(\xi) = \hat{\Gamma}_{ijkl}^{sym}(\xi) \hat{\varphi}_{kl}(\xi), \quad (30)$$

986 where  $\hat{\Gamma}_{ijkl}^{sym} = \text{sym}(\hat{G}_{ik,jl})$ . The tensors  $\hat{G}_{ik}(\xi)$  and  $\hat{\Gamma}_{ijkl}^{sym}(\xi)$  are only func-  
 987 tions of  $\mathbf{L}^0$  and can be readily obtained for every point belonging to  $\{\xi^d\}$   
 988 (for details, see Lebensohn et al. (2008)). Now, taking into account the  
 989 definition 27 of  $\varphi(\mathbf{x})$ , Eq. 29 is an integral equation where the velocity  
 990 gradient appears in both sides, and, thus, it can be solved iteratively. As-  
 991 signing initial guess values to the strain-rate field in the regular grid (e.g.  
 992  $\tilde{\epsilon}(\mathbf{x}^d) = 0 \Rightarrow \dot{\epsilon}^{(0)}(\mathbf{x}^d) = \dot{\tilde{\epsilon}}$ ), and computing the corresponding stress field  
 993  $\sigma^{(0)}(\mathbf{x}^d)$  from the local constitutive relation (18) allows to obtain an initial  
 994 guess for the polarization field in direct space  $\varphi^{(0)}(\mathbf{x}^d)$  (27), which in turn  
 995 can be Fourier-transformed to obtain  $\hat{\varphi}^{(0)}(\xi^d)$ .

996 The rate of convergence of this fixed point technique is rather poor for  
 997 nonlinear constitutive relations such as power-law relations between the  
 998 stress and the strain-rate. Accelerated schemes based on augmented La-  
 999 grangians have been proposed to improve this rate of convergence originally  
 1000 by Michel et al. (2000, 2001) for composites, and later adapted by Lebensohn  
 1001 (2001) for polycrystals to which the interested reader is referred for details.  
 1002 Upon convergence, the stress at each material point can be used to calculate  
 1003 the shear rates associated with each slip system (Eq. 4), from which fields  
 1004 of relative activity of the basal, prismatic and pyramidal slip modes can be

1005 obtained, as well. While it is certainly possible to use the FFT-based for-  
1006 mulation for the prediction of microstructure evolution, in this section we  
1007 have restricted our analysis to the local fields that are obtained for a fixed  
1008 configuration. In this sense, the high strain-rate regions predicted by the  
1009 model (see below) should be regarded as precursors of localization bands.  
1010 Evidently, microstructural changes that are not considered under this ap-  
1011 proximation, like the eventual grain's and subgrain's morphologic evolution  
1012 and rotation, as well as the possible occurrence of local strain hardening,  
1013 may modify some of the trends observed in the initial micromechanical fields.  
1014 In order to account for these microstructural changes, the FFT-based for-  
1015 mulation has been coupled with the front-tracking numerical platform Elle  
1016 (Bons et al., 2001). Results of this coupled model are reported in Section  
1017 5.2.2.

#### 1018 *4.1.2. Application to columnar ice deforming in the secondary creep regime.*

1019 Lebensohn et al. (2009) and Montagnat et al. (2011) applied this FFT  
1020 method to simulate strain rate and stress fields, and local lattice misorienta-  
1021 tions obtained at secondary creep in columnar ice polycrystals. Lebensohn  
1022 et al. (2009) compared the simulated fields to a series of compression creep  
1023 experiments performed by Mansuy et al. (2000, 2002) on laboratory-grown  
1024 columnar ice samples characterized by multicrystals of controlled shape and  
1025 orientations. The specimen used for this comparison (see Fig. 13) was a  
1026 plate of 210×140 mm with a relatively thick (8 mm) section, consisting of  
1027 a multicrystalline cluster, located in the center of the plate, with c-axes  
1028 lying on the plane of the plate, and embedded in a matrix of fine-grained  
1029 ice. This specimen was deformed under a compressive stress of 0.75 MPa  
1030 exerted vertically in the plane at -10°C under plane strain conditions. Fig.

1031 13 shows, after 0.07 strain, three types of localization bands: basal shear  
1032 bands, kink bands and sub-boundaries, that change orientation to follow  
1033 crystallographic directions when they cross from one grain to another.  
1034 In this configuration, kink band boundaries are seen mainly inside grains  
1035 oriented close to  $45^\circ$  from the imposed compression direction. Kink bands,  
1036 described as a sharp or discontinuous change in orientation of the active  
1037 slip surface, had been reported in experimental studies conducted on 2-D  
1038 ice polycrystals (Wilson et al., 1986; Wilson and Zhang, 1994; Montagnat  
1039 et al., 2011). Sub-boundaries parallel to the c-axis were also observed.

1040

1041 The FFT-based calculation as described in the previous section was run  
1042 to obtain the overall and local mechanical response of the above-described  
1043 unit cell representing a columnar ice polycrystal, to the following imposed  
1044 strain-rate tensor (see also Fig. 14):

$$\dot{\tilde{\epsilon}}_{ij} = \begin{bmatrix} 1 \times 10^{-8} & 0 & 0 \\ 0 & -1 \times 10^{-8} & 0 \\ 0 & 0 & 0 \end{bmatrix} s^{-1} \quad (31)$$

1045 The crystallographic texture of the 2-D ice polycrystal consisting of colum-  
1046 nar grains with c-axes perpendicular to the axial (vertical) direction  $x_3$  was  
1047 described in terms of a collection of Euler-angle triplets of the form  $(\varphi_1, 90^\circ,$   
1048  $\varphi_2)$  (Bunge convention). The application of the FFT method required the  
1049 generation of a periodic unit cell or representative volume Element (RVE),  
1050 by repetition along  $x_1$  and  $x_2$  of a square domain. This square domain was  
1051 constructed in such a way that it contained the cross-sections of 200 colum-  
1052 nar grains, generated by Voronoi tessellation (see Fig. 14). This square do-  
1053 main is the cross-section of the unit cell, consisting of columnar grains with

1054 axes along  $x_3$  and sections in the  $x_1$ - $x_2$  plane. This unit cell was discretized  
1055 using a  $1024 \times 1024 \times 1$  grid of regularly-spaced Fourier points, resulting in  
1056 an average of around 5250 Fourier points per grain. Note that the periodic  
1057 repetition of this unit cell along  $x_3$  determines infinitely long grains along  
1058 this direction. Three specific orientations with c-axis respectively at  $0^\circ$ ,  $45^\circ$ ,  
1059 and  $90^\circ$  from the compression direction were forced to be among the set of  
1060 200 (otherwise random) orientations assigned to the grains. For a plane-  
1061 strain state, such that  $x_1$  is the tensile direction and  $x_2$  is the compression  
1062 direction, the grain with  $\varphi_1 = 45^\circ$  (45 deg grain in what follows) is theo-  
1063 retically favorably oriented to deform by soft basal slip, while in the 0 deg  
1064 and 90 deg grains, the hard pyramidal systems are the only ones favorably  
1065 oriented to accommodate deformation. It is worth noting that due to the  
1066 above plane-strain condition and the in-plane orientation of the c-axes, the  
1067 prismatic slip systems are not well-oriented, for any  $\varphi_1$  angle.

1068 The computed effective response of this kind of isotropic columnar ice  
1069 polycrystal deformed in-plane is twice softer compared to an isotropic 3-D  
1070 polycrystalline ice (Lebensohn et al., 2007). The computed overall relative  
1071 activities of the different slip modes (i.e. 90.7%, 7.6% and 1.7% for basal,  
1072 pyramidal and prismatic slip, respectively) show a preeminence of basal slip,  
1073 a minor contribution of pyramidal slip and a very low activity of prismatic  
1074 slip. Fig. 15 shows the computed equivalent strain-rate field for the entire  
1075 unit cell, normalized with respect to the average equivalent strain rate ( $\dot{\epsilon}_{eq} =$   
1076  $1.15 \times 10^{-8} \text{s}^{-1}$ ). The main feature observed in this plot is a network of high  
1077 strain-rate bands, precursors of localization bands (in what follows we will  
1078 sometimes refer to them simply as "localization bands"). These bands are  
1079 transmitted from grain to grain and are, in general, inclined with respect  
1080 to the shortening and extension directions. They follow tortuous paths,

1081 sometimes with large deviations from  $\pm 45^\circ$  (i.e. the macroscopic directions  
1082 of maximum shear stress). They follow crystallographic directions (basal  
1083 poles or basal planes) inside each grain. The predicted bands parallel or  
1084 perpendicular to the c-axis were reasonably assumed to be kink or shear  
1085 bands, respectively (see Lebensohn et al. (2009) for details). Some segments  
1086 of these bands also follow favorably-oriented grain boundaries and frequently  
1087 go through triple or multiple points between grains, in good agreement with  
1088 some of the observations of (Mansuy et al., 2002) (Fig. 13). Fig. 16 shows in  
1089 more details the predicted fields of equivalent strain rate (normalized to  $\dot{\epsilon}_{eq}$ ),  
1090 equivalent stress (in units of  $\tau^{bas}$ ) and relative basal activity, in the vicinities  
1091 of the 45 deg grain. Two very intense (i.e. local strain rates higher than 10  
1092 times the macroscopic strain rate) and parallel kink bands are seen inside  
1093 the 45 deg grain, connected by several less intense shear bands (orthogonal  
1094 to the pair of kink bands, lying on to the basal plane), in good agreement  
1095 with Mansuy's experiments (see Fig. 13). The basal activity in the 45 deg  
1096 grain is very high, although some regions of high non-basal activity can be  
1097 observed between shear bands and immediately outside the kink bands. The  
1098 latter is compatible with a low or even vanishing resolved shear stress on  
1099 basal planes in those locations, which may be responsible for the formation  
1100 of basal dislocation walls that are at the origin of a kink band (Mansuy  
1101 et al., 2002). This correlation between kink band precursors and nearby  
1102 localized high non-basal activity is systematic in these results. From the  
1103 same detailed analysis performed around the 0 and 90 deg grains, a good  
1104 match was found with experimental observations.

1105 In (Montagnat et al., 2011), the viscoplastic FFT-based approach was  
1106 applied to the exact experimental microstructure of a compressive test per-  
1107 formed on a 2D columnar sample. Samples (dimensions  $\approx 10 \times 10 \times 1.5 \text{ cm}^3$ )

1108 were grown in the laboratory under a uniaxial temperature gradient to reach  
1109 a columnar microstructure with all  $c$ -axes lying parallel to the sample sur-  
1110 face. In this work, the observed kink bands could be associated with mis-  
1111 orientations between adjacent regions of a grain interior of more than  $5^\circ$ ,  
1112 and their exact nature in term of dislocation arrangements were confirmed  
1113 by EBSD measurements. Although the boundary conditions of the model-  
1114 ing were slightly different from the experimental one, the model was able  
1115 to predict the exact location of the localization bands. The bands were as-  
1116 sociated with stress concentration that could reach five times the applied  
1117 macroscopic stress, and to high levels of local non basal activity (see Fig.  
1118 17). Nevertheless, the amplitude of the modeled lattice misorientations were  
1119 always overestimated, and this was associated with the fact that very local  
1120 grain boundary migration and new grain nucleation (dynamic recrystalliza-  
1121 tion mechanisms) observed experimentally were not considered in the model  
1122 (see Section 5.2.2).

#### 1123 *4.2. Elasto-viscoplastic FFT approach*

1124 The full-field FFT approach described above has been extended very re-  
1125 cently to the case of elasto-viscoplasticity, see (Idiart et al., 2006; Suquet  
1126 et al., 2011; Lebensohn et al., 2012). As for purely viscoplastic behaviors,  
1127 its application to highly anisotropic material like ice allows investigating the  
1128 accuracy of elasto-viscoplastic mean-field models (see Section 3.6) since, as  
1129 already mentioned, the FFT technique provides the “exact” (in a numerical  
1130 sense) response of the specimen with the actual microstructure and local con-  
1131 stitutive relations. Application to ice allows studying transient creep effects  
1132 with more detail. Comparison with experimental strain field measured with  
1133 an intragranular spatial resolution has been provided in (Grennerat et al.,



1134 2012) making use of the relative ease of producing samples with controlled  
 1135 2-D microstructure, compared to other polycrystalline materials.

1136 *4.2.1. The mechanical problem*

1137 The method described in Suquet et al. (2011) considers the same mi-  
 1138 crostructure description as in Section 4.1: a polycrystalline volume  $V$  com-  
 1139 posed of several grains of different orientations, each grain obeying con-  
 1140 stitutive relations defined in Section 2.3. The volume  $V$  is subjected to  
 1141 a macroscopic loading path, which can be a prescribed history of average  
 1142 strain, or a history of average stress or a combination of both. For simplicity,  
 1143 the method is presented here assuming a prescribed history of macroscopic  
 1144 strain  $\bar{\boldsymbol{\varepsilon}}(t), t \in [0, T]$ . Other types of loadings can be handled by different  
 1145 methods described in (Michel et al., 1999) for instance.

1146 The local problem to be solved to determine the local stress and strain  
 1147 fields in the volume element  $V$  consists of the equilibrium equations, com-  
 1148 patibility conditions, constitutive relations and periodicity boundary condi-  
 1149 tions:

$$\left\{ \begin{array}{ll} (\dot{\boldsymbol{\sigma}}, \dot{\boldsymbol{\tau}}_0, \dot{\mathbf{X}}) = \mathbf{F}(\dot{\boldsymbol{\varepsilon}}, \boldsymbol{\sigma}, \boldsymbol{\tau}_0, \mathbf{X}, \mathbf{x}, t), & \text{for } (\mathbf{x}, t) \in V \times [0, T], \\ \boldsymbol{\varepsilon}(\mathbf{x}, t) = \frac{1}{2}(\nabla \mathbf{u}(\mathbf{x}, t) + {}^T \nabla \mathbf{u}(\mathbf{x}, t)), & \\ \operatorname{div} \boldsymbol{\sigma}(\mathbf{x}, t) = 0 & \text{for } (\mathbf{x}, t) \in V \times [0, T], \\ \mathbf{u}(\mathbf{x}, t) - \bar{\boldsymbol{\varepsilon}}(t) \cdot \mathbf{x} \text{ periodic on } \partial V, & \text{for } t \in [0, T] \end{array} \right. \quad (32)$$

1150 The data of interest are the effective response  $\bar{\boldsymbol{\sigma}}(t), t \in [0, T]$  of the poly-  
 1151 crystal, the history of the average strain  $\bar{\boldsymbol{\varepsilon}}(t), t \in [0, T]$ , but also the local  
 1152 fields  $\boldsymbol{\sigma}(\mathbf{x}, t), \boldsymbol{\varepsilon}(\mathbf{x}, t)$  and other significant fields (internal variables, thermo-  
 1153 dynamic forces etc...).

