

1 **Time for anisotropy: The significance of mechanical anisotropy for the**  
2 **development of deformation structures**

3

4 Hao Ran<sup>1,2</sup>, Tamara de Riese<sup>1</sup>, Maria-Gema Llorens<sup>1,3</sup>, Melanie A. Finch<sup>1</sup>, Lynn A.  
5 Evans<sup>4</sup>, Enrique Gomez-Rivas<sup>5,6</sup>, Albert Griera<sup>3</sup>, Mark W. Jessell<sup>7</sup>, Ricardo A.  
6 Lebensohn<sup>8</sup>, Sandra Piazzolo<sup>9</sup>, Paul D. Bons<sup>1,\*</sup>

7

8 <sup>1</sup>Department of Geosciences, Eberhard Karls University Tübingen, Germany

9 <sup>2</sup>School of Earth Sciences and Resources, China University of Geosciences, Beijing,  
10 China

11 <sup>3</sup>Departament de Geologia, Universitat Autònoma de Barcelona, Spain

12 <sup>4</sup>School of Earth, Atmosphere and Environmental Sciences, Monash University,  
13 Clayton, Victoria, Australia

14 <sup>5</sup>Department of Mineralogy, Petrology and Applied Geology, University of  
15 Barcelona, Barcelona, Spain

16 <sup>6</sup>School of Geosciences, King's College, University of Aberdeen, Aberdeen, UK

17 <sup>7</sup>Centre for Exploration Targeting, School of Earth Sciences, The University of  
18 Western Australia, Crawley, Western Australia, Australia

19 <sup>8</sup>Material Science and Technology Division, Los Alamos National Laboratory, USA

20 <sup>9</sup>School of Earth and Environment, University of Leeds, Leeds, UK

21

22 \*Corresponding author: Department of Geosciences, Eberhard Karls University,  
23 Wilhelmstr. 56, 72074 Tübingen, Germany. Tel.: +49-7071-2976469.

24 paul.bons@uni-tuebingen.de

25

26 **Keywords**

27

28 Mechanical anisotropy; porphyroclasts; strain localisation; folds; shear zones

29

30 **Abstract**

31

32 The forty-year history of the *Journal of Structural Geology* has recorded an  
33 enormous increase in the description, interpretation and modelling of

34 deformation structures. Amongst factors that control deformation and the  
35 resulting structures, mechanical anisotropy has proven difficult to tackle. Using a  
36 Fast Fourier Transform-based numerical solver for viscoplastic deformation of  
37 crystalline materials, we illustrate how mechanical anisotropy has a profound  
38 effect on developing structures, such as crenulation cleavages, porphyroblast  
39 geometry and the initiation of shear bands and shear zones.

40

## 41 **1. Introduction**

42

43 Structural geologists have used a range of structures to determine deformation  
44 histories of rocks (e.g. Treagus, 1982; Ramsay and Huber, 1987; Hudleston and  
45 Lan, 1993; Passchier and Trouw, 2005). Many of these structures, such as folds  
46 and structures around rigid objects (i.e. porphyroclasts and porphyroblasts) are  
47 controlled by contrasts in the mechanical properties of the different minerals  
48 involved. These structures are therefore typically treated as inclusion-matrix  
49 (IM) systems, with typically a stronger inclusion phase (porphyroclasts, boudins,  
50 folding layers) embedded in a softer matrix.

51 To improve and quantify the interpretation of structures observed in the  
52 field, geologists have developed increasingly complex models for IM systems.  
53 Initially these were based on pioneering analytical models, such as those by  
54 Jeffery (1922), Eshelby (1957) and Ramberg (1962) for rotation of elliptical  
55 inclusions and Biot (1961) for folding of a single layer in a softer matrix. Taylor  
56 (1938) recognised the importance of the anisotropy of crystal plasticity to the  
57 development of crystallographic preferred orientations, and Kamb (1972) first  
58 explained how this could modify dynamic recrystallization in ice. The 40-year  
59 history of the *Journal of Structural Geology* has seen the advent and blossoming  
60 of numerical modelling to simulate a range of IM structures, thus helping  
61 geologists to understand how they form. Since the earliest computer simulations,  
62 models have steadily increased in sophistication and resolution. Early computers  
63 were usually restricted to linear, Newtonian rheology (e.g. Dieterich, 1970). Non-  
64 linear rheology, assumed common in rocks (Kirby, 1983; Carter and Tsenn,  
65 1987), has now become a standard ingredient in models (Hudleston and Lan,  
66 1994; Bons et al., 1997; Jessell et al., 2009; Mancktelow, 1999; 2011; Schmalholz

67 and Maeder, 2012; Llorens et al., 2013a; Gardner et al. 2017). Boundary  
68 conditions in early models were usually restricted to pure shear conditions.  
69 However, many natural high-strain structures of interest typically develop in  
70 mylonites that deform close to simple shear (e.g. Passchier and Trouw, 2005;  
71 Gomez-Rivas et al., 2007). Simple shear deformation was therefore already  
72 applied to these IM systems early on (Jezek, 1994; Bons et al. 1997), but, for  
73 example, systematic modelling of folding in simple shear started much later  
74 (Viola and Mancktelow, 2005; Llorens et al., 2013a,b). The steadily increasing  
75 calculation speed of computers has allowed modellers to reach ever-higher finite  
76 strains (e.g. Schmalholz et al., 2001; Jessell et al., 2009; Dabrowski and Schmid,  
77 2011; Dabrowski et al., 2012; Grasemann and Dabrowski, 2015). Additional  
78 factors and processes, such as shear heating, strain softening, slipping phase  
79 boundaries, grain-size effects, etc. have also been incorporated in models  
80 (Schmalholz and Podladchikov, 1999; Marques et al., 2005a,b, 2014; Schmalholz,  
81 2006; Hobbs et al., 2008; Mancktelow, 2013; Montagnat et al., 2014; Gardner et  
82 al., 2017, among others).