1154 The extension of the simplest version of the FFT-based method, also

1155 called the *basic scheme*, to constitutive relations including crystalline elasto-  
1156 viscoplasticity relies on two ingredients:

1157 1. A time-integration scheme for the constitutive differential equations.  
1158 The time interval of interest  $[0, T]$  is split into time steps  $[t_n, t_{n+1}]$ . All  
1159 quantities are assumed to be known at time  $t_n$ , and the quantities at  
1160 time  $t_{n+1}$  are unknown. This time integration is performed at every  
1161 point  $\mathbf{x}^d$  of the discretized polycrystal and the evolution problem is  
1162 reduced to a problem for the stress and strain fields  $\boldsymbol{\sigma}$  and  $\boldsymbol{\varepsilon}$  at time  
1163  $t_{n+1}$  in the form

$$\boldsymbol{\sigma}_{n+1}(\mathbf{x}^d) = \mathcal{F}_{n+1}(\mathbf{x}^d, \boldsymbol{\varepsilon}_{n+1}(\mathbf{x}^d)) \quad (33)$$

1164 2. A FFT global scheme to solve the local problem for a nonlinear com-  
1165 posite obeying Eq. (33).

1166 The algorithm developed applies to a wide class of constitutive relations,  
1167 see (Suquet et al., 2011). As before, it is limited to specimens submitted  
1168 to periodic boundary conditions. Results presented below are performed  
1169 with the FFT-based program Craft (freely available at [http://craft.lma.cnrs-](http://craft.lma.cnrs-mrs.fr)  
1170 [mrs.fr](http://craft.lma.cnrs-mrs.fr)). For application to elastoviscoplasticity in ice, the local constitutive  
1171 relation is the one provided above, see Eqs (2, 3, 6, 7, 8). It can also be  
1172 formulated via the following differential equation:

$$\dot{\mathbf{Y}} = \mathbf{F}(\dot{\boldsymbol{\varepsilon}}, \mathbf{Y}, t), \quad (34)$$

1173 where

$$\mathbf{Y} = \begin{pmatrix} \boldsymbol{\sigma} \\ \tau_0^{(k)}, k = 1, \dots, M \\ X^{(k)}, k = 1, \dots, M \end{pmatrix},$$

$$\mathbf{F}(\dot{\boldsymbol{\epsilon}}, \mathbf{Y}, t) = \begin{pmatrix} \mathbf{C} : \left( \dot{\boldsymbol{\epsilon}} - \sum_{k=1}^M \dot{\gamma}^{(k)}(\mathbf{Y}) \boldsymbol{\mu}^{(k)} \right) \\ \left( \tau_{sta}^{(k)} - \tau_0^{(k)} \right) \sum_{\ell=1}^M h^{(k,\ell)} |\dot{\gamma}^{(\ell)}(\mathbf{Y})| \\ c^{(k)} \dot{\gamma}^{(k)}(\mathbf{Y}) - d^{(k)} X^{(k)} |\dot{\gamma}^{(k)}(\mathbf{Y})| - e^{(k)} |X^{(k)}|^m \text{sign} \left( X^{(k)} \right) \end{pmatrix} \quad (35)$$

1174 with  $\mathbf{C}$  the elastic stiffness ( $\mathbf{C} = \mathbf{S}^{-1}$ ). The set of parameters used are  
 1175 given in Table 1.

#### 1176 4.2.2. Application to strain field prediction in a 2D-1/2 configuration.

1177 The elasto-viscoplastic FFT approach was used to predict strain and  
 1178 stress field evolution during transient creep tests on ice polycrystals, in  
 1179 comparison with experimental measurements performed by Grennerat et al.  
 1180 (2012).

1181 Samples were grown following (Montagnat et al., 2011) (see Section 4.1.2).  
 1182 This way, when compressed, (i) plastic deformation can be approximate as 2-  
 1183 D, and (ii) strain fields measured at the specimen surface are representative  
 1184 for the sample volume owing to the minimisation of in-depth microstructure  
 1185 gradients. Average grain size (section perpendicular to the column direction)  
 1186 was about 5 mm and most of the c-axes were oriented parallel to the surface

1187 ( $\pm 15^\circ$ ). The microstructure and grain orientation were measured using an  
1188 Automatic Fabric Analyzer (Russell-Head and Wilson, 2001) which provides  
1189 orientation values with about  $50 \mu\text{m}$  resolution, and  $1^\circ$  accuracy. A Digital  
1190 Image Correlation technique (Vacher et al., 1999) was applied to measure  
1191 the strain heterogeneities on the surface perpendicular to the column direc-  
1192 tion. From displacement measurements performed during transient creep in  
1193 ice, i.e. up to 1 to 2%, at  $-10^\circ\text{C}$ , under 0.5 MPa, strain fields were evaluated  
1194 with a resolution of about 0.2%, and at a spatial resolution of about 1 mm.

1195

1196 The experimental microstructures were implemented in the code using  
1197 the fabric analyzer data of  $2000 \times 2000$  pixels (but the model input does not  
1198 need to be square). One pixel in the third dimension (column direction) is  
1199 enough to reproduce the 2D-1/2 geometry thanks to the periodic boundary  
1200 conditions.

1201 Fig. 18 presents the strain field measured experimentally at the end of  
1202 the transient creep, and the simulated fields of strain and stress. Although  
1203 simulated boundary conditions did not precisely match the experimental  
1204 ones, the heterogeneities of the strain field that develop during transient  
1205 creep of polycrystalline ice were reproduced well by the model (Grennerat  
1206 et al., 2012). In particular, the model was able to reproduce the characteris-  
1207 tic length of the heterogeneities being larger than the grain size, and scaling  
1208 with the sample dimensions. Furthermore, both experimental and modeled  
1209 results showed no correlation between the orientation of the c-axis and the  
1210 strain intensity (see Fig. 19). This result casts doubt on the relevance of  
1211 the distinction between "hard grains" and "soft grains" classically made for  
1212 the analysis of ice mechanical behavior, and more generally for anisotropic  
1213 materials.

1214 Fig. 20 represents the evolution of the simulated equivalent strain field from  
1215 0.25 to 0.60% of compression during transient creep. As observed experi-  
1216 mentally, the strain heterogeneities develop early during the transient creep  
1217 and are reinforced up to about 10 times the imposed strain.

## 1218 **5. Modeling of dynamic recrystallization mechanisms**

1219 Under laboratory conditions (described in Section 1), dynamic recryst-  
1220 tallization (DRX) dominates the changes of microstructures and fabrics in  
1221 the tertiary creep regime, that is after about 1% macroscopic strain (Du-  
1222 val, 1981; Jacka and Maccagnan, 1984; Jacka and Li, 1994). During DRX,  
1223 grain nucleation and grain boundary migration are two processes that con-  
1224 tribute to the reduction of the dislocation density, therefore of the stored  
1225 deformation energy (Humphreys and Hatherly, 2004). In the laboratory,  
1226 tertiary creep is a continuous sequence of deformation and recrystallization  
1227 that gradually results in a steady state. This steady state is associated with  
1228 an equilibrium grain size (Jacka and Li, 1994) and a girdle-type fabric with  
1229 c-axes at about  $30^\circ$  from the compression axis (Jacka and Maccagnan, 1984),  
1230 or with two maxima in simple shear (Bouchez and Duval, 1982).

1231 In polar ice sheets, DRX was identified from observation on ice thin sections  
1232 along ice cores (Alley, 1992; Thorsteinsson et al., 1997; de la Chapelle et al.,  
1233 1998; Kipfstuhl et al., 2006). Three regions are usually defined: (i) normal  
1234 grain growth driven by the reduction of grain-boundary energy in the upper  
1235 hundreds meters of the core, (ii) rotation recrystallization during which new  
1236 grains are formed by the progressive lattice rotation of the subgrains in the  
1237 main part of the core and (iii) migration recrystallization similar to the one  
1238 observed in the laboratory, in the bottom part where the temperature is

1239 above  $-10^{\circ}\text{C}$  (see Montagnat et al. (2009) and Faria et al. (this issue) for a  
1240 review).

1241 Recrystallization and grain growth significantly influence the microstruc-  
1242 ture, the fabric and therefore the mechanical properties. To be able to in-  
1243 tegrate these mechanisms in the modeling of ice deformation is therefore  
1244 crucial for an accurate prediction of its behavior.

### 1245 *5.1. Dynamic recrystallization within mean-field approaches*

1246 Several attempts were made to integrate dynamic recrystallization mech-  
1247 anisms into mean-field approaches as described in Section 3.

1248 On the basis of the VPSC scheme (tangent version) described in Section 3  
1249 for the description of the mechanical behavior, Wenk et al. (1997) developed  
1250 a nucleation and grain-growth model to represent DRX in anisotropic ma-  
1251 terials such as ice. The model is based on the hypothesis that grains with  
1252 a high stored energy (highly deformed) are likely to nucleate new grains  
1253 and become dislocation-free. They may also be invaded by their neighbors  
1254 which have a lower stored energy. Depending on the respective importance  
1255 of nucleation and grain boundary migration processes, the recrystallization  
1256 textures are expected to favor either highly deformed components or less  
1257 deformed ones.

1258 One must first remember that, in the VPSC scheme, grains are represented  
1259 by inclusions in an homogenous equivalent medium (HEM). Grain interac-  
1260 tions are therefore represented "averaged" through the interaction between  
1261 the inclusion and the HEM.

1262 In this model, nucleation is represented, by a probability of nucleation  $P$   
1263 per time increment  $\Delta t$  for each deformation step:

$$P \propto \Delta t \times \exp(-A/E^2) \quad (36)$$

1264 The constant  $A$  depends on the grain boundary energy and was taken as  
 1265 an adjustable parameter.  $E$  is a proxy of the stored energy,  $E \propto \sum_s (\Delta\tau_0^s)$   
 1266 with  $\Delta\tau_0^s$  the variation of the critical resolved shear stress on the system  $s$   
 1267 during the deformation step. This calculation supposes a hardening law for  
 1268 each slip system to be defined. An isotropic hardening law was chosen in the  
 1269 form  $\dot{\tau}_0^s = H \sum_s \dot{\gamma}^s$ , with hardening matrix  $H$  being isotropic. A threshold  
 1270 was then defined for the minimum strain energy to nucleate, and the new  
 1271 grain completely replaced the old one (same size, same orientation), with a  
 1272 stored energy equal to zero.

1273 The grain boundary migration rate was taken proportional to the difference  
 1274 in stored energy between the grain and the average, i.e., the HEM. The de-  
 1275 velopment of the microstructure is therefore a balance between nucleation  
 1276 and growth. Adjustable parameters were varied arbitrarily for comparison  
 1277 purpose.

1278 Applied to ice, this model resulted into weaker fabrics than the one ob-  
 1279 tained by the classical VPSC tangent approach, mostly because grains near  
 1280 the compression axis disappeared (high stored energy) and only a few girdle  
 1281 grains, and a few grains exactly aligned with the compression axis from the  
 1282 beginning, remained.

1283

1284 Thorsteinsson (2002) included some DRX in its Nearest-Neighbor Inter-  
 1285 action (NNI) model described in Section 3. Polygonization associated with  
 1286 rotation (or continuous) recrystallization is accounted for by comparing the  
 1287 resolved shear stress in the crystal ( $|\sum_s \tau_s \hat{\mathbf{b}}_s|$ ) to the applied stress (with  
 1288  $\tau_s$  the shear stress on system  $s$ , and  $\hat{\mathbf{b}}_s$  a unit vector in the direction of the  
 1289 Burgers vector). If the ratio is smaller than a given value, and the disloca-  
 1290 tion density higher than a given value, then the crystal size is halved and

1291 both new grains are rotated by a fixed  $\Delta\theta$  of  $5^\circ$ . Grain growth occurs by  
1292 normal grain growth according to (Gow, 1969; Alley et al., 1986) parabolic  
1293 law ( $D^2 - D_0^2 = Kt$ ). The grain growth factor  $K$  follows an Arrhenius-type  
1294 dependence on the temperature. To take into account the grain growth as-  
1295 sociated with the difference in dislocation-stored energy between the grain  $i$   
1296 and the average, this growth factor was modified into ( $\tilde{K} = (E_{disl}^{av} - E_{disl}^i)K'$ )  
1297 with  $K'$  a constant depending on temperature and impurities.

1298 Migration recrystallization is included in the model by considering the bal-  
1299 ance between grain-boundary energy, and stored energy associated with dis-  
1300 locations (the stored energy is calculated following (Wenk et al., 1997), as  
1301 just described, and translated into dislocation density). A crystal recrystal-  
1302 lizes (i.e. is replaced by a crystal with initial dislocation density  $\rho_0$ ) when  
1303 the dislocation energy is higher than the grain-boundary energy. This as-  
1304 sumption relies on the hypothesis that stored energy is released by normal  
1305 grain growth (driven by GB energy), and that dynamic recrystallization only  
1306 occurs if this relaxation is not efficient enough to decrease the dislocation  
1307 density. The size of the new crystal is adjusted with the effective stress fol-  
1308 lowing (Guillopé and Poirier, 1979; Jacka and Li, 1994) and its orientation  
1309 is chosen at random in the range of the "softest" orientations in the applied  
1310 stress state.

1311 Modeling results were obtained for comparison to a case similar to the GRIP  
1312 ice core, with vertical compression, and rotation recrystallization domi-  
1313 nating. The introduction of polygonization allows for the preferential re-  
1314 moval of "hard" grains, which leads to a weaker fabric compared to the  
1315 "no-recrystallization" case. In particular, when associated with the NNI  
1316 formulation, the model is able to reproduce fabrics quite similar to those  
1317 measured along the GRIP ice core at several depths. "Girdle-type" fabric



1318 similar to the experimental fabrics, results from the introduction of migra-  
1319 tion recrystallization. However, parametrization remains weak, in particular  
1320 the estimation of the dislocation density, and of the recrystallized grain ori-  
1321 entations.

1322

1323 The last example presented here is the cellular automaton model for  
1324 fabric development by Ktitarev et al. (2002) and Faria et al. (2002). The  
1325 application was mostly to reproduce the fabric measured along deep ice  
1326 cores, with the assumption of deformation under uniaxial compression. The  
1327 cellular automaton (CA) frame is especially suitable for simulation of sys-  
1328 tems represented by a certain number of cells, which are associated with  
1329 generalized state variables and arranged in regular environment. The con-  
1330 sidered material is a thin horizontal layer of ice located along the ice core,  
1331 thin enough so that it is considered homogeneous in the vertical dimension.  
1332 To discretize the problem according to the CA method, the authors took a  
1333 one-dimensional lattice of equal cells representing the grains, described by  
1334 their size, and their orientation. The basic dynamical quantity of the al-  
1335 gorithm is the dislocation density. This density increases with deformation  
1336 and depends on the orientation of the grain. Recrystallization mechanisms  
1337 proceed when a critical value is reached. Normal grain growth is accounted  
1338 for following Gow (1969) and is apparently the only growth mechanism asso-  
1339 ciated with polygonization mechanisms. The increase in dislocation density  
1340 is associated with the resolved shear stress on the basal system and the re-  
1341 crystallization model developed in Montagnat and Duval (2000) is used to  
1342 estimate the evolution of the density in relation with grain size and polygo-  
1343 nization mechanisms. Rotation of grains is ruled by a kinematic equation  
1344 based on the inelastic spin, assuming a compressive stress proportional to the

1345 depth along the core, and a linear dependence between the shearing rate of  
1346 sliding on the basal system and the resolved shear stress. The time evolution  
1347 was related to the depth along the core using the Dansgaard et al. (1993)  
1348 relation. Following Duval and Castelnau (1995), migration recrystallization  
1349 was only applied below 2800 m depth. During migration recrystallization,  
1350 new grains were allowed to grow much faster by consuming up to ten cells  
1351 at every time step, until it is impinged by another growing grain, or until it  
1352 reaches the critical size of the steady state.

1353 The model was able to provide a good qualitative evolution of the grain  
1354 size, by separating the influence of normal grain growth, polygonization and  
1355 migration recrystallization similarly to what was suggested from the mea-  
1356 surements along the GRIP ice core (Thorsteinsson et al., 1997; de la Chapelle  
1357 et al., 1998). Concerning the fabric evolution, the model was able to pre-  
1358 dict the evolution toward a single maximum, but the kinetics is too strongly  
1359 influenced by the polygonization, and further by migration recrystallization.

1360

## 1361 *5.2. Dynamic recrystallization within full-field approaches*

1362 This section presents a coupling between a platform for structural change  
1363 in materials (Elle) with the full-field FFT approach presented in Section 4.1,  
1364 to predict the microstructure evolution of ice polycrystals during dynamic  
1365 recrystallization. A critical step in the development of generic models linking  
1366 plastic deformation and recrystallization is the incorporation of the interac-  
1367 tion between intra- and intergranular heterogeneities of the micromechanical  
1368 fields (i.e. strain rate and stress) and the recrystallization processes. Be-  
1369 cause local rotations of the crystal lattice are controlled by local gradients of  
1370 plastic deformation, heterogeneous distributions of lattice orientations are

1371 observed at the grain and subgrain scale, see Section 4. This has a strong  
1372 influence on recrystallization as this is a process driven by the local gradi-  
1373 ents of energy (e.g. grain boundary or stored strain energy). Traditional  
1374 mean-field models used to predict microstructure evolution during recryst-  
1375 tallization are based on a simplified description of the medium and cannot  
1376 fully describe intragranular heterogeneities (Section 5.1). Therefore, explicit  
1377 full-field approaches are required for a better understanding of dynamic re-  
1378 crystallization and prediction of microstructure evolution at large strain.

1379

#### 1380 *5.2.1. The Elle modeling platform*

1381 Elle is a platform for the numerical simulation of processes in rocks  
1382 and grain aggregates, with particular focus on (micro-) structural changes  
1383 (Jessell et al., 2001; Jessell and Bons, 2002; Bons et al., 2008; Piazzolo et al.,  
1384 2010). The simulations act on an actual 2D image of the microstructure  
1385 (Fig. 21.a). Elle is currently restricted to 2D cases although the underlying  
1386 principles for 2D are equally valid in 3D (Becker et al., 2008), and therefore  
1387 the approach could be converted for 3D simulations.

1388 The central philosophy of Elle is to enable the coupling of processes  
1389 that act on the material, recognizing that the effect of one process may  
1390 significantly alter that of a concurrent process. Dynamic recrystallization,  
1391 for example, can greatly change crystallographic preferred orientations in  
1392 mineral aggregates deforming by dislocation creep (Jessell, 1988a,b). Cou-  
1393 pling of processes is achieved in Elle using the principle of operator splitting,  
1394 whereby individual processes successively act on the model in isolation, for  
1395 a small time step. This approach greatly simplifies coding, as the coupling  
1396 between processes needs not be programmed itself, but emerges from their

1397 alternating effect on the model.

1398 Each process in Elle is an individual program or module. A shell-script  
1399 takes the starting model and then passes it in a loop to the individual pro-  
1400 cesses, which each in turn modify the model slightly. Each loop represents  
1401 one time step. The user can freely determine the mix of processes that op-  
1402 erate by choosing which ones to include in the loop. The relative activity  
1403 of individual processes is determined by the parameters passed on to each  
1404 process.

1405 The model is essentially defined by two types of nodes: boundary nodes  
1406 (bnodes) and unconnected nodes (unodes) (Fig. 21.b). Bnodes define the  
1407 boundaries of a contiguous set of polygons (termed flynns). These flynns  
1408 typically represent single grains, but can also represent regions within a  
1409 material, for example rock layers (Llorens et al., 2012). The boundaries of  
1410 the flynns are formed by straight segments that connect neighboring bnodes.  
1411 One bnode can be connected by either two or three other bnodes. The use  
1412 of bnodes and flynns makes the model suitable for a range of Finite Element  
1413 and front-tracking models.

1414 Unodes form a second layer of the model. These are nodes that do not  
1415 necessarily have fixed neighborhood relationships and typically represent  
1416 points within the material. Some processes are not amenable to be modeled  
1417 with polygons, but are best simulated with a regular grid of unodes. The  
1418 FFT code is an example. Nodes and flynns can have a range of attributes  
1419 assigned to them, such as c-axis orientation, boundary properties, etc.

1420 Elle uses fully wrapping boundaries. A flynn that touches one side of  
1421 the model continues on the other side (Fig. 21.a). The model is thus effec-  
1422 tively a unit cell that is repeated infinitely in all directions. Although Elle  
1423 typically uses a square model, deformation may change the unit cell into a

1424 parallelogram shape.

1425 Elle now includes a large and ever growing number of process modules for  
1426 a variety of processes that mostly relate to microstructural developments in  
1427 mineral aggregates. Each process can essentially act on the model in only  
1428 two ways: changing the position of a node (e.g. a bnode in case of grain  
1429 boundary migration) or changing the value(s) of attributes of flynns or nodes  
1430 (e.g. concentration at a unode in a diffusion simulation). Some of the most  
1431 relevant current processes are:

1432 • Normal grain growth driven by the reduction of surface energy, and  
1433 hence curvature of grain boundaries. This process was used by Roes-  
1434 siger et al. (2011) to address the issue of the competition between  
1435 grain growth and grain size reduction in the upper levels of polar ice  
1436 caps (Mathiesen et al., 2004). Surface energy can be anisotropic, i.e.  
1437 depending on the lattice orientation of the grains on either side of the  
1438 boundary (Bons et al., 2001). Two-phase grain growth has been ap-  
1439 plied to grain growth in rocks with a small proportion of melt (Becker  
1440 et al., 2008) and to ice with air bubbles (Fig. 21)(Roessiger et al. this  
1441 volume).

1442

1443 • The Finite Element module Basil is used for incompressible power-law  
1444 viscous deformation (Barr and Houseman, 1996). Using viscosities  
1445 that are assigned to flynns, it calculates the stress and velocity fields  
1446 resulting from applied boundary conditions. It has been used to study  
1447 the behaviour of rigid inclusions in a deforming matrix (Bons et al.,  
1448 1997), the behaviour of deforming two-phase materials as a function of  
1449 viscosity contrast and composition (Jessell et al., 2009) and for folding

1450 of layers (Llorens et al., 2012). The wrapping boundaries of the Elle  
1451 model, in combination with continuous remeshing allows for arbitrarily  
1452 high strains (Jessell et al., 2009). In combination with grain growth  
1453 and dynamic viscosity, Jessell et al. (2005) studied strain localisation  
1454 behaviour. Durand et al. (2004) investigated the influence of uniaxial  
1455 deformation on grain size evolution in polar ice cores and its influence  
1456 on ice dating methods.

1457 • Dynamic recrystallisation includes grain boundary migration driven  
1458 by strain energy (dislocation density) and the formation of new grain  
1459 boundaries by progressive subgrain rotation or polygonisation (Urai  
1460 et al., 1986). In the next section (5.2.2 ) we will describe how these  
1461 processes, employing a front-tracking model for grain-boundary mi-  
1462 gration, are linked with the FFT approach (Griera et al., 2011, 2012;  
1463 Piazzolo et al., 2012) to model the stress and strain-rate fields and the  
1464 driving forces for recrystallization.

1465 • A final Elle module of potential relevance to ice is that developed by  
1466 Schmatz (2010) for the interaction between migrating grain bound-  
1467 aries and small particles (e.g. dust or clathrates). The particles are  
1468 represented by unodes, which, when swept by a grain boundary, can  
1469 latch onto that boundary. Particles can slow down grain boundary  
1470 movement, but can also be dragged along and eventually be released  
1471 by a grain boundary.

1472 Summarizing, Elle provides a large number of routines to simulate grain-  
1473 scale processes in minerals and rocks, and hence in glacial or polar ice. The  
1474 open and versatile code allows for more process modules to be added or  
1475 existing ones to be tailored for application to ice. A significant advantage of

1476 the code is that it enables the investigation of the complex microstructural  
1477 and mechanical effects of multiple, concurrent and coupled processes.

### 1478 *5.2.2. Coupling Elle platform to FFT approach*

1479 Most of the numerical approaches used to simulate deformation and mi-  
1480 crostructural evolution of rocks and metals are based on combining defor-  
1481 mation approaches based on the Finite Element Method with Monte Carlo,  
1482 cellular automaton, phase field, network or level-set methods to simulate  
1483 recrystallization (Jessell, 1988a,b; Raabe and Becker, 2000; Piazzolo et al.,  
1484 2002, 2010, 2012; Solas et al., 2004; Battaile et al., 2007; Logé et al., 2008).  
1485 An alternative to these methods is the numerical scheme used in this study  
1486 based on the coupling between the crystal plasticity FFT-based code (Leben-  
1487 sohn, 2001) (section 4.1) and the Elle modeling platform just described  
1488 (Bons et al., 2008). Both codes have been previously explained and here  
1489 we only concentrate on some particularities of the coupling between them.  
1490 The FFT-based formulation is integrated within the Elle platform using  
1491 a direct one-to-one mapping between data structures. The polycrystalline  
1492 aggregate is discretized into a periodic, regular array of spaced and uncon-  
1493 nected nodes (Fourier Points in the FFT and "unconnected nodes", unodes,  
1494 in Elle; Fig. 21).

1495 Numerical simulation is achieved by iterative application of small time  
1496 steps of each process. After numerical convergence of the FFT model, data is  
1497 transferred to Elle assuming that the micromechanical fields are constant in  
1498 the incremental time step. The position and material information of unodes  
1499 are directly updated because they are equivalent to the Fourier points, while  
1500 position of boundary nodes (bnodes) are calculated using the velocity field.  
1501 Based on the evolution of the predicted local lattice rotation field, the dislo-

1502 cation density can be estimated using strain gradient plasticity theory (e.g.  
1503 Gao et al. (1999); Brinckmann et al. (2006)) or using the dislocation density  
1504 tensor or Nye tensor (Nye, 1953; Arsenlis and Parks, 1999; Pantleon, 2008).  
1505 With this approach, only geometrical necessary dislocations required to en-  
1506 sure strain compatibility are estimated. To simplify the problem, we use  
1507 a scalar approach where all dislocations are assumed to be related to the  
1508 basal plane. The lattice-orientation and dislocation-density fields provide  
1509 the input parameters to predict recrystallization in the aggregate.

1510 Recrystallization is simulated by means of three main processes: nucle-  
1511 ation, subgrain rotation and grain boundary migration. Using the kinematic  
1512 and thermodynamic instability criteria of classical recrystallization theory  
1513 (Humphreys and Hatherly, 2004; Raabe and Becker, 2000), nucleation is  
1514 simulated by the creation of a small new, dislocation-free flynn when the  
1515 local misorientation or dislocation density exceeds a defined threshold. The  
1516 lattice orientation of the new grain is set to that of the critical unode. When  
1517 a cluster of unodes within a grain share the same orientation that is different  
1518 from the rest of the unodes in that grain, a new grain boundary is created,  
1519 while preserving the lattice orientations of the unodes. A technical limita-  
1520 tion is that nucleation of grains and subgrains is only allowed along grain  
1521 boundaries. Nucleation within grains are therefore not possible.

1522 Grain boundary migration is described by a linear relationship between  
1523 velocity ( $v$ ) and driving force per unit area ( $\Delta f$ ), by  $v = M\Delta f$  where  $M$   
1524 corresponds to the grain boundary mobility, which has an Arrhenius-type  
1525 dependency on temperature. Grain boundary curvature and stored strain  
1526 energies are used as driving forces for grain boundary motion. For this



1527 situation, the driving force can be defined as

$$\Delta f = \Delta E - 2\gamma/r \quad (37)$$

1528 where  $\Delta E$  is the difference of stored strain energy across the boundary,  $\gamma$   
1529 is the boundary energy and  $r$  is the local radius of curvature of the grain  
1530 boundary. Stored strain energy is the energy per unit volume associated  
1531 with lattice distortions and depends on the dislocation density ( $\rho$ ) and dis-  
1532 location type. Grain boundary motion is simulated using the free-energy  
1533 minimization front-tracking scheme of (Becker et al., 2008). When an un-  
1534 ode is swept by a moving grain boundary, it is assumed that dislocations  
1535 are removed and the new lattice orientation is that of the nearest unode  
1536 belonging to the growing grain.