83         Despite the enormous progress in IM-system modelling, there seems to be  
84 one elephant left in the room that is still commonly overlooked or ignored in  
85 these numerical models: anisotropy. Many material properties are known to be  
86 highly anisotropic in rocks and minerals, including magnetism, thermal  
87 expansion, elasticity, surface energy and mineral slip system activity. Early  
88 numerical simulations studies recognised the importance of mechanical  
89 anisotropy to the production of crystallographic preferred orientations in rocks  
90 (Taylor, 1938; Kröner, 1961; Etchecopar, 1977; Lister et al., 1978), and these  
91 have also been shown to be significant in the formation of larger-scale geological  
92 structures. For example, a field geologist would probably interpret the structure  
93 in Fig. 1a as follows (Druguet et al., 1997): the rock is a foliated biotite schist  
94 with a first foliation  $S_1$  formed by aligned biotite grains. The foliated schist and a  
95 younger quartz vein were then deformed in a second event ( $D_2$ ), which led to  
96 buckle folds in the vein and the formation of an axial-planar crenulation cleavage  
97 ( $S_2$ ) in the schist. The quartz vein folds are comparable with those in numerical  
98 simulations and these folds from Cap de Creus (Spain) have indeed been used to  
99 compare with and validate numerical models (Llorens et al., 2013a,b). However,

100 folds in the matrix look completely different. Whereas the quartz vein forms  
101 approximately parallel buckle folds, the crenulations in the schist are closer to  
102 similar folds (Fig. 1a). Structural geologists are aware that this is because the  
103 schist already has a distinct  $S_1$ -foliation, and is, therefore, strongly anisotropic.  
104 Although the importance of anisotropy for folding is known for decades (e.g.  
105 Baily, 1970; Cobbold et al., 1971; Fletcher, 1974; Watkinson, 1983; Weijermars,  
106 1992; Zhang et al., 1993), most numerical simulations have been of buckle folds  
107 in isotropic matrices (see Hudleston and Treagus (2010) for a review), with  
108 relatively few exceptions, mostly dealing with chevron folds (Mühlhaus et al.,  
109 2002; Kocher et al., 2006, 2008; Jansen et al., 2016; Schmalholz and Mancktelow,  
110 2016). This example illustrates clearly that mechanical anisotropy needs to be  
111 taken into account when realistically modelling geological structures. Below we  
112 give examples of incorporating the effect of mechanical anisotropy in simulations  
113 of folding,  $\sigma$ -/ $\delta$ -clast formation and shear localisation.

114 In the following section, we present a numerical method that allows  
115 geologists to assess the influence of anisotropy in the development of geological  
116 structures. This is followed by a number of examples of models highlighting the  
117 fact that anisotropy of material properties may be one of the “missing” keys to  
118 understand geological structures, holding much promise for future  
119 investigations.

120

## 121 **2. The full-field crystal plasticity approach**

122 At the grain scale, the crystal structure results in anisotropic behaviour of many  
123 physical properties. This is particularly relevant for viscous deformation  
124 accommodated by dislocation glide along particular slip systems (Frost and  
125 Ashby, 1983). Montagnat et al. (2014) provide an example of the many  
126 approaches that have been applied to model single- and polycrystal deformation  
127 of the mechanically highly anisotropic mineral ice Ih. Here, our simulations of  
128 polycrystalline aggregates with intrinsic anisotropy (i.e. anisotropy well  
129 developed at all scales) are based on the full-field VPFFT crystal plasticity code  
130 (Lebensohn, 2001), which calculates the viscoplastic deformation for a  
131 polycrystalline aggregate using a Fast Fourier Transform-based numerical solver.  
132 The VPFFT code solves the micromechanical problem by finding the strain rate

133 and stress fields that minimize the average local work-rate satisfying the  
134 constitutive relation at local level, under the constraints of strain compatibility  
135 and stress equilibrium (see Lebensohn (2001), Lebensohn et al. (2008; 2009)  
136 and Montagnat et al. (2014) for a more detailed description of the theoretical  
137 framework and the numerical algorithm, and Griera et al. (2013) and Llorens et  
138 al. (2016a,b) for the coupling with the ELLE microstructural simulation  
139 platform).

140 In geology the coupling of the full-field crystal plasticity VPFFT  
141 (Viscoplastic Full-Field Transform) method by Lebensohn (2001), Lebensohn et  
142 al. (2008) and the ELLE microstructural simulation platform (Jessell et al., 2001;  
143 Bons et al., 2008; Piaolo et al. 2010; <http://www.elle.ws>) has allowed the  
144 systematic simulation of deformation and recrystallization of polycrystalline  
145 rocks (such as ice and halite, e.g. Griera et al., 2011; 2013; Llorens et al., 2016a,b;  
146 2017; Steinbach et al., 2016, 2017; Gomez-Rivas et al., 2017). In these cases, the  
147 polycrystalline aggregate is discretised into a periodic, regular mesh of nodes  
148 that store properties such as lattice orientation and dislocation density. These  
149 nodes act as Fourier Points in the VPFFT code and as unconnected nodes  
150 (*unodes*) in ELLE routines. Therefore, the integration between VPFFT and ELLE  
151 is based on the direct one-to-one mapping between the data structures of the  
152 two approaches. It is important to note that the VPFFT method is essentially  
153 scale independent and can therefore be used to simulate geological structures  
154 that have an inherent mechanical anisotropy ranging from small-scale (e.g. shear  
155 sense indicators, grain scale stress heterogeneities) to large-scale features (e.g.  
156 layers with contrasting rheology).

157 Here, we present a number of examples utilizing the VPFFT-ELLE method.  
158 In these examples the mechanical properties of the polycrystal are simulated  
159 assuming a "numerical mineral" with hexagonal symmetry, as was used by  
160 Griera et al. (2011; 2013) to model porphyroclast/-blast systems. With this  
161 symmetry, deformation is allowed to be accommodated by glide on the basal  
162 plane (basal slip) and along non-basal planes (pyramidal and prismatic slip). In  
163 this approach the grain anisotropy parameter ( $A$ ) that accounts for the degree of  
164 anisotropy is defined as the ratio of the critical resolved stresses ( $\tau_{cr}$ ) of the non-  
165 basal basal and basal slip systems (e.g. Lebensohn et al., 2009).  $A$  is comparable

166 to the ratio between normal and shear viscosity as employed by e.g. Mühlhaus  
167 (2002) and Kocher et al. (2006, 2008). For all examples, a stress exponent of  $n=3$   
168 is assumed for all slip systems.

169

### 170 **3. Examples**

171

172 In the following, examples we contrast the effect of different material behaviour  
173 in terms of anisotropy on the characteristics of developing geological structures  
174 during deformation.

175

#### 176 *3.1. Single layer folding: The effect of matrix anisotropy*

177

178 In our example, we first show deformation of a layer embedded in an isotropic  
179 matrix, using a non-linear viscous finite element method (BASIL, Houseman et al.,  
180 2008) within ELLE (Fig. 1b-c). BASIL is a finite element deformation module that  
181 simulates viscous deformation of a 2D sheet in plane-strain. BASIL can be  
182 coupled within ELLE in order to calculate the viscous strain rates and the  
183 associated stress field for different boundary conditions (i.e. from pure to simple  
184 shear). The grid of regularly spaced unconnected nodes (*unodes*) is used to track  
185 the deformation history and deformation field through passive lines initially  
186 parallel to the folding layer. ELLE uses both horizontally and vertically wrapping  
187 boundaries, allowing the model to be periodic in all directions. This approach  
188 reduces detrimental boundary effects and simplifies visualisation of the model at  
189 very high strains. See Jessell et al. (2005), Bons et al. (2008), and Jessell et al.  
190 (2009) for details about BASIL and ELLE.

191 In our simulations, we assigned homogeneous rheological properties to  
192 the polygons (Fig. 1b-c) that define the layer and matrix. With no variation in  
193 properties within the material, perturbations in the layer surface are critical for  
194 the resulting folds (Mancktelow, 1999; Zhang et al., 2000). Small variations in  
195 layer thickness were therefore introduced to initiate folding, as in Llorens et al.  
196 (2013a,b).

197            Figures 1b and 1c show the results for folding a single layer in simple and  
198 in pure shear, respectively. In BASIL, the rheology is defined by a power-law of  
199 the type:

$$200 \quad \dot{\epsilon} = \sigma^n / B, \quad (1)$$

201 with  $\dot{\epsilon}$  the strain rate and  $\sigma$  the differential stress. The competence contrast  
202 between layer and matrix is defined here by the ratio of  $B_{layer}/B_{matrix}$ , set to 50  
203 here (Table 1). Passive grid lines, originally parallel to the competent layer, show  
204 the deformation within the matrix. Folding decreases in intensity away from the  
205 "zone of contact strain" (Ramberg, 1962) near the layer, and strain is  
206 approximately homogeneous at the lateral edges of the model.

207            In Fig. 1d-e, we present two numerical simulations of single competent  
208 layer folding in an anisotropic matrix using the VPFFT-ELLE code with power-  
209 law rheology. Initially, the basal slip plane of grains (individual square elements  
210 in the 256x256 element model) in the matrix were aligned approximately  
211 parallel to the layer. Therefore, starting models can be regarded as representing  
212 a foliated or mica-rich rock with anisotropy. The noise to initiate folding now  
213 derives from the small random variations in lattice orientation in the layer and  
214 matrix. The competent layer was set to be isotropic, with a  $\tau_{cr}$  five times higher  
215 than the non-basal slip systems of the matrix. Their  $\tau_{cr}$  in turn was set at 20 times  
216 that of the basal slip system, giving an anisotropy factor  $A$  of 20 (Table 1). Under  
217 pure and simple shear, the geometry of the folded single layer in the anisotropic  
218 matrix is similar to that in isotropic matrix (Fig. 1b-c). However, the geometry of  
219 microfolds represented by passive gridlines in the anisotropic matrix is very  
220 different from those in isotropic cases. The grid lines are folded in similar-type  
221 folds or crenulations that do not decay away from the competent layer (similar  
222 to results obtained by Kocher et al., 2006). Fold hinges align to form an axial-  
223 planar crenulation cleavage. The resulting geometry is similar to that of the  
224 natural example (Fig. 1a), with the passive gridlines representing  $S_1$  and the  
225 crenulation cleavage  $S_2$ .

226

227 *3.2. Mantled porphyroclasts:  $\delta$ - or  $\sigma$ -clasts?*

228

229  $\sigma$ - and  $\delta$ -clasts, or more general mantled porphyroclasts are extremely useful  
230 shear-sense indicators (Passchier and Simpson, 1986; Hanmer and Passchier,  
231 1991; Grasemann and Dabrowski, 2015). These typically consist of a core  
232 porphyroclast with wings or tails of recrystallised material. Most studies  
233 addressed the rotation rate of isolated competent inclusions during deformation  
234 as a function of factors such as the object shape, stress exponent, and slipping  
235 object-matrix boundaries (e.g. Ghosh and Ramberg, 1976; Bons et al., 1997;  
236 Mandal et al., 2000; ten Grotenhuis et al., 2002; Schmid and Podladchikov, 2005;  
237 Fay et al., 2008; Dabrowski and Schmid, 2011; Griera et al., 2011, 2013;  
238 Mancktelow, 2011, 2013; Jiang, 2016). Although the role of anisotropy was  
239 recognised early on (e.g. Passchier et al., 1992), only Dabrowski and Schmid  
240 (2011) and Griera et al. (2011; 2013) actually included anisotropic flow  
241 properties in their numerical models. Main outcomes of these studies are that  
242 the rotation rate and the strain field around an object are affected by anisotropy.

243         With a strong emphasis on the ongoing rotation versus non-rotation of  
244 porphyroblasts debate (Bell et al., 1992; Passchier et al., 1992), little attention has  
245 been given to the question what causes mantles porphyroclasts to either form  $\delta$   
246 or  $\sigma$  geometries. The main model is that this depends on the weakness of the  
247 mantle (or slipping interface) and its thickness relative to the size of the central  
248 object, with thick mantles forming  $\sigma$ -clasts and thin ones  $\delta$ -clasts (Passchier and  
249 Sokoutis, 1993; and review of Marques et al., 2014). Bons et al. (1997) already  
250 suggested that anisotropy of the matrix would inhibit rotation, leading to the  
251 formation of  $\sigma$ -clasts. Here we show an example of the effect of anisotropy on the  
252 developing shape of a mantled porphyroclast, again using the VPFFT-ELLE code.

253         In the isotropic case (all slip systems of one phase have the same  $\tau_{cr}$ ; Table  
254 1), the core object's  $\tau_{cr}$  was set at 50x that of the matrix, while that of the mantle  
255 was 0.8x that of the matrix. Deformation is homogeneous in case of an isotropic  
256 mantle and the central object rotates at a rate close to the analytical solution of  
257 Jeffery (1922) (Griera et al., 2011; 2013) (Fig. 2a). Wings develop by smearing  
258 out of the mantle and as the points where the wings attach to the object rotate  
259 along with the object, a  $\delta$ -clast develops (Fig. 2a). When the mantle is distinctly  
260 softer ( $\tau_{cr}=4$ ) than the object ( $\tau_{cr}=50$ ), and the matrix is anisotropic ( $A=10$ , with



261  $\tau_{cr}=1$  for the basal slip system and  $\tau_{cr}=10$  for non-basal slip systems),  
262 deformation in the matrix is highly heterogeneous and folds and shear bands  
263 develop (Griera et al., 2011; 2013). Rotation of the object is now inhibited  
264 (contrary to the analytical model of Fletcher, 2009) and the attachment points of  
265 the wings do not rotate enough to develop the distinct embayments of  $\delta$ -clasts  
266 (Fig. 2b). Instead, a  $\sigma$ -clast forms.

267         These results confirm the observations of Griera et al (2013) that the  
268 incorporation of anisotropy provides an elegant way to explain controversies in  
269 structural geology regarding the duality between rotation or non-rotation of  
270 porphyroblasts (Bell et al., 1992; Passchier et al., 1992). Spiral geometries of  
271 inclusions preferentially develop in isotropic conditions, while an increase in  
272 anisotropy tends to reduce rotation of porphyroblasts of which the inclusion  
273 trails then indicate growth over a crenulated matrix.