1537 Following the Elle philosophy, each process runs individually, following a  
1538 pre-established sequence. After all Elle processes have run, the unodes layer  
1539 is used to define the new input microstructure to be deformed viscoplasti-  
1540 cally by the FFT code. A drawback is that the unodes are not following a  
1541 regular mesh, a requirement needed by the FFT approach. For this reason,  
1542 as proposed by Lahellec et al. (2003), and later adapted in the context of  
1543 Elle by Grier et al. (2011, 2012), a particle-in-cell method is used to remap  
1544 all material and morphological information to a new regular computational  
1545 mesh. In order to avoid unrealistic crystallographic orientations, these are  
1546 not interpolated during remapping. The crystallographic orientation of a  
1547 new Fourier Point that belongs to a specific grain is that of the nearest un-  
1548 ode that belongs to the same grain. This allows to run numerical simulation  
1549 up to large strains.

1550 *5.2.3. Application to creep experiments and natural ice*

1551 An example of numerical simulation using the FFT/Elle approach is  
1552 shown in Fig. 22. The simulation is based on a creep experiment of poly-  
1553 crystalline columnar ice. Samples and experimental conditions are those  
1554 of (Montagnat et al., 2011) described in Section 4.1.2. The specimen was  
1555 deformed at  $-10^{\circ}\text{C}$  under uniaxial conditions with a constant load of 0.5  
1556 MPa up to an axial strain of 4%. A thin section of the initial and the  
1557 final microstructure was analyzed using the Automatic Ice Texture Ana-  
1558 lyzer method (Russell-Head and Wilson, 2001) to obtain the local c-axis  
1559 orientations. After a 4% of shortening, the onset of local recrystallization  
1560 is evident in the experiment (Fig. 22a), in the form of irregular and ser-  
1561 rated grain boundaries and small new grains that are preferentially located  
1562 at triple junctions and along grain boundaries. Localized variations in the  
1563 orientation of the basal plane form sharp and straight subgrain boundaries  
1564 that indicate intracrystalline deformation. The experimental c-axis map was  
1565 used as input for the FFT/Elle simulation. The experimental starting mi-  
1566 crostructure was discretized into a grid of  $256 \times 256$  Fourier points. As only  
1567 the c-axis orientation is known, the other axes are given a random orienta-  
1568 tion. Crystal plasticity is described with an incompressible rate-dependent  
1569 equation for basal, prismatic and pyramidal slip (see Section 3). Critical  
1570 resolved shear stress for basal slip was set 20 times lower than for non-basal  
1571 systems. The physical properties used for recrystallization are as follows:  
1572 mobility  $M = 1 \times 10^{-10} \text{ m}^2\text{Kg}^{-1}\text{s}^{-1}$  (e.g. Nasello et al., 2005), isotropic  
1573 boundary energy  $\gamma = 0.065 \text{ Jm}^{-2}$  (Ketcham and Hobbs, 1969), shear mod-  
1574 ulus  $G = 3 \times 10^9 \text{ Pa}$  and critical dislocation density  $\rho = 1 \times 10^{12} \text{ m}^{-2}$  (de la  
1575 Chapelle et al., 1998). Pure shear boundary conditions were imposed with

1576 vertical constant strain rate of  $-1 \times 10^{-8} \text{ s}^{-1}$  up to a 4% of strain in 1%  
1577 increments.

1578 The computed orientation map and grain boundary misorientation are  
1579 shown in Fig. 22b. Several features of the experiment are seen in the  
1580 numerical simulation, such as the development of sharp misorientations or  
1581 kink bands, bulging and serrated grain boundaries, and new grains at triple  
1582 junction and grain boundaries. There is a good correlation between loca-  
1583 tion of kink bands in the experiment and the simulation. However, the  
1584 width of kink bands in the simulation is dependent on the numerical reso-  
1585 lution. A relationship between grain boundary motion/nucleation and high  
1586 dislocation-density regions is observed (Fig. 23). Variations in dislocation  
1587 densities across grain boundaries lead to migration of these boundaries in  
1588 the direction of the dislocation density gradient. However, some discrepan-  
1589 cies are also seen, such as, for example, grain boundary motion (e.g. at the  
1590 bottom-left part) that was not observed in the experiment. One explanation  
1591 may be that low and high angle grain boundaries were not differentiated in  
1592 the simulation and, therefore, both types had similar mobility.

1593

1594 A second example aims to show the strong effect recrystallization can  
1595 have on the final microstructure. A  $10 \times 10 \text{ cm}^2$  microstructure with 1600  
1596 grains with random c-axis orientations (Fig. 24a) was deformed to 40%  
1597 shortening in plane-strain pure shear. The values of mechanical (slip sys-  
1598 tems, CRSS, etc) and recrystallization (mobility, surface energy, etc) prop-  
1599 erties are similar to those of the model described before, but adjusted to a  
1600 natural strain rate of  $10^{-12} \text{ s}^{-1}$  at about  $-30^\circ\text{C}$ . Fig. 24b shows the c-axis and  
1601 relative misorientation maps for an extreme case with no recrystallization  
1602 (FFT only). Dominant red and purple colors indicate that the c-axis of crys-

1603 tallites are preferentially oriented at low angles to the shortening direction.  
1604 Elongated grains are oriented parallel to the stretching direction. Remark-  
1605 able differences are observed when recrystallization is activated (Fig. 24c).  
1606 Grain boundaries are smooth and grains larger and more equidimensional.  
1607 Despite the significant difference in microstructure, both simulations show a  
1608 single maximum c-axis distribution at low angle to the shortening direction.  
1609 The strong resemblance of the simulated microstructure with that of natural  
1610 ice (Thorsteinsson et al., 1997; de la Chapelle et al., 1998; Weikusat et al.,  
1611 2009) shows the strong potential of modeling of ice deformation based on  
1612 an actual map of the microstructure.

## 1613 **6. Toward large scale ice flow modeling**

1614 A number of models have been developed in glaciology to simulate the  
1615 flow of anisotropic ice and the strain-induced development of fabric within  
1616 polar ice-sheets. Accounting for ice anisotropy in an ice-flow model implies  
1617 to (i) build a macroscopic anisotropic flow law whose response will depend  
1618 on the local fabric and (ii) have a proper description of the ice fabric at  
1619 each node of the mesh domain and be able to model the fabric evolution as  
1620 a function of the flow conditions. We hereafter present the main issues to  
1621 address these two points.

1622 Due to the scale of these large ice-masses, the implementation of a poly-  
1623 crystalline law must stay simple enough and numerically tractable. At  
1624 present, full-field or even homogenization models presented previously are  
1625 computationally too demanding and cannot realistically be used to estimate  
1626 the mechanical response in an ice-sheet flow model. Here we present two ap-  
1627 proaches to build a simple and efficient macroscopic law for polycrystalline

1628 ice. The first one is based on the concept of a scalar enhancement factor  
1629 function so that the collinearity between the strain-rate and the deviatoric  
1630 stress tensors is conserved (Placidi and Hutter, 2006), see Section 6.1. The  
1631 second polycrystalline law is fully orthotropic and depends on six relative  
1632 viscosities, function of the fabric (Gillet-Chaulet et al., 2005, 2006), see Sec-  
1633 tion 6.2. Both models are phenomenological and must be calibrated using  
1634 experimental or numerical results, as described below.

1635     With regards to other materials, the advantage of the hexagonal symme-  
1636 try of ice is that the crystal rheology can be assumed transversally isotropic  
1637 (only true for a linear rheology). Under this assumption, only one unit vector  
1638 suffices to describe the lattice orientation, thus simplifying the mathemat-  
1639 ical description of fabrics. With regards to other materials, the advantage  
1640 of the hexagonal symmetry of ice is that only one unit vector suffices to de-  
1641 scribe the lattice orientation, thus simplifying the mathematical description  
1642 of fabrics. The discrete description of the fabric, *i.e.* a couple of angles for  
1643 each crystal, would require too large a number of variables to be stored at  
1644 each node of the domain mesh. Typical mesh size are hundreds of thousand  
1645 nodes in 3D (Seddik et al., 2011) up to few millions for the most recent appli-  
1646 cations (Gillet-Chaulet et al., 2012). The use of a parameterized orientation  
1647 distribution function (ODF) would decrease the number of parameters, but  
1648 evolution equations for these parameters to describe the fabric evolution  
1649 cannot be obtained in a general case (Gagliardini et al., 2009). The ori-  
1650 entation tensors, which describe the fabric at the macroscopic scale in a  
1651 condensed way are more suitable. Five parameters are needed to describe  
1652 an orthotropic fabric (the two eigenvalues of the second-order orientation  
1653 tensor and the three Euler angles to specify the position of the material  
1654 symmetry basis), and an evolution equation for the second-order orienta-

1655 tion tensor can be easily derived from the macroscopic stress and strain-rate  
1656 fields.

### 1657 *6.1. Continuous Diversity and the CAFFE model*

1658 The CAFFE model (Continuum-mechanical Anisotropic Flow model based  
1659 on an anisotropic Flow Enhancement factor) results from a suitable com-  
1660 bination of two basic concepts: a power law description of ice rheology  
1661 resembling the well-known Glen’s flow law (Glen, 1955); and a multiscale  
1662 approach to model the evolution of the polycrystalline microstructure of ice  
1663 based on the general theory of continuous diversity (Faria, 2001; Faria and  
1664 Hutter, 2002; Faria et al., 2003).

1665 The ideas leading to the CAFFE model have been elaborated in a series  
1666 of works by Luca Placidi and his collaborators (Placidi, 2004, 2005; Placidi  
1667 and Hutter, 2005, 2006; Placidi et al., 2004). These ideas culminated in the  
1668 definitive CAFFE formulation, presented by Placidi et al. (2010), in which  
1669 the so-called enhancement factor of Glen’s flow law becomes a function of  
1670 the material anisotropy (fabric), and the evolution of the latter is governed  
1671 by an orientation-dependent mass balance equation derived from the theory  
1672 of continuous diversity applied to glacier and ice-sheet dynamics (Faria,  
1673 2006a,b; Faria et al., 2006).

1674 The greatest strength of the CAFFE model is its successful compromise  
1675 between accuracy and flexibility, which allows one to upgrade existing com-  
1676 puter models of isotropic ice-sheet dynamics based on Glen’s flow law into  
1677 efficient anisotropic models, without profound changes in the original code.  
1678 In fact, due to its relative simplicity, the CAFFE model has already been  
1679 implemented in several numerical ice-flow simulations. For instance, it has  
1680 been used by Seddik et al. (2008) and Bargmann et al. (2011) to simulate

1681 the ice flow at the site of the EPICA-DML drill site at Kohnen Station,  
 1682 Dronning Maud Land, East Antarctica, while Seddik et al. (2011) used it  
 1683 to simulate the ice flow in the vicinity of the Dome Fuji drill site in central  
 1684 East Antarctica.

1685 In the following, we review the CAFFE formulation presented by Placidi  
 1686 et al. (2010). The fundamental idea is to regard polycrystalline ice as a  
 1687 "mixture" of lattice orientations, following the philosophy of the theory  
 1688 of Mixtures with Continuous Diversity (MCD) proposed by Faria (2001,  
 1689 2006a). Succinctly, a mixture with continuous diversity is a multicompo-  
 1690 nent medium made up of an infinite number of mutually interacting species,  
 1691 whose distinctive properties vary smoothly from one to another.

1692 In the case of polycrystalline ice, species are distinguished by their c-axis  
 1693 orientations. Each point of the continuous body is interpreted as a represen-  
 1694 tative volume element, which encompasses a large number of crystallites with  
 1695 their own c-axis orientations. Each of such orientations is mathematically  
 1696 identified with a point on the surface of the unit sphere  $\mathcal{S}^2$  and represented  
 1697 by a unit vector  $\mathbf{n} \in \mathcal{S}^2$ . As a consequence, for each species one can intro-  
 1698 duce a mass density field  $\varrho^*(\mathbf{x}, t, \mathbf{n})$ , given at a certain position  $\mathbf{x}$  within the  
 1699 polycrystal, and at time  $t$ , sometimes called orientational mass density, such  
 1700 that, when integrated over the whole unit sphere, the usual mass density  
 1701 field of the polycrystal (i.e. of the "mixture") results:

$$\varrho(\mathbf{x}, t) = \int_{\mathcal{S}^2} \varrho^*(\mathbf{x}, t, \mathbf{n}) d^2n, \quad (38)$$

1702 where  $d^2n$  ( $= \sin \theta d\theta d\phi$  in spherical coordinates) is the infinitesimal solid  
 1703 angle on the unit sphere  $\mathcal{S}^2$ . The product  $\varrho^*(\mathbf{x}, t, \mathbf{n}) d^2n$  is the mass fraction  
 1704 of crystalline material in the volume element with c-axis directed towards  
 1705  $\mathbf{n}$  within the solid angle  $d^2n$ . Therefore, assuming that the material is

1706 incompressible, the mass (or volume) fraction  $\varrho^*/\varrho$  can be interpreted as  
 1707 the usual orientation distribution function (ODF) in the context of materials  
 1708 science (Bunge, 1993; Zhang and Jenkins, 1993; Raabe and Roters, 2004).  
 1709 It should be remarked that in the glaciological literature the term "ODF"  
 1710 sometimes refers to the relative number, instead of the mass (or volume)  
 1711 fraction, of grains with a certain orientation.

1712 The time evolution of  $\varrho^*$  is governed by the balance equation of species  
 1713 (orientational) mass

$$\frac{\partial \varrho^*}{\partial t} + \operatorname{div}(\varrho^* \mathbf{v}) + \operatorname{div}_{\mathbf{n}}(\varrho^* \mathbf{u}^*) = \varrho^* \Gamma^* \quad (39)$$

1714 with

$$\begin{aligned} \operatorname{div}_{\mathbf{n}}(\Phi^*) &= \operatorname{tr}[\operatorname{grad}_{\mathbf{n}}(\Phi^*)], \\ \operatorname{grad}_{\mathbf{n}}(\Phi^*) &= \frac{\partial \Phi^*}{\partial \mathbf{n}} - \left( \frac{\partial \Phi^*}{\partial \mathbf{n}} \cdot \mathbf{n} \right) \mathbf{n} \end{aligned} \quad (40)$$

1715 for any scalar-, vector- or tensor-valued field  $\Phi^*(\mathbf{x}, t, \mathbf{n})$ . In (39),  $\mathbf{u}^*(\mathbf{x}, t, \mathbf{n})$   
 1716 denotes a sort of "velocity" on the unit sphere (with  $\mathbf{u}^* \cdot \mathbf{n} = 0$ ), called  
 1717 orientational transition rate. Further,  $\Gamma^*(\mathbf{x}, t, \mathbf{n})$  is the specific recrystal-  
 1718 lization rate, which describes the rate of change of mass (per unit mass) of  
 1719 one species into another one with different orientation. Integration of (39)  
 1720 over the unit sphere  $\mathcal{S}^2$  gives rise to the usual mass balance equation for the  
 1721 polycrystal (i.e. the "mixture")

$$\begin{aligned} \frac{\partial \varrho}{\partial t} + \operatorname{div}(\varrho \mathbf{v}) &= 0 \quad \text{with} \\ \int_{\mathcal{S}^2} \varrho^* \Gamma^* \, d^2 n &= \int_{\mathcal{S}^2} \operatorname{div}_{\mathbf{n}}(\varrho^* \mathbf{u}^*) \, d^2 n = 0, \end{aligned} \quad (41)$$

1722 Notice that the first integral in (41) is a consequence of mass conservation,  
 1723 while the second integral follows from Gauss' theorem.

1724 As shown by Faria (2001, 2006a) and Faria and Hutter (2002), the tran-  
 1725 sition rate  $\mathbf{u}^*$  is governed by its own balance equation, involving couple



1726 stresses and body couples. In the development of the CAFFE model, how-  
 1727 ever, an abridged approach has been adopted by postulating a constitutive  
 1728 equation for the transition rate

$$\mathbf{u}^* = \mathbf{W}\mathbf{n} - \iota [\dot{\boldsymbol{\epsilon}}\mathbf{n} - (\mathbf{n} \cdot \dot{\boldsymbol{\epsilon}}\mathbf{n}) \mathbf{n}] - \frac{\lambda}{\varrho^*} \text{grad}_{\mathbf{n}}(\varrho^* H^*) \quad (42)$$

1729 where

$$\mathbf{W} = \frac{1}{2} (\text{grad } \mathbf{v} - (\text{grad } \mathbf{v})^T), \dot{\boldsymbol{\epsilon}} = \frac{1}{2} (\text{grad } \mathbf{v} + (\text{grad } \mathbf{v})^T) \quad (43)$$

1730 are the tensors of rotation and strain rate, respectively. The first term on  
 1731 the right hand side of (42) represents a rigid-body rotation, while the second  
 1732 term describes the process of strain-induced lattice rotation (Dafalias, 2001),  
 1733 with  $\iota > 0$  denoting the so-called "shape factor" of the theory of rotational  
 1734 diffusion (Faria, 2001). According to Placidi et al. (2010), fabric evolution  
 1735 simulations of the GRIP and EPICA-DML ice cores suggest that best results  
 1736 are obtained for  $0.6 > \iota > 0.4$ . Finally, the third term on the right hand  
 1737 side of (42) models rotation recrystallization as a diffusive process, with  
 1738  $\lambda > 0$  being the orientational diffusivity and  $H^*(\mathbf{x}, t, \mathbf{n})$  an orientational  
 1739 ("chemical") potential, also called "hardness function" by Gödert (2003). In  
 1740 principle  $H^*$  should be a constitutive function, but, based on microstructural  
 1741 analyses of the NorthGRIP ice core (Durand et al., 2008), Placidi et al.  
 1742 (2010) suggest that one may simply set  $H^* = 1$ .

1743 In the original application of the MCD theory to the flow of glaciers and  
 1744 ice sheets (Faria, 2006b), the specific recrystallization rate  $\Gamma^*$  is regarded as  
 1745 a dissipative variable. However, for simplicity, in the CAFFE model Placidi  
 1746 (2004, 2005) has proposed the following relation between  $\Gamma^*$  and the strain

1747 rate

$$\Gamma^* = G(D^* - D), \quad \text{with} \quad (44)$$

$$D^* = 5 \frac{(\dot{\boldsymbol{\varepsilon}} \mathbf{n})^2 - (\mathbf{n} \cdot \dot{\boldsymbol{\varepsilon}} \mathbf{n})^2}{\text{tr}(\dot{\boldsymbol{\varepsilon}}^2)} \quad \text{and} \quad D = \frac{1}{\varrho} \int_{S^2} \varrho^* D^* d^2 n,$$

1748 where  $G > 0$  is a material parameter, while  $5/2 \geq D^* \geq 0$  and  $5/2 \geq D \geq 0$   
 1749 are called the species and polycrystal "deformability", respectively.

1750 As remarked by Placidi et al. (2010), owing to the difficulties in determin-  
 1751 ing the values of the material parameters  $\lambda$  and  $G$  from experiments, they  
 1752 are usually determined by fitting numerical simulations of ice core fabrics  
 1753 and grain stereology. This concludes the description of the fabric evolution.

1754 As for the flow law, in contrast to the full stress–strain rate relation with  
 1755 tensorial fluidity (viscosity) predicted by the theory of continuous diversity  
 1756 (Faria, 2006b), the CAFFE model adopts a much simplified generalization  
 1757 of Glen's flow law:

$$\dot{\boldsymbol{\varepsilon}} = E(D) A(T) \sigma_{eq}^{n-1} \boldsymbol{\sigma}', \quad (45)$$

1758 where  $\boldsymbol{\sigma}'$  is the deviatoric part of the Cauchy stress tensor  $\boldsymbol{\sigma}$ ,  $\sigma_{eq}$  is the  
 1759 effective stress invariant,  $n$  is the power law exponent (usually set equal  
 1760 3),  $T$  is the temperature, and  $A(T)$  is a temperature-dependent rate factor.  
 1761 Clearly, (45) implies that all anisotropy effects are contained in the scalar-  
 1762 valued, deformability-dependent flow enhancement factor  $E(D)$ , such that  
 1763 stress and strain rate are collinear and (45) reduces to the classical form of  
 1764 Glen's flow law when  $E(D) \equiv \text{const.}$

1765 A detailed functional form for the enhancement factor  $E(D)$  has been  
 1766 proposed by Seddik et al. (2008) and Placidi et al. (2010), which is con-  
 1767 tinuously differentiable at  $D = 1$  and is compatible with the experimental

1768 results of Azuma (1995) and Miyamoto (1999)

$$E(D) = \begin{cases} (1 - E_{\min}) D^\zeta + E_{\min} & 1 \geq D \geq 0, \\ \frac{4D^2 (E_{\max} - 1) + 25 - 4E_{\max}}{21} & 5/2 \geq D > 1, \end{cases} \quad (46)$$

1769 with

$$\zeta = \frac{8}{21} \left( \frac{E_{\max} - 1}{1 - E_{\min}} \right), \quad E_{\max} \approx 10, \quad E_{\min} \approx 0.1. \quad (47)$$

1770 By introducing the orientation tensors (essentially equivalent to the  
1771 dipole and quadrupole moments of  $\varrho^*/\varrho$ )

$$\mathbf{a}^{(2)} = \frac{1}{\varrho} \int_{\mathbb{S}^2} \varrho^* \mathbf{n} \otimes \mathbf{n} \, d^2n, \quad \mathbf{a}^{(4)} = \frac{1}{\varrho} \int_{\mathbb{S}^2} \varrho^* \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \, d^2n \quad (48)$$

1772 to reformulate the CAFFE flow law (45) in an explicitly anisotropic form

$$\dot{\boldsymbol{\varepsilon}} = \hat{E}(\boldsymbol{\sigma}') A(T) \sigma_{eq}^{n-1} \boldsymbol{\tau}, \quad (49)$$

1773 In plain words, (49) tells us that the CAFFE model can be applied to all  
1774 anisotropies (fabrics) that can satisfactorily be represented by a multipole  
1775 expansion up to fourth order. Fortunately, most anisotropies observed in  
1776 glaciers and ice sheets.

## 1777 6.2. GOLF law and Elmer/Ice

1778 In this section, we present the anisotropic ice flow model developed at  
1779 LGGE. This model has been used for various applications (Gillet-Chaulet  
1780 et al., 2005, 2006; Durand et al., 2007; Martín et al., 2009; Ma et al., 2010).  
1781 In this approach, the fabric is described using the second and fourth-order  
1782 orientation tensors (48). In this continuum description of the fabric, the  
1783 polycrystal represents the local behavior of a representative elementary ice  
1784 volume. By assuming that the fourth-order orientation tensor  $\mathbf{a}^{(4)}$  is given

1785 as a tensorial function of  $\mathbf{a}^{(2)}$  (Gillet-Chaulet et al., 2005), the fabric can  
 1786 be described in a very condensed way using  $\mathbf{a}^{(2)}$  solely. By definition,  
 1787  $\text{tr } \mathbf{a}^{(2)} = 1$ , so that only the first two eigenvalues  $a_1^{(2)}$  and  $a_2^{(2)}$  and three  
 1788 Euler angles are needed to completely define the fabric. As a consequence,  
 1789 modeled fabrics are orthotropic, *i.e.* the c-axes distribution presents three  
 1790 orthogonal symmetry planes. Although orthotropy is a simple form of the  
 1791 most general anisotropy, it is thought to be a good compromise between  
 1792 physical adequateness and simplicity. The second-order orientation tensor  
 1793 allows to describe all the observed fabric patterns: for random c-axes dis-  
 1794 tribution the diagonal entries of  $\mathbf{a}^{(2)}$  are  $a_{11}^{(2)} = a_{22}^{(2)} = a_{33}^{(2)} = 1/3$ , for a  
 1795 single maximum fabric with its maximum in the third direction,  $a_{33}^{(2)} > 1/3$   
 1796 and  $a_{11}^{(2)} \approx a_{22}^{(2)} < 1/3$ , and for a girdle type fabric in the plane  $(x_1, x_2)$ ,  
 1797  $a_{33}^{(2)} < 1/3$  and  $a_{11}^{(2)} \approx a_{22}^{(2)} > 1/3$ . When the material symmetry axes are  
 1798 those of the general reference frame, as for the three particular previous  
 1799 fabrics, the non-diagonal entries of  $\mathbf{a}^{(2)}$  are zero.

1800 The behavior of the polycrystal is described by the general orthotropic  
 1801 linear flow law (GOLF, Gillet-Chaulet et al., 2005). In its initial form, ice  
 1802 was assumed to behave as a linearly viscous orthotropic material. In more  
 1803 recent works (Martín et al., 2009; Ma et al., 2010), the GOLF law has been  
 1804 extended to a nonlinear form by adding an invariant in the anisotropic linear  
 1805 law. The simple choice is either to add the second invariant of the strain  
 1806 rate (Martín et al., 2009) or the second invariant of the deviatoric stress  
 1807 (Pettit et al., 2007). No theoretical or experimental results are available  
 1808 today to discard one of these two solutions, and other solutions based on  
 1809 anisotropic invariants of the deviatoric stress and/or the strain rate are  
 1810 also possible. In (Ma et al., 2010) approach, the nonlinearity of the law is  
 1811 introduced through the second invariant of the deviatoric stress. With this

1812 definition, the anisotropy factors of the polycrystalline law for a given stress  
 1813 are identical in the linear and nonlinear cases. In other words, for a given  
 1814 fabric and a given state of stress, the corresponding strain rate relative to  
 1815 the isotropic response is the same for the linear and nonlinear cases. Using  
 1816 the strain-rate invariant in the same way as Martín et al. (2009) did, leads  
 1817 to different anisotropy factors (as defined here) in the linear and nonlinear  
 1818 cases. Therefore, the proposed expression of the nonlinear GOLF law is as  
 1819 follows:

$$\sum_{r=1}^3 [\eta_r \text{tr}(\mathbf{M}_r \cdot \dot{\boldsymbol{\epsilon}}) \mathbf{M}'_r + \eta_{r+3} (\dot{\boldsymbol{\epsilon}} \cdot \mathbf{M}_r + \mathbf{M}_r \cdot \dot{\boldsymbol{\epsilon}})'] = 2A\sigma_{eq}^{n-1} \boldsymbol{\sigma}', \quad (50)$$

1820 where  $A$  is the temperature-dependent Glen's law parameter for isotropic ice.  
 1821 The six dimensionless anisotropy viscosities  $\eta_r(\mathbf{a}^{(2)})$  and  $\eta_{r+3}(\mathbf{a}^{(2)})$  ( $r = 1,$   
 1822  $2, 3$ ) are functions of eigenvalues of the second-order orientation tensor  $\mathbf{a}^{(2)}$ ,  
 1823 which represent a measure of the anisotropy strength. The three structure  
 1824 tensors  $\mathbf{M}_r$  are given by the dyadic products of the three eigenvectors of  $\mathbf{a}^{(2)}$ ,  
 1825 which then represent the material symmetry axes. In the method proposed  
 1826 by Gillet-Chaulet et al. (2005), the six dimensionless viscosities  $\eta_r(\mathbf{a}^{(2)})$  are  
 1827 tabulated as a function of the fabric strength (*i.e.*, the  $a_i^{(2)}$ ) using a micro-  
 1828 macro model. When ice is isotropic,  $\eta_r = 0$  and  $\eta_{r+3} = 1$  ( $r = 1, 2, 3$ ), and  
 1829 Eq. (50) reduces to the isotropic Glen's flow law.

1830 Following Gillet-Chaulet et al. (2005), the six dimensionless viscosities  
 1831  $\eta_r(\mathbf{a}^{(2)})$  are tabulated using the visco-plastic self-consistent model (VPSC,  
 1832 Castelnau et al., 1996a, 1998), see Section 3. The two crystal parameters  
 1833 in the VPSC model used to tabulate the GOLF law were chosen so that  
 1834 the experimentally observed polycrystal anisotropy is reproduced. Gillet-  
 1835 Chaulet et al. (2005) use the shear-strain rates ratio for a polycrystal with  
 1836 a single maximum fabric and an isotropic polycrystal both experiencing

1837 the same shear stress. This anisotropy factor in shear is hereafter noted  
1838  $k_s$  and, according to the experimental results of Pimienta et al. (1987), its  
1839 value is approximately  $k_s = 10$ . In other words, the VPSC parameters  
1840 are chosen so that the response under simple shear of a polycrystal with a  
1841 single maximum fabric is  $k_s$  times easier to deform than the corresponding  
1842 isotropic polycrystal. The experimental results of Pimienta et al. (1987) also  
1843 indicate that an isotropic polycrystal is much easier to deform than a single  
1844 maximum fabric polycrystal experiencing the same uniaxial compressional  
1845 stress. These experiments allow to define a second anisotropy factor for  
1846 uniaxial compressional stress, which is noted  $k_c$ . A value  $k_c = 0.4$  is in  
1847 accordance with the experimental results of Pimienta et al. (1987). As  
1848 discussed before, the anisotropy factors  $k_s$  and  $k_c$  are independent of Glen's  
1849 flow law exponent  $n$  with the adopted nonlinear formulation.