274

### 275 *3.3. Shear bands in composite materials*

276

277 Structures in natural and modelled shear zones are determined in part by the  
278 strength contrast between minerals and slip systems within minerals. Weak  
279 minerals define the foliation (S-surface) at  $45^\circ$  from the shear zone boundary,  
280 and planes progressively rotate into parallelism with the shear zone boundary  
281 and the C-surface (Fig. 3a). Less well understood is the development of C' shear  
282 bands (fig. 3a), despite their ubiquity in shear zones in nature, experiments, and  
283 models (White, 1979; Platt and Vissers, 1980; Platt, 1984; Dennis and Secor,  
284 1987). C' shear bands dip at an angle of  $\sim 15\text{--}35^\circ$  from the shear zone boundary,  
285 in the opposite direction to the main foliation (or S plane; White, 1979; Platt and  
286 Vissers, 1980) and show synthetic, normal shear sense (Fig. 3a). They are most  
287 common in well-foliated rocks such as schists and phyllites (Passchier, 1991;  
288 Delle Piane et al., 2009) and so it has been suggested that anisotropy is required  
289 for their development (Wilson, 1984; Goodwin and Tikoff, 2002).

290         We used VPFFT-ELLE to model the development of C' shear bands in  
291 anisotropic materials, building on the work of Jessell et al. (2009) by testing the  
292 proportion of weak phase required for the development of C' shear bands in  
293 three-phase models and by introducing anisotropy to the crystallography of the

294 weakest phase. The model shown (Fig. 3b) included a strong, intermediate, and a  
295 weak phase, the latter of which had a basal plane ten times weaker than  
296 prismatic and pyramidal planes (i.e.  $A=10$ ). We found that C' shear bands formed  
297 in all models with  $>1\%$  weak phase and were more abundant in models with a  
298 higher proportion of weak phase. In nature (Fig. 3a) and in models (Fig. 3b) C'  
299 shear bands are dominantly defined by the weakest phase.

300

### 301 *3.4. Shear localisation*

302

303 Shear localisation develops at almost all scales in ductile rocks. For example, the  
304 shear zones in Cap de Creus (NE Spain) are linked in an anastomosing  
305 framework with self-similar properties, where a pre-existing foliation in the  
306 metasediments have led to instabilities, forming shear zones at a wide range of  
307 scales (Druguet et al., 1997; Carreras, 2001; Fousseis et al., 2006; Schrank et al.,  
308 2008). In polar ice sheet dynamics, the behaviour of large ice masses is strongly  
309 influenced by visco-plastic anisotropy of grains and their ability to form a lattice  
310 preferred orientation (LPO) by lattice rotation (Azuma and Higashi, 1985; Alley,  
311 1988). The flow of glaciers and polar ice sheets is controlled by the highly  
312 anisotropic rheology of Ice Ih crystals (Azuma, 1994; Bons et al., 2016; Llorens et  
313 al., 2016a,b; Llorens et al., 2017), which may lead to high strain zones in the  
314 glaciers and polar ice sheets (Marmo and Wilson, 1998) and folding (Bons et al.,  
315 2016; Jansen et al., 2016).

316 To show how anisotropy (defined by the parameter  $A$ ) affects localisation,  
317 we simulate the deformation of a pure, single-phase polycrystal in dextral simple  
318 shear (Fig. 4) up to a shear strain of 1.5 with VPFIT-ELLE described above. Basal  
319 planes were initially randomly oriented. Strain localisation occurs only in  
320 anisotropic cases ( $A>1$ ), as can be seen by the passive deformation of the  
321 polygon boundaries that originally had a foam texture (Fig. 4a) and the map of  
322 the normalised Von Mises strain rate field (Fig. 4b). High strain-rate bands  
323 oriented at a low angle to the horizontal shear plane are clearly visible (Fig. 4a  
324 and b), especially at high anisotropy values ( $A>>1$ ).

325 The frequency distribution of normalised strain rates, at a shear strain of  
326 three, in the isotropic material ( $A=1$ ) is approximately normal (Fig. 4c).

327 Simulations with  $A > 1$  show frequency distribution that deviate from normal  
328 distribution (Fig. 4c) and are closer to log-normal. However, they are not exactly  
329 log-normal, as they become heavy tailed for large strain-rate values. Higher  
330 strain rate values become overrepresented with values up to 20 times the mean  
331 for  $A=20$ . Therefore, a material with a higher degree of anisotropy will reach  
332 significantly higher strain rate values due to strain localisation. As a result, most  
333 of the material deforms at a significantly lower rate than the mean strain rate, as  
334 can be seen by the leftward shift of the frequency peak in Fig. 4c.

335

#### 336 **4. Discussion and conclusions**

337

338 The examples described in previous sections provide a brief glimpse into the  
339 effect of intrinsic mechanical anisotropy (Griera et al. 2013) on deformation  
340 structures in rocks. In all cases, anisotropy caused heterogeneous strain:  
341 expressed in the axial planar crenulation cleavage in Fig. 1d-e; folds and shear  
342 bands in the matrix of the  $\sigma$ -clast in Fig. 2b; and shear bands in shearing  
343 multiphase (Fig. 3) and single-phase (Fig. 4) models. The strain localisation may  
344 be the most interesting aspect here. Processes such as shear heating and grain-  
345 size reduction have been considered in detail as causes for strain localisation  
346 (Tullis and Yund, 1985; Braun et al., 1999; de Bresser et al., 2001; Bercovici,  
347 2003; Jessell et al., 2005; Kaus and Podladchikov, 2006; Platt and Behr, 2011;  
348 Montési 2013). Mechanical anisotropy may be of equal importance, leading to  
349 shear zones from the grain scale (Fig. 3) to possibly continental sutures, similar  
350 to the damage model of Bercovice (2014).

351 In this paper we have used the VPFFT+ELLE numerical code to illustrate  
352 the effect of intrinsic mechanical anisotropy. We do not claim that this is the only  
353 available approach. We use this anniversary issue to encourage structural  
354 geologists to develop more analytical and numerical models to finally elucidate  
355 the role of mechanical anisotropy on all scales.

356

#### 357 **Acknowledgments**

358

359 HR acknowledges financial support by the China Scholarship Council (CSC; grant  
360 nr. 201506400014). EGR acknowledges the support of the Beatriu de Pinós  
361 programme of the Government of Catalonia's Secretariat for Universities and  
362 Research of the Department of Economy and Knowledge (2016 BP 00208). We  
363 thank Bruce Hobbs and an anonymous reviewer for their suggestions to improve  
364 this article.

365

366

## 367 **References**

368

369 Alley, R.B., 1988. Fabrics in polar ice sheets: development and prediction. *Science*  
370 240, 493-495.

371 Azuma, N., 1994. A flow law for anisotropic ice and its application to ice sheets.  
372 *Earth and Planetary Science Letters* 128, 601-614.

373 Azuma, N. Higashi, A., 1985. Formation processes of ice fabric pattern in ice  
374 sheets. *Annals of Glaciology* 6, 130-134.

375 Bayly, M.B., 1970. Viscosity and anisotropy estimates from measurements on  
376 chevron folds. *Tectonophysics* 9, 459-474.

377 Bell, T.H., Johnson, S.E., Davis, B., Forde, A., Hayward, N., Wilkins, C., 1992.  
378 Porphyroblast inclusion-trail orientation data: eppure-non-son-girate.  
379 *Journal of Metamorphic Geology* 10, 295-307.

380 Bercovici, D., 2003. The generation of plate tectonics from mantle convection.  
381 *Earth and Planetary Science Letters* 205, 107-121.

382 Bercovici, D., 2014. Plate tectonics, damage and inheritance. *Nature* 508, 513–  
383 516.

384 Biot, M.A., 1961. Theory of folding of stratified viscoelastic media and its  
385 implication in tectonics and orogenesis. *Geological Society of America*  
386 *Bulletin* 72, 1595-1632.

387 Bons, P.D., Barr, T.D., ten Brink, C.E., 1997. The development of delta-clasts in  
388 non-linear viscous materials: a numerical approach. *Tectonophysics* 270,  
389 29-41.

390 Bons, P.D., Koehn, D., Jessell, M.W. (Eds.), 2008. Microdynamics simulation. In:  
391 *Lecture Notes in Earth Science* 106. Springer, Berlin.

- 392 Bons, P.D., Jansen, D., Mundel, F., Bauer, C.C., Binder, T., Eisen, O., Jessell, M.W.,  
393 Llorens, M.-G., Steinbach, F., Steinhage, D., Weikusat, I., 2016. Converging  
394 flow and anisotropy cause large-scale folding in Greenland ice sheet.  
395 Nature Communications 7, doi: 10.1038/ncomms11427.
- 396 Braun, J., Chery, J., Poliakov, A., Mainprice, D., Vauchez, A., Tommasi, A.,  
397 Daignieres, M., 1999. A simple parameterization of strain localization in  
398 the ductile regime due to grain size reduction: a case study for olivine.  
399 Journal of Geophysical Research 104, 25167-25181.
- 400 Carreras, J., 2001. Zooming on Northern Cap de Creus shear zones. Journal of  
401 Structural Geology 23, 1457-1486.
- 402 Carter, N.L., Tsenn, M.C., 1987. Flow properties of the continental lithosphere.  
403 Tectonophysics 136, 27-63.
- 404 Cobbold, P.R., Cosgrove, J.W., Summers, J.M., 1971. Development of internal  
405 structures in deformed anisotropic rocks. Tectonophysics 12, 23-53.
- 406 Dabrowski, M., Schmid, D.W., 2011. A rigid circular inclusion in an anisotropic  
407 host subject to simple shear. Journal of Structural Geology 33, 1169-1177.
- 408 Dabrowski, M., Schmid, D.W., Podladchikov, Y.Y., 2012. A two-phase composite in  
409 simple shear: Effective mechanical anisotropy development and  
410 localization potential. Journal of Geophysical Research 117, B08406, doi:  
411 10.1029/2012JB009183.
- 412 de Bresser, J.H.P., ter Heege, J.H., Spiers, C.J., 2001. Grain size reduction by  
413 dynamic recrystallization: can it result in major rheological weakening?  
414 International Journal of Earth Sciences 90, 28-45.
- 415 Delle Piane, C., Wilson, C.J.L., Burlini, L., 2009. Dilatant plasticity in high-strain  
416 experiments on calcite–muscovite aggregates. Journal of Structural  
417 Geology 31, 1084-1099.
- 418 Dennis, A.J., Secor, D.T., 1987. A model for the development of crenulations in  
419 shear zones with applications from the Southern Appalachian Piedmont.  
420 Journal of Structural Geology 9, 809-817.
- 421 Dieterich, J.H., 1970. Computer experiments on mechanics of finite-amplitude  
422 folds. Canadian Journal of Earth Sciences 7, 467-476.

- 423 Druguet, E., Passchier, C.W., Carreras, J., Victor, P., den Brok, S.W.J., 1997. Analysis  
424 of a complex high-strain zone at Cap de Creus, Spain. *Tectonophysics* 280,  
425 31–45.
- 426 Eshelby, J.D., 1957. The determination of the elastic field of an ellipsoidal  
427 inclusion and related problems. *Proceedings of the Royal Society of*  
428 *London Series A* 241, 376-396.
- 429 Etchecopar, A., 1977. A plane kinematic model of progressive deformation in a  
430 polycrystalline aggregate. *Tectonophysics* 39, 121-139.
- 431 Fay, C., Bell, T.H., Hobbs, B.E., 2008, Porphyroblast rotation versus nonrotation:  
432 Conflict resolution! *Geology* 36, 307–310.
- 433 Fletcher, R.C., 1974. Wavelength selection in the folding of a single layer with  
434 power-law rheology. *American Journal of Science* 274, 1029-1043.
- 435 Fletcher, R.C., 2009. Deformable, rigid, and inviscid elliptical inclusions in a  
436 homogeneous incompressible anisotropic viscous fluid. *Journal of*  
437 *Structural Geology* 31, 382-387.
- 438 Frost, H.J., Ashby, M.F., 1983. *Deformation-Mechanism Maps: the Plasticity and*  
439 *Creep of Metals and Ceramics*. Pergamon, Oxford.
- 440 Fousseis, F., Handy, M. R., Schrank, C., 2006. Networking of shear zones at the  
441 brittle-to-viscous transition (Cap de Creus, NE Spain). *Journal of*  
442 *Structural Geology* 28, 1228-1243.
- 443 Gardner, R., Piazzolo, S., Evans, L., Daczko, N., 2017. Patterns of strain localization  
444 in heterogeneous, polycrystalline rocks – a numerical perspective. *Earth*  
445 *and Planetary Science Letters* 463, 253-265.
- 446 Ghosh, S.K., Ramberg, H., 1976. Reorientation of inclusions by combination of  
447 pure and simple shear. *Tectonophysics* 34, 1-70.
- 448 Gomez-Rivas, E., Bons, P.D., Griera, A., Carreras, J., Druguet, E. Evans, L., 2007.  
449 Strain and vorticity analysis using small-scale faults and associated drag  
450 folds. *Journal of Structural Geology* 29, 1882-1899.
- 451 Gomez-Rivas, E., Griera, A., Llorens, M.-G., Bons, P. D., Lebensohn, R. A., Piazzolo, S.,  
452 2017. Subgrain rotation recrystallization during shearing: Insights from  
453 full-field numerical simulations of halite polycrystals. *Journal of*  
454 *Geophysical Research: Solid Earth* 122, doi: 10.1002/2017JB014508.