1850 Assuming that recrystallization processes do not occur and that the ice  
1851 fabric is induced solely by deformation, the evolution of the second-order  
1852 orientation tensor  $\mathbf{a}^{(2)}$  can be written as

$$\frac{D\mathbf{a}^{(2)}}{Dt} = \mathbf{W} \cdot \mathbf{a}^{(2)} - \mathbf{a}^{(2)} \cdot \mathbf{W} - (\mathbf{C} \cdot \mathbf{a}^{(2)} + \mathbf{a}^{(2)} \cdot \mathbf{C}) + 2\mathbf{a}^{(4)} : \mathbf{C}, \quad (51)$$

1853 where  $\mathbf{W}$  is the spin tensor defined as the antisymmetric part of the velocity  
1854 gradient. The tensor  $\mathbf{C}$  is defined as

$$\mathbf{C} = (1 - \alpha)\dot{\boldsymbol{\varepsilon}} + \alpha k_s A \sigma_{eq}^{n-1} \boldsymbol{\sigma}'. \quad (52)$$

1855 The *interaction parameter*  $\alpha$  controls the relative weighting of the strain  
1856 rate  $\dot{\boldsymbol{\varepsilon}}$  and the deviatoric stress  $\boldsymbol{\sigma}'$  in the fabric evolution Eq. (51). When  
1857  $\alpha = 0$ , the fabric evolution is solely controlled by the state of strain rate,  
1858 whereas in the case where  $\alpha = 1$  the fabric evolves under the influence of  
1859 the deviatoric stress solely. In between, as for the VPSC, both the strain

1860 rate and deviatoric stress contribute to the fabric evolution. In what fol-  
1861 lows, the interaction parameter is  $\alpha = 0.06$  in accordance with the crystal  
1862 anisotropy and the VPSC model used to derive the polycrystal behaviour  
1863 (Gillet-Chaulet et al., 2005). In Eq. (51), the fourth-order orientation ten-  
1864 sor is evaluated assuming a closure approximation giving  $\mathbf{a}^{(4)}$  as a tensorial  
1865 function of  $\mathbf{a}^{(2)}$  (Gillet-Chaulet et al., 2005).

1866 The anisotropic polycrystalline law described above and the associated  
1867 fabric evolution equations have been implemented in the Finite Element  
1868 code Elmer/Ice, the glaciological part of the open source Finite Element  
1869 software Elmer developed by CSC (<http://www.elmerfem.org/>). Ice flow  
1870 (velocity and isotropic pressure) are obtained solving the anisotropic Stokes  
1871 equations and coupled with the fabric evolution equation (51) and the upper  
1872 free surface equation in the case of transient simulations. In Gillet-Chaulet  
1873 et al. (2006), the model was applied to synthetic geometries in order to  
1874 show the influence of coupling the Stokes and fabric evolution equations on  
1875 the flow of ice over a bumpy bedrock. In Durand et al. (2007), the model  
1876 was used to explain the fabric evolution in the Dome C ice core, in the  
1877 framework of the EPICA project. The authors showed that to explain the  
1878 fabric evolution at Dome C, shear stress must be invoked. The model was  
1879 also applied to evaluate the value of the ad-hoc enhancement factor that  
1880 should be incorporated in large-scale isotropic ice-sheet flow model in Ma  
1881 et al. (2010). In Martín et al. (2009), the anisotropic ice flow model was  
1882 applied to explain observed shapes of isochrones below ridges or domes.

## 1883 **7. Synthesis and perspectives**

1884       Applications of ice mechanical behavior modeling extend from below the  
1885 single-crystal scale to the ice sheet scale. Upwards, this scale range far ex-  
1886 ceeds that of engineering material sciences but is similar to the geological  
1887 one. Within this scale range, many physical processes come into play, some  
1888 of which are not yet very well described. Furthermore, there exist strong in-  
1889 teractions between these processes that create bridges between the different  
1890 levels of complexity. Modeling of ice has strongly benefited from advances  
1891 in materials science. In return, as shown by the results presented in this pa-  
1892 per, the contribution of the ice community to the theoretical understanding  
1893 and modeling of the mechanical behavior of anisotropic materials is signif-  
1894 icant. With the large viscoplastic anisotropy of the ice crystal, ice is now  
1895 considered a model material. The advances presented here may equally well  
1896 be applied to, for example, mantle flow, where the anisotropy due to fabric  
1897 (CPO) development in olivine is thought to play a significant role (Tommasi  
1898 et al., 2009; Long and Becker, 2010).

1899       The presented modeling methods are basically of two types; some that  
1900 aim to precisely reproduce the physical mechanisms as observed experimen-  
1901 tally, and some with a more phenomenological approach. Going through  
1902 scales, it clearly appears that individual dislocation interactions cannot be  
1903 taken into account at the scale of the polycrystal imbedded in a glacier envi-  
1904 ronment. Nevertheless, modeling at the scale of dislocation interactions pro-  
1905 vides a better estimate of the interactions between slip systems at the single  
1906 crystal scale, which, in turn, is essential to reproduce an accurate mechanical  
1907 response of the polycrystal with mean-field and full-field approaches. Fur-  
1908 thermore, full-field approaches are necessary to validate the approximations



1909 made using mean-field models, as they provide the "exact" (in a numerical  
1910 sense) response of the specimen with a real microstructure, integrating the  
1911 inter- and intra-granular interactions. Finally, large-scale flow models are  
1912 now getting to a sufficient level of complexity to be able to take into account  
1913 and represent the anisotropy associated with the fabrics induced by the flow  
1914 conditions. To do so, they integrate mean-field approaches that correctly  
1915 reproduce the viscoplastic anisotropy and a non-linear mechanical behavior.

1916 A summary of the main domains of application, advantages, and limita-  
1917 tions of the main modeling tools presented in the paper is given on tables  
1918 2, 3 and 4

1919 Much progress has recently been made in the modeling of dynamic re-  
1920 crystallization processes and their interactions with flow anisotropy. Never-  
1921 theless, due to the complexity of the physical processes involved, to jump  
1922 the gap between scales is a strong challenge. The field dislocation mechanics  
1923 approach appears very promising to associate the internal stress field and  
1924 dislocation arrangements to the nucleation and grain boundary migration  
1925 mechanisms. However, field dislocation mechanics cannot yet be applied to  
1926 scales larger than the polycrystal. Full-field models, including the FFT-Elle  
1927 coupling, have the same scale limitation, but may play an important role  
1928 in parameterizing small-scale processes (dislocation glide, grain boundary  
1929 migration, etc.) for mean-field models. They are also important tools to  
1930 test models of mechanical and microstructural evolution.

1931 Compared to other minerals, ice shows remarkably strong transient be-  
1932 havior (Duval et al., 1983; Castelnau et al., 2008b). Continuum flow models,  
1933 such as Glen law (Glen, 1955) have so far not been able to incorporate the  
1934 resulting mechanical complexity of polycrystalline ice deformation. Only  
1935 recently have mechanical models reached a level of sophistication to address

1936 transient behavior. This development is promising and probably highly rel-  
1937 evant in cases where ice flow changes at rates for where both elastic and  
1938 viscoplastic behavior may interact. In particular, this concerns the very  
1939 topical subject of ice shelves, ice streams or extra-terrestrial ice submitted  
1940 to tide forcing. Which model will be able to correctly take into account  
1941 these transient, and event cyclic behavior, and at which scale?

1942 A next step will likely be the multi-scale coupling of models of increas-  
1943 ing complexity. We can expect dislocation dynamics and field dislocation  
1944 mechanics to provide the local criteria for slip system interactions, nucle-  
1945 ation, grain boundary migration as local input to full-field approaches that  
1946 will be further used in interaction with mean-field approaches to calibrate  
1947 dynamic recrystallization variables influencing the mechanical response and  
1948 fabric development.

1949 An interesting example of such model interweaving is given by the large-  
1950 scale flow modeling presented in this paper. Nevertheless, a strong effort  
1951 is still required concerning the flow law of ice and its dependency on fab-  
1952 rics (CPO) and strain. Recent velocity measurements in Greenland (Gillet-  
1953 Chaulet et al., 2011) questioned the relevance of a stress exponent equal  
1954 to three as classically considered for large scale flow modeling (for instance  
1955 Paterson (1994); Hooke (2005); Greve and Blatter (2009), ...). Owing to  
1956 the variety of processes that accommodate strain along an ice core path,  
1957 one could also expect several regimes to occur with depth, as suggested by  
1958 some authors (see for instance Lipenkov et al. (1989); Faria et al. (2009);  
1959 Pettit et al. (2011)). Such modeling - observation comparisons mainly raise  
1960 the complexity of the physical processes involved that can probably not be  
1961 summarized in a single universal law.

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1970

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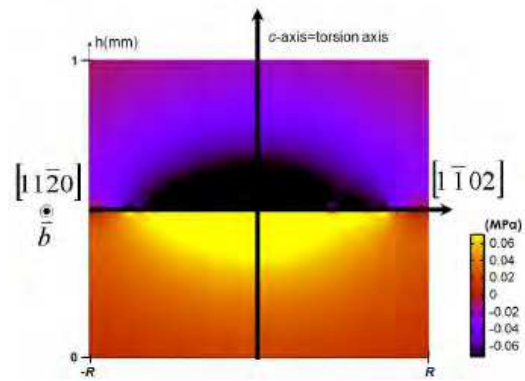


Figure 1: Map of the resolved shear stress in the prismatic system for a torsion boundary made of basal screw dislocations. The cylinder diameter is 1 mm, and the maximum applied stress is 0.1 MPa. From (Chevy et al., 2012)



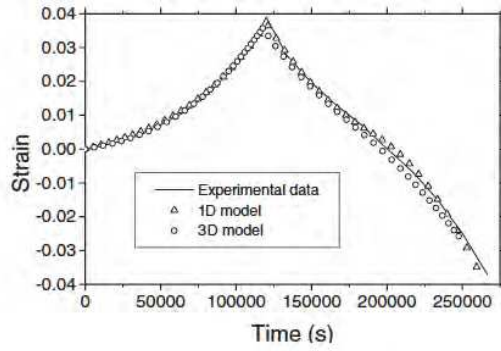


Figure 2: Creep curves in forward and reverse torsion from experiments on single crystals, obtained by 1D and 3D FDM models. From (Taupin et al., 2007)

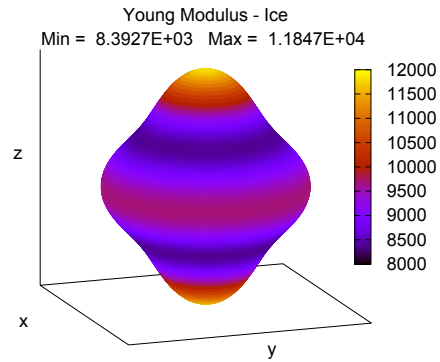


Figure 3: Young's modulus in [MPa] of an ice single crystal with its c-axis aligned with z, at  $-16^{\circ}\text{C}$ .

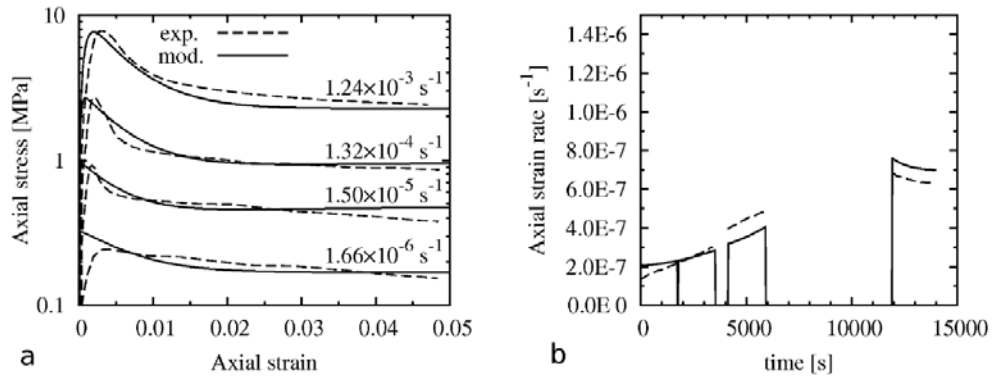


Figure 4: Behavior of an ice single crystal deformed by basal slip. a) Predictions of the model, based on Eq. (6) and with parameters given in Table 1, in comparison with the experimental data of Weertman (1973). Axial strain rates are indicated. b) Prediction of the model in comparison with the results of the recovery tests of Taupin et al. (2008). Temperature is  $-10^{\circ}\text{C}$ . From (Suquet et al., 2011)

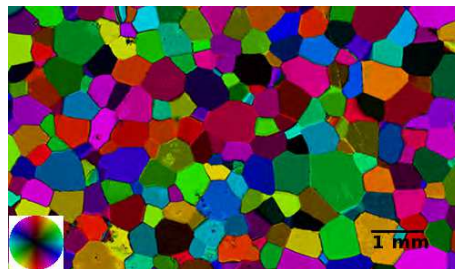


Figure 5: Typical 2D microstructure of an ice polycrystal grown in the laboratory. The color wheel gives the color-code for the c-axis orientation.

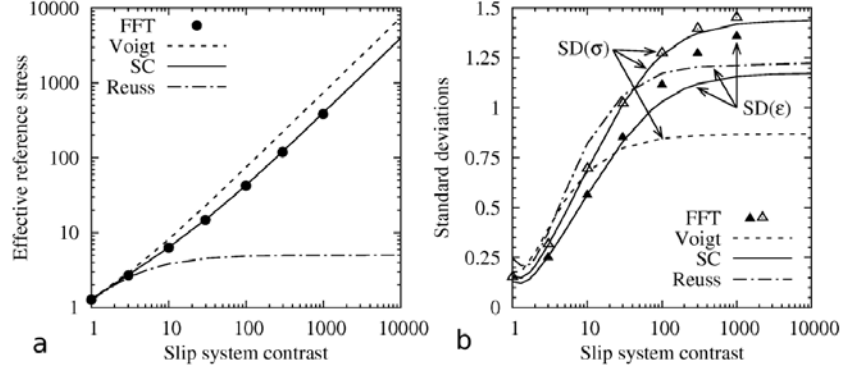


Figure 6: Full-field vs. mean-field behavior for ice polycrystals with random fabric, for a linear viscous behavior ( $n = 1$ ) and various viscoplastic anisotropy (or slip system contrasts) at the grains level. a) Effective flow stress  $\bar{\sigma}_0$ . b) Standard deviation of equivalent stress and strain rate, normalized by  $\bar{\sigma}_{eq}$  and  $\bar{\dot{\epsilon}}_{eq}$ , respectively, characterizing field heterogeneities at the polycrystal scale. Results from the linear SC scheme are compared to reference numerical solutions provided by the FFT approach. Reuss and Voigt bounds are also indicated. Note that, for these bounds, standard deviations of stress and strain rate, respectively, do vanish.

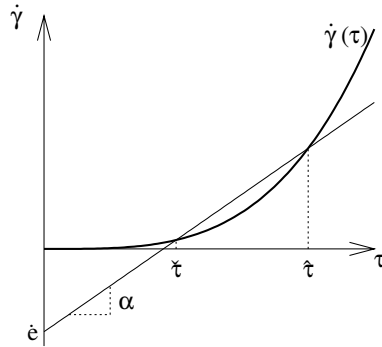


Figure 7: Schematic representation of the linearization between the shear rate ( $\dot{\gamma}$ ) and the stress ( $\tau$ ), to illustrate Eq. (21).

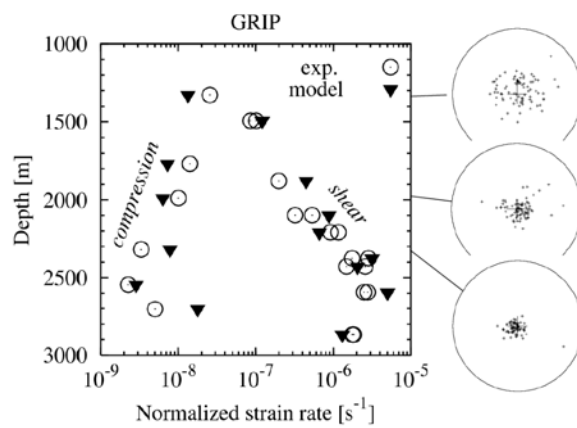


Figure 8: Stationary creep behavior at  $-10^{\circ}\text{C}$  calculated by the affine SC model, and compared to experimental data obtained on anisotropic specimens from the GRIP ice core. The  $c$ -axis pole figures on the right show an increasing concentration of  $c$ -axes towards the *in situ* vertical direction from the surface of the ice sheet down to  $\sim 2600\text{m}$  depth. Experimental data from Castelnau et al. (1998) are expressed for a stress of  $1\text{MPa}$  using a stress sensitivity  $n = 3$ . Points on the left hand side reflect the (hard) behavior under vertical compression, whereas data on the right correspond to (soft) horizontal shear.

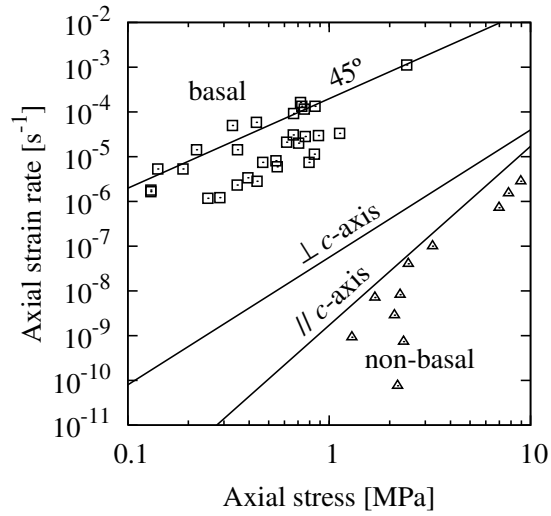


Figure 9: Stationary creep behavior of single crystals at  $-10^{\circ}\text{C}$  input in the AFF SC model to get results of Fig. 8 (lines), compared to the data set compiled by Duval et al. (1983) (symbols). Results are indicated for uniaxial compression at  $45^{\circ}$  from the  $c$ -axis (activation of basal slip), as well as for compression perpendicular (activation of prismatic slip) and parallel (activation of pyramidal systems) to the  $c$ -axis. From (Castelneau et al., 2008b)

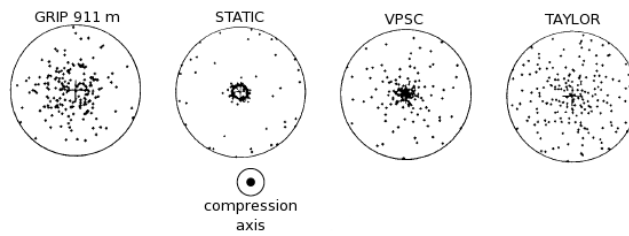


Figure 10: Comparison between fabrics measured along the GRIP ice core (911 m depth), simulated by the static (Reuss), VPSC-tangent, and Taylor (Voigt) approaches.

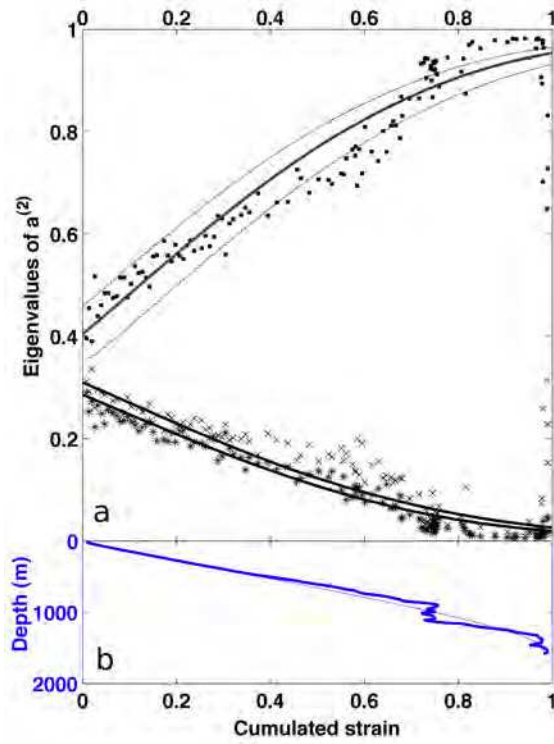


Figure 11: a) Evolution of the eigenvalues of the orientation tensor  $\mathbf{a}^{(2)} = \mathbf{c} \otimes \mathbf{c}$  of the fabric along the Talos Dome ice core, as a function of the cumulated compressive strain. Lines = VP-SO model results, dashed line represents the range of fabric evolution modeled with variation of the initial orientation tensor eigenvalue from isotropic (bottom line), as measured at 18 m (central line), more concentrated than measured (top line). Dots, crosses and plus = measurements performed with the Automatic Ice Texture Analyzer (Russell-Head and Wilson, 2001). b) Cumulated in-situ compressive strain as a function of depth as model by the TALDICE-1 chronology (full line) (Buiron et al., 2011).

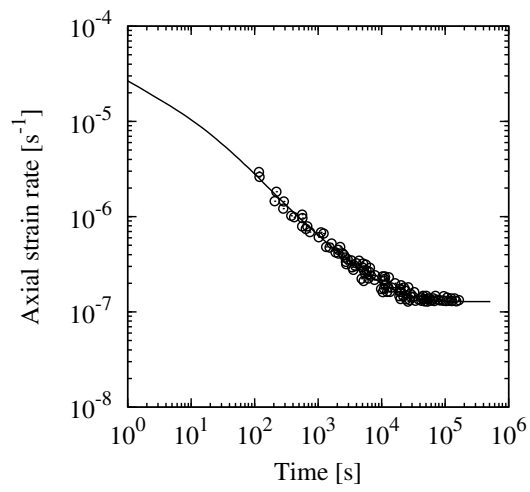


Figure 12: Transient creep response of isotropic ice under an uniaxial compressive stress of 1 MPa predicted with the affine elasto-viscoplastic extension of the self-consistent scheme (line). Model results are compared to the data of Ashby and Duval (1985), expressed for the same loading conditions (points). Strain hardening of prismatic and pyramidal slip systems is taken into account. From (Castelnau et al., 2008b)

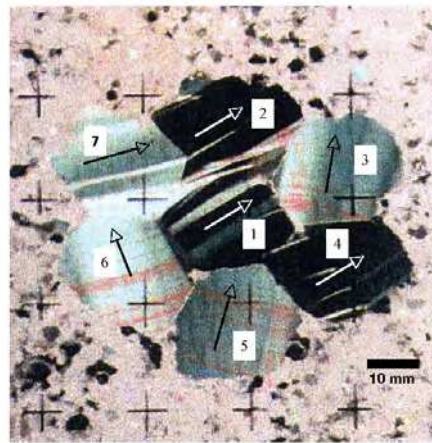


Figure 13: Photograph of a compression creep specimen (after (Mansuy et al., 2000)) between crossed polarizers, after a deformation of  $6.6 \times 10^{-2}$  at  $-10^\circ\text{C}$ . The corresponding strain rate was  $6.0 \times 10^{-8} \text{ s}^{-1}$ . The compression direction is vertical in the plane of the photograph. The mean size of each hexagonal grain was 20 mm. Black and white arrows indicate the initial c-axis orientations. Kink bands appear as abrupt changes in color parallel to the c-axis, shear bands are perpendicular to the c-axis direction.



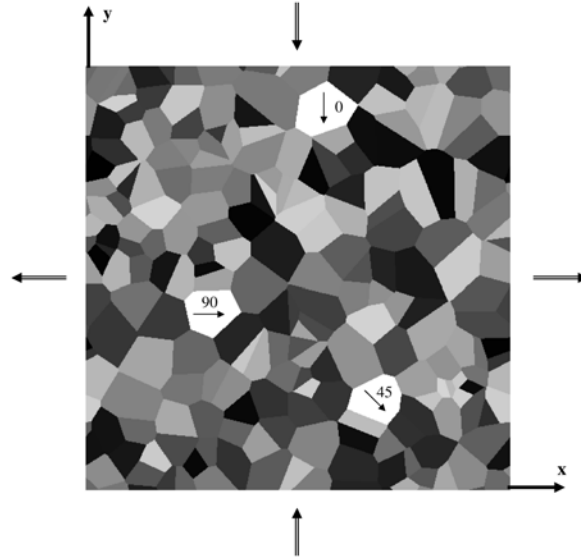


Figure 14: Unit cell containing the cross-sections of 200 columnar grains generated by Voronoi tessellation. The three hand-picked orientations:  $(0^\circ, 90^\circ, 0^\circ)$ ,  $(45^\circ, 90^\circ, 0^\circ)$  and  $(90^\circ, 90^\circ, 0^\circ)$ , and the extension and shorting directions are also indicated.

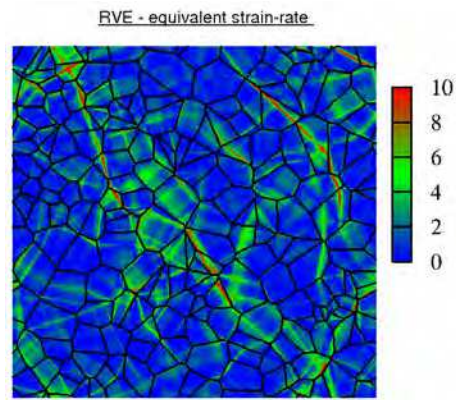


Figure 15: Predicted equivalent strain-rate field over the entire unit cell of Fig. 14, normalized with respect to the average equivalent strain rate ( $\dot{\epsilon}_{eq} = 1.15 \times 10^{-8} \text{s}^{-1}$ ).

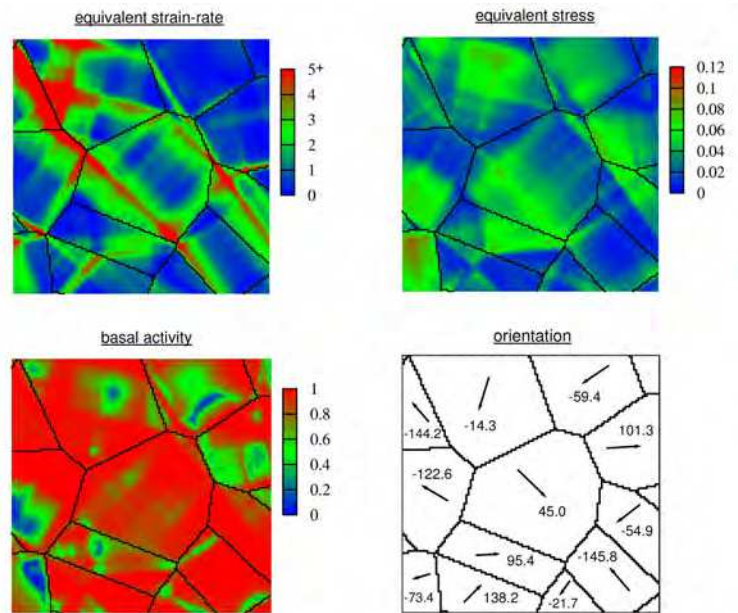


Figure 16: Predicted fields of equivalent strain rate (normalized to  $\dot{\epsilon}_{eq}$ ), equivalent stress (in units of  $\tau^{bas}$ ), relative basal activity, and map of neighbor orientations, for the 45 deg grain and its surroundings.