- 455 Goodwin, L.B., Tikoff, B., 2002. Competency contrast, kinematics, and the  
456 development of foliations and lineations in the crust. *Journal of Structural*  
457 *Geology* 24, 1065-1085.
- 458 Grasemann, B., Dabrowski, M., 2015. Winged inclusions: Pinch-and-swell objects  
459 during high-strain simple shear. *Journal of Structural Geology* 70, 78-94.
- 460 Griera, A., Bons, P.D., Jessell, M.W., Lebensohn, R.A., Evans, L., Gomez-Rivas, E.,  
461 2011. Strain localization and porphyroclast rotation. *Geology* 39, 275-278.
- 462 Griera, A., Llorens, M.-G., Gomez-Rivas, E., Bons, P.D., Jessell, M.W., Evans, L.A.,  
463 Lebensohn, R., 2013. Numerical modelling of porphyroclast and  
464 porphyroblast rotation in anisotropic rocks. *Tectonophysics* 587, 4-29.
- 465 Hanmer, S., Passchier, C.W., 1991. Shear sense indicators: a review. *Geological*  
466 *Survey of Canada* 90, 1-71.
- 467 Hobbs, B., Regenauer-Lieb, K., Ord, A., 2008. Folding with thermal-mechanical  
468 feedback. *Journal of Structural Geology* 30, 1572-1592.
- 469 Houseman, G., Barr, T., Evans, L., 2008. Basil: stress and deformation in a viscous  
470 material. In: Bons, P.D., Koehn, D., Jessell, M.W. (Eds.), *Microdynamics*  
471 *Simulation*. In: *Lecture Notes in Earth Sciences* 106. Springer, Berlin.
- 472 Hudleston, P.J., Lan, L., 1993. Information from fold shapes. *Journal of Structural*  
473 *Geology* 15, 253-264.
- 474 Hudleston, P.J., Lan, L.B., 1994. Rheological control on the shapes of single-layer  
475 folds. *Journal of Structural Geology* 16, 1007-1021.
- 476 Hudleston, P.J., Treagus, S.H., 2010. Information from folds: A review. *Journal of*  
477 *Structural Geology* 32, 2042-2071.
- 478 Jansen, D., Llorens, M.-G, Westhoff, J., Steinbach, F., Kipfstuhl, S., Bons, P.D., Griera,  
479 A., Weikusat, I., 2016. Small-scale disturbances in the stratigraphy of the  
480 NEEM ice core: observations and numerical model simulations. *The*  
481 *Cryosphere* 10, 359-370.
- 482 Jeffery, G.B., 1922. The motion of ellipsoidal particles immersed in a viscous fluid.  
483 *Proceedings of the Royal Society of London Series A* 102, 161-179.
- 484 Jessell, M., Bons, P.D., Evans, L., Barr, T., Stüwe, K., 2001. Elle: the numerical  
485 simulation of metamorphic and deformation microstructures. *Computers*  
486 *& Geosciences* 27, 17-30.

- 487 Jessell, M.W., Siebert, E., Bons, P.D., Evans, L., Piazzolo, S., 2005. A new type of  
488 numerical experiment on the spatial and temporal patterns of localization  
489 of deformation in a material with a coupling of grain size and rheology.  
490 Earth and Planetary Science Letters 239, 309-326.
- 491 Jessell, M.W., Bons, P.D., Griera, A., Evans, L.A., Wilson, C.J.L., 2009. A tale of two  
492 viscosities. Journal of Structural Geology 31, 719-736.
- 493 Jezek, J., 1994. Software for modeling the motion of rigid triaxial ellipsoidal  
494 particles in viscous-flow. Computers & Geosciences 20, 409-424.
- 495 Jiang, D. 2016. Viscous inclusions in anisotropic materials: Theoretical  
496 development and perspective applications. Tectonophysics 693, 116-142.
- 497 Kamb, W. B. 1972. Experimental recrystallization of ice under stress. American  
498 Geophysical Union Monograph 16, 221-241.
- 499 Kaus, B.K.P., Podladchikov, Y.Y., 2006. Initiation of localized shear zones in  
500 viscoplastic rocks. Journal of Geophysical Research 111, B04412, doi :  
501 10.1029/2005JB003652.
- 502 Kirby, S.H., 1983. Rheology of the lithosphere. Reviews of Geophysics and Space  
503 Physics 21, 1458-1487.
- 504 Kocher, T., Schmalholz, S.M., Mancktelow, N.S., 2006. Impact of mechanical  
505 anisotropy and power-law rheology on single layer folding.  
506 Tectonophysics 421, 71-87.
- 507 Kocher, T., Mancktelow, N.S., Schmalholz, S.M., 2008. Numerical modelling of the  
508 effect of matrix anisotropy orientation on single layer fold development.  
509 Journal of Structural Geology 30, 1013-1023.
- 510 Kröner, E. 1961. On the plastic deformation of polycrystals. Acta Metallurgica 9,  
511 155-161.
- 512 Lebensohn, R.A., 2001. N-site modelling of a 3D viscoplastic polycrystal using fast  
513 Fourier transform. Acta Materialia 49, 2723-2737.
- 514 Lebensohn, R.A., Brenner, R., Castelnau, O., Rollett, A.D., 2008. Orientation image-  
515 based micromechanical modelling of subgrain texture evolution in  
516 polycrystalline copper. Acta Materialia 56, 3914-3926.
- 517 Lebensohn, R.A., Montagnat, M., Mansuy, P., Duval, P., Meysonnier, J., Philip, A.,  
518 2009. Modeling viscoplastic behavior and heterogenous intracrystalline  
519 deformation of columnar ice polycrystals. Acta Materialia 57, 1405-1415.