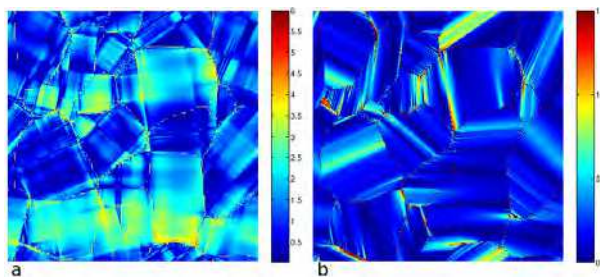


Figure 17: a) Predicted equivalent stress field (in units of  $\tau^{bas}$ ), and b) the misorientation, compared with initial orientation, obtained after 1% strain in a laboratory made microstructure. From (Montagnat et al., 2011)

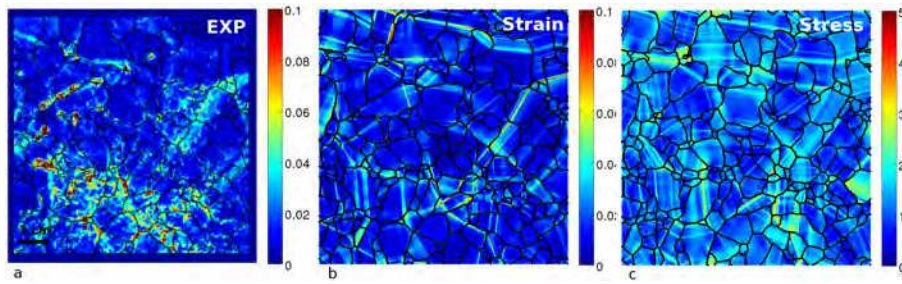


Figure 18: a) Strain field measured experimentally, b) simulated, and c) stress field simulated, after 0.85 % of axial compression. Experimental resolution is about  $75 \times 75$  pixels, the modeling one is  $1024 \times 1024$  pixels. From (Grennerat et al., 2012)

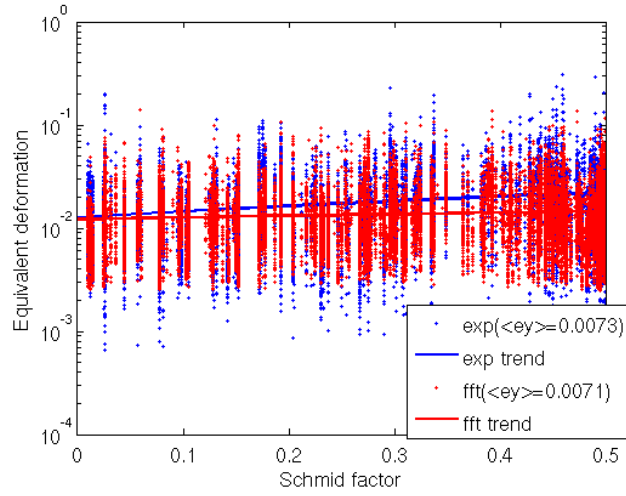


Figure 19: Equivalent strain as a function of the Schmid factor (as a proxy of the orientation). Experimental results are in blue, modeling results in red. Each point is one pixel of the microstructure. The macroscopic strain was 0.7%. From (Grennerat et al., 2012)

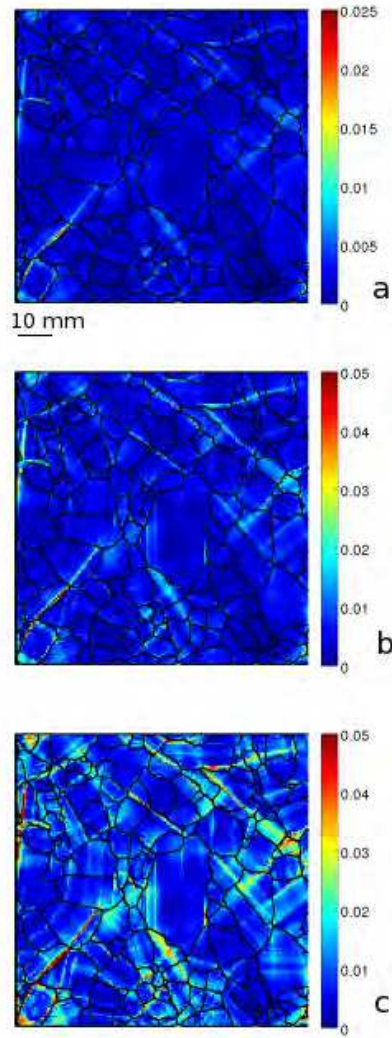


Figure 20: Evolution of the FFT-simulated equivalent strain field during the transient creep of a "2D-1/2" sample of ice, after (a) 0.15%, (b) 0.35% and (c) 0.60% compressive strain (see Grennerat et al. (2012)).

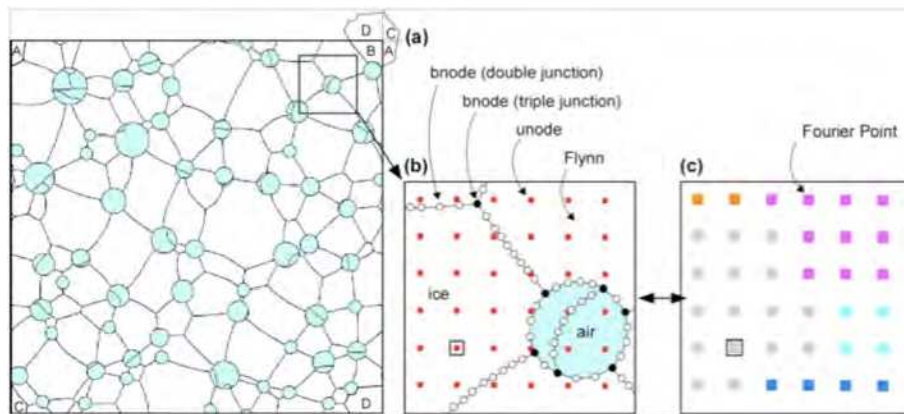


Figure 21: (a) Example of an Elle model: ice (white) with air bubbles (pale blue) (Roesiger et al., this volume). The Elle model has fully wrapping boundaries and grains A to D are in fact one single grain. (b) Close-up showing that grains are defined by flynns (polygons), themselves defined by straight segments that connect boundary nodes (bnodes). A second layer of unconnected nodes (unodes) can be added to keep track of material points. (c) For the FFT module, the microstructure is discretized into a periodic, regular mesh of Fourier Points defined by a characteristic lattice orientation. A direct mapping between unodes layer and Fourier points is established between both codes.

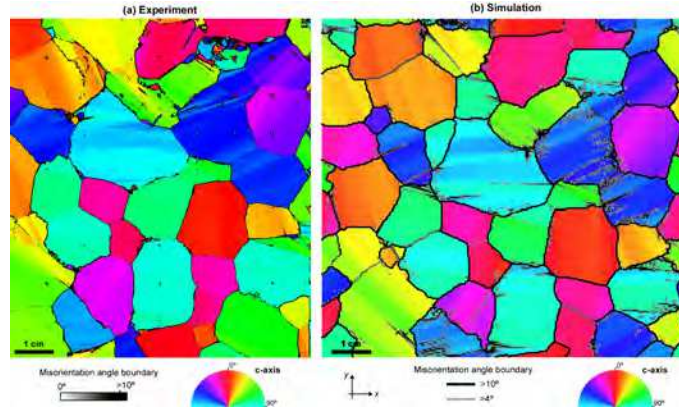


Figure 22: Comparison of (a) physical experiment and (b) numerical simulation after a vertical shortening of 4%. A qualitative equivalence between experiment and simulations is observable, such as correspondence of kink-bands or discontinuous subgrain boundaries at sharp grain boundaries asperities. Colors indicate the orientation of the c-axis respect to the sample reference. Misorientation angle between nodes are indicated in grey ( $> 4^\circ$ ) and black ( $> 10^\circ$ ). Triangular patches seen in the experiment are due to erroneous misfit during Automatic Ice Texture Analyzer acquisition.

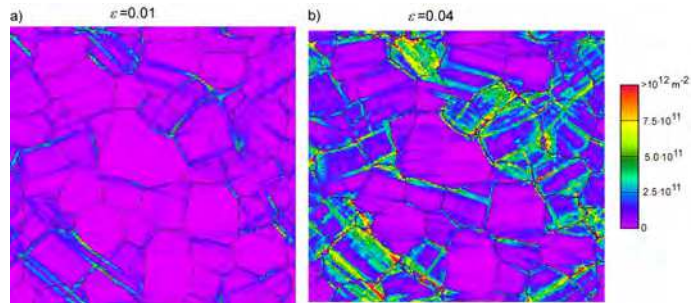


Figure 23: Dislocation density maps after (a) 1% and (b) 4% of shortening. Grain microstructure is indicated by dark lines. Serrated and bulging grain boundaries develop due to grain boundary migration into regions of high dislocation density. New recrystallized grains develop preferentially at triple points and along grain boundaries. Low dislocation densities are typically observed at bulge areas and new grains.

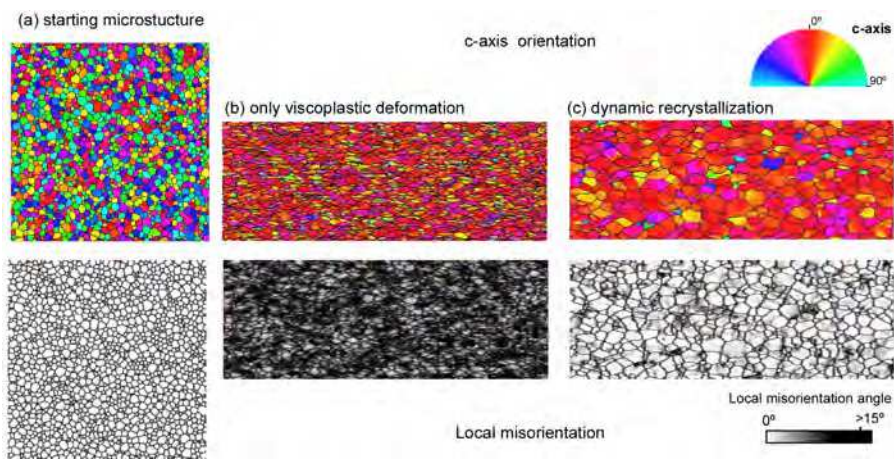


Figure 24: Numerical simulation of polar ice microstructure using the FFT/Elle scheme. (a) Starting microstructure. (b) 40% vertical shortening with only viscoplastic deformation. (c) 40% shortening with viscoplastic deformation coupled with recrystallization. Top row shows c-axis orientations in color and local misorientation in grey. Bottom row shows local misorientation only. C-axis orientation distributions are shown in lower-hemisphere stereoplots.



	$\tau_{ini}$	$\tau_{sta}$	$\dot{\gamma}_0$	$n$	$c$	$d$	$e$
Basal	0.1	0.022	$10^{-6}$	2	9	60	0.0003
Prismatic	0.13	1.5	$10^{-6}$	2.85	9	60	0.0003
Pyramidal	3.875	3.875	$10^{-6}$	4	9	60	0.0003

Hardening matrix:

	Basal	Prismatic	Pyramidal
Basal	70	125	0
Prismatic	125	110	0
Pyramidal	0	0	0

Table 1: Material parameters used in the full-field simulations for single crystals of ice at  $-10^\circ C$ . Units are MPa and  $s^{-1}$ .

Model	Scale	Type	Applications	Advantages	Limitations
DD	Single crystal (mesoscopic)	Finite Element (FE)	Dislocation dynamics and interactions	Solve physics of plasticity at the dislocation scale - Provide slip system activities and interactions	Computing time-intensive. Small samples. Simplified configurations
FDM	Single to poly-crystal	Full-field (FE)	Plasticity modeling taking into account heterogeneous internal stress field associated with dislocations	Length scaling, makes the link between the complexity of the dislocation field dynamics and the macroscopic behavior - Provide intra-crystalline fields	Computing time-intensive - Limited number of grains
VPSC	Polycrystal	Mean-field	Provides effective visco-plastic behavior of polycrystals, based on a given single-crystal behavior	Texture-induced polycrystal anisotropy, texture evolution for secondary creep, can reach large strains	Very limited information on intra-crystalline fields, elasticity and recrystallization neglected
EVPSC	Polycrystal	Mean-field	Provides effective elasto-visco-plastic behavior at polycrystal level, based on known single-crystal behavior	Captures texture-induced anisotropy during transient creep regime	Very limited information on intra-crystalline fields, limited to small strains

Table 2: Summary of techniques application domains, interest and limitations. DD: Dislocation Dynamics, FDM: Field Dislocation Mechanics, VPSC: Homogenized Polycrystal Visco-Plasticity, EVPSC: Homogenized Polycrystal Elasto-Visco-Plasticity

Model	Scale	Type	Applications	Advantages	Limitations
VPSC + DRX	Polycrystal	Mean-field	DRX mechanisms with phenomenological laws, fabric evolution	Fast to run for high strain - easily adaptable to various DRX laws	Too simplified description of DRX mechanisms. No account for intra-crystalline fields
VPFFT	Polycrystal	Full-field	Provides effective visco-plastic behavior and local intra- crystalline fields, 2D and 3D	Microstructural effects on local fields distribution in the secondary creep regime	Microstructure evolution at large strains can only be captured in a crude way. No elasticity and DRX
EVPFFT	Polycrystal	Full-field	Provides effective elasto-visco-plastic behavior and local intra-crystalline fields, 2D and 3D	Microstructural effects on local fields distribution and their evolution during transient creep	Limited to small strains, no microstructure evolution yet, no DRX
VPFFT - Elle	Polycrystal	Full-field	Provides local intra-crystalline fields and microstructure evolution in 2D	Couple local field predictions to DRX mechanisms in the secondary creep regime	No account for local field evolution during transient creep. Limited to 2D (Elle). Rough update of the dislocation field during DRX

Table 3: Summary of techniques application domains, interest and limitations. DRX: dynamic recrystallization, VPFFT: FFT-based formulation for Visco-Plastic polycrystals , EVPFFT: FFT-based formulation for Elasto-Visco-Plastic polycrystals

Model	Scale	Type	Applications	Advantages	Limitations
Mixture with Continuous Diversity (MCD)	Large scale	General continuum theory	General overview of the interactions between microstructure evolution, DRX and ice flow	Effects of microstructure and its evolution via internal variables. Secondary and tertiary creep regimes. Thermodynamically consistent	Mathematically complex. Not implemented numerically yet
CAFEE	Large Scale	Continuum model	Provides effective visco-plastic behavior on the large scale, including fabric development	Captures the effects of fabric development in the secondary and tertiary creep regimes, easy to implement	Stress and strain rate are colinear (scalar effective viscosity). Limited to fabrics represented by a multipole expansion up to fourth order only.
GOLF law	Polycrystal	Phenomenological orthotropic non-linear law	Provides orthotropic viscous behavior and fabric development	Efficient, easy-to-use and able to reproduce the response of micro-macro models	Orthotropic fabric restricted to the assumed closure approximation. Non-linear case not validated against micro-macro models yet
Elmer/Ice	Large scale	FE code including GOLF and CAFEE law	Flow of anisotropic polar ice and its fabric evolution	Fabric evolution consistent with the stress field and strain-rate field	Can not be used to simulate the localization of the deformation (diffusion of the fabric induced by interpolation)

Table 4: Summary of techniques application domains, interest and limitations. DRX: dynamic recrystallization