- 520 Lister, G.S., Paterson, M.S., Hobbs, B.E., 1978. The simulation of fabric  
521 development during plastic deformation and its application to quartzite:  
522 the model. *Tectonophysics* 45, 107-158.
- 523 Llorens, M.-G., Bons, P.D., Griera, A., Gomez-Rivas, E., 2013a. When do folds  
524 unfold during progressive shearing? *Geology* 41, 563-566.
- 525 Llorens, M.-G., Bons, P.D., Griera, A., Gomez-Rivas, E., 2013b. Single layer folding  
526 in simple shear. *Journal of Structural Geology* 50, 209-220.
- 527 Llorens, G.-M., Griera, A., Bons, P.D., Lebensohn, R.A., Evans, L.A., Jansen, D.,  
528 Weikusat, I. 2016a. Full-field predictions of ice dynamic recrystallisation  
529 under simple shear conditions. *Earth and Planetary Science Letters* 450,  
530 233-242.
- 531 Llorens, G.-M., Griera, A., Weikusat, I., Bons, P.D., Roessiger, J., Lebensohn, R.A.  
532 2016b. Dynamic recrystallisation of ice aggregates during co-axial  
533 viscoplastic deformation: a numerical approach. *Journal of Glaciology* 62,  
534 359-377.
- 535 Llorens, M.-G., Griera, A., Steinbach, F., Bons, P.D., Gomez-Rivas, E., Jansen, D.,  
536 Roessiger, J., Lebensohn, R.A., Weikusat, I., 2017. Dynamic  
537 recrystallization during deformation of polycrystalline ice: insights from  
538 numerical simulations. *Philosophical Transactions Series A: Mathematical,*  
539 *physical, and engineering sciences* 375, 2086, doi:  
540 10.1098/rsta.2015.0346.
- 541 Mancktelow, N.S., 1999. Finite-element modelling of single-layer folding in  
542 elastoviscous materials; the effect of initial perturbation geometry.  
543 *Journal of Structural Geology* 21, 161-177.
- 544 Mancktelow, N.S., 2011. Deformation of an elliptical inclusion in two-dimensional  
545 incompressible power-law viscous flow. *Journal of Structural Geology* 33,  
546 1378-1393.
- 547 Mancktelow, N.S., 2013. Behaviour of an isolated rimmed elliptical inclusion in  
548 2D slow incompressible viscous flow. *Journal of Structural Geology* 46,  
549 235-254.
- 550 Mandal, N., Samanta, S.K., Chakraborty, C., 2000. Progressive development of  
551 mantle structures around elongate porphyroclasts: insights from  
552 numerical models. *Journal of Structural Geology* 22, 993-1008.

- 553 Marmo, B.A., Wilson, C.J., 1998. Strain localisation and incremental deformation  
554 within ice masses, Framnes Mountains, east Antarctica. *Journal of*  
555 *Structural Geology* 20, 149-162.
- 556 Marques, F.O., Taborda, R., Antunes, J., 2005a. Influence of a low-viscosity layer  
557 between rigid inclusion and viscous matrix on inclusion rotation and  
558 matrix flow: a numerical study. *Tectonophysics* 407, 101-115.
- 559 Marques, F.O., Taborda, R., Bose, S., Antunes, J., 2005b. Effects of confinement on  
560 matrix flow around a rigid inclusion in viscous simple shear: insights from  
561 analogue and numerical modelling. *Journal of Structural Geology* 27, 379-  
562 396.
- 563 Marques, F.O., Mandal, N., Taborda, R., Antunes, J.V., Bose, S., 2014. The behaviour  
564 of deformable and non-deformable inclusions in viscous flow. *Earth-*  
565 *Science Reviews* 134, 16-69.
- 566 Montagnat, M., Castelnau, O., Bons, P.D., Faria, S.H., Gagliardini, O., Gillet-Chaulet,  
567 F., Grennerat, F., Griera, A., Lebensohn, R.A., Moulinec, H., Roessiger, J.,  
568 Suquet, P., 2014. Multiscale modeling of ice deformation behavior. *Journal*  
569 *of Structural Geology* 61, 78-108.
- 570 Montési, L.G.J., 2013. Fabric development as the key for forming ductile shear  
571 zones and enabling plate tectonics. *Journal of Structural Geology* 50, 254-  
572 266.
- 573 Mühlhaus, H.-B., Moresi, L., Hobbs, B., Dufour, F., 2002. Large amplitude folding in  
574 finely layered viscoelastic rock structures. *Pure and Applied Geophysics*  
575 159, 2311-2333.
- 576 Passchier, C. W., 1991. The classification of dilatant flow types. *Journal of*  
577 *Structural Geology* 13, 101-104.
- 578 Passchier, C.W., Simpson, C., 1986. Porphyroclast systems as kinematic indicators.  
579 *Journal of Structural Geology* 8, 831-843.
- 580 Passchier, C.W., Sokoutis, D., 1993. Experimental modelling of mantle  
581 porphyroclasts. *Journal of Structural Geology* 15, 895-909.
- 582 Passchier, C.W., Trouw, R.A.J., 2005. *Deformation mechanisms. Microtectonics,*  
583 *Springer, Berlin.*
- 584 Passchier, C.W., Trouw, R.A.J., Zwart, H.J., Vissers, R.L.M., 1992. Porphyroblast  
585 rotation - Eppur-Si-Muove. *Journal of Metamorphic Geology* 10, 283-294.

- 586 Piazzolo, S., Jessell, M.W., Bons, P.D., Evans, L., Becker, J.K., 2010. Numerical  
587 simulations of microstructures using the Elle platform: A modern  
588 research and teaching tool. *Journal of the Geological Society of India* 75,  
589 110-127.
- 590 Platt, J.P., 1984. Secondary cleavages in ductile shear zones. *Journal of Structural*  
591 *Geology* 6, 439-442.
- 592 Platt, J.P., Vissers, R.L.M., 1980. Extensional structures in anisotropic rocks.  
593 *Journal of Structural Geology* 2, 397-410.
- 594 Platt, J.P., Behr, W.M., 2011. Grainsize evolution in ductile shear zones:  
595 Implications for strain localization and the strength of the lithosphere.  
596 *Journal of Structural Geology* 33, 537-550.
- 597 Ramberg, H., 1962. Contact strain and folding instability of a multilayered body  
598 under compression. *Geologische Rundschau* 51, 405-439.
- 599 Ramsay, J.G., Huber, M.I., 1987. *The Techniques of modern structural geology*, vol.  
600 2: *Folds and Fractures*. Academic Press, London.
- 601 Schmalholz, S.M., 2006. Finite amplitude folding of single layers: elastica,  
602 bifurcation and structural softening. *Philosophical Magazine* 86, 3393-  
603 3407.
- 604 Schmalholz, S.M., Maeder, X., 2012. Pinch-and-swell structure and shear zones in  
605 viscoplastic layers. *Journal of Structural Geology* 37, 75-88.
- 606 Schmalholz, S.M., Mancktelow, N.S., 2016. Folding and necking across the scales:  
607 a review of theoretical and experimental results and their applications.  
608 *Solid Earth* 7, 1417-1465.
- 609 Schmalholz, S.M., Podladchikov, Y., 1999. Buckling versus folding: Importance of  
610 viscoelasticity. *Geophysical Research Letters* 26, 2641-2644.
- 611 Schmalholz, S.M., Podladchikov, Y.Y., Schmid, D.W., 2001. A spectral/finite  
612 difference method for simulating large deformations of heterogeneous,  
613 viscoelastic materials. *Geophysical Journal International* 145, 199-208.
- 614 Schmid, D.W., Podladchikov, Y.Y., 2005. Mantled porphyroclast gauges. *Journal of*  
615 *Structural Geology* 27, 571-585.
- 616 Schrank, C.E., Handy, M.R., Füsseis, F., 2008. Multiscaling of shear zones and the  
617 evolution of the brittle-to-viscous transition in continental crust. *Journal*  
618 *of Geophysical Research: Solid Earth* 113, doi: 10.1029/2006JB004833.

- 619 Steinbach, F., Bons, P.D., Griera, A., Jansen, D., Llorens, M.-G., Roessiger, J.,  
620 Weikusat, I., 2016. Strain localisation and dynamic recrystallisation in the  
621 ice-air aggregate: A numerical study. *The Cryosphere* 10, 3071-3089.
- 622 Steinbach, F., Kuiper, E.J.N., Eichler, J., Bons, P.D., Drury, M.R., Griera, A., Pennock,  
623 G.M., Weikusat, I., 2017. The Relevance of Grain Dissection for Grain Size  
624 Reduction in Polar Ice: Insights from Numerical Models and Ice Core  
625 Microstructure Analysis. *Frontiers in Earth Science* 5, 66, doi:  
626 10.3389/feart.2017.00066.
- 627 Taylor, G.I., 1938. Plastic strain in metals. *J. Inst. Metals*, 62, 307-324.
- 628 ten Grotenhuis, S.M., Passchier, C.W., Bons, P.D., 2002. The influence of strain  
629 localisation on the rotation behaviour of rigid objects in experimental  
630 shear zones. *Journal of Structural Geology* 24, 485-499.
- 631 Treagus, S.H., 1982. A new isogon-cleavage classification and its application to  
632 natural and model fold studies. *Geological Journal* 17, 49-64.
- 633 Tullis, J., Yund, R.A., 1985. Dynamic recrystallization of feldspar: a mechanism for  
634 ductile shear zone formation. *Geology* 13, 238-241.
- 635 Viola, G., Mancktelow, N.S., 2005. From XY tracking to buckling: axial plane  
636 cleavage fanning and folding during progressive deformation. *Journal of*  
637 *Structural Geology* 27, 409-417.
- 638 Watkinson, A.J., 1983. Patterns of folding and strain influenced by linearly  
639 anisotropic bands. *Journal of Structural Geology* 5, 449-454.
- 640 Weijermars, R., 1992. Progressive deformation in anisotropic rocks. *Journal of*  
641 *Structural Geology* 14, 723-742.
- 642 White, S., 1979. Large strain deformation: report on a tectonic studies group  
643 discussion meeting held at Imperial College, London on 14 November  
644 1979. *Journal of Structural Geology* 1, 333-339.
- 645 Wilson, C.J.L., 1984. Shear bands, crenulations and differentiated layering in ice-  
646 mica models. *Journal of Structural Geology* 6, 303-319.
- 647 Zhang, Y., Hobbs, B.E., Jessell, M.W., 1993. Crystallographic preferred orientation  
648 development in a buckled single layer: a computer simulation. *Journal of*  
649 *Structural Geology* 15, 265-276.
- 650 Zhang, Y., Mancktelow, N.S., Hobbs, B.E., Ord, A., Mühlhaus, H.B., 2000. Numerical  
651 modelling of single-layer folding: clarification of an issue regarding the

652 possible effects of computer codes and the influence of initial  
653 irregularities. *Journal of Structural Geology* 22, 1511-1522.  
654  
655

656 **Figure captions**

657

658 **Fig. 1. (a)** Folded quartz vein in biotite-schist matrix at Puig Culpit (Cap de Creus,  
 659 Eastern Pyrenees, Spain). The matrix has a first cleavage ( $S_1$ , solid yellow lines)  
 660 that is crenulated to develop an  $S_2$ -cleavage (white dashed lines), axial planar to  
 661 the vein folds. One Euro coin for scale,  $\varnothing=23$  mm. **(b-c)** Finite-element  
 662 simulations of folding of a single competent layer embedded in a weaker,  
 663 isotropic matrix (same as presented in Llorens et al., 2013a,b). (b) dextral simple  
 664 shear up to a shear strain of 2, and (c) vertical pure shear up to 55% shortening.  
 665 **(d-e)** VPFFT-ELLE simulations of single layer folding in an anisotropic matrix  
 666 ( $A=20$ ) in (d) dextral simple shear up to a shear strain of 1, and (e) vertical pure  
 667 shear up to 50% shortening. Note that the anisotropy in the matrix results in an  
 668 axial planar crenulation cleavage, comparable to the one shown in (a). Grey area  
 669 in insets is area of model shown.

670

671 **Fig. 2.** VPFFT-ELLE-simulations of a circular hard object (dark red), deformed to  
 672 a dextral simple shear strain of ten, with a softer mantle (black), embedded in an  
 673 **(a)** isotropic or **(b)** anisotropic matrix ( $A=10$ ). Strain distribution is illustrated  
 674 by the boundaries of the originally equidimensional elements. White arrows  
 675 show the total amount of rotation of the objects. Ongoing rotation of the object in  
 676 the isotropic matrix leads to the development of a  $\delta$ -clast, while an anisotropic  
 677 matrix leads to strongly heterogeneous matrix deformation, reduced object  
 678 rotation and, hence, development of a  $\sigma$ -clast.

679

680 **Fig. 3.** C' shear bands in **(a)** a naturally deformed rock and **(b)** an VPFFT-ELLE  
 681 simulation with a weak (black), intermediate (white) and strong (pink) phase. St  
 682 = staurolite, Qtz = quartz, Bt = biotite. The S-foliation is highlighted with blue  
 683 lines, C-planes with green lines and C'-planes with dashed green lines.

684

685 **Fig. 4.** VPFFT-ELLE simulations of polycrystals deformed in dextral simple shear  
 686 up to a shear strain of 3 and with increasing degree of grain anisotropy ( $A$ ) from  
 687 1 to 20. Anisotropy is defined as the ratio between the critical resolved shear  
 688 stress ( $\tau_{cr}$ ) required to activate the non-basal and basal slip systems. **(a)** Grain

689 boundary network and **(b)** Von-Mises shear strain rate field, normalized with  
690 respect to the bulk value. For better visibility figures of Von Mises strain rate  
691 field have been enlarged two times, only showing the lower right quarter of the  
692 model. **(c)** Frequency distribution of normalised Von-Mises strain rates for  
693 different anisotropy values. Whereas the distribution for  $A=1$  is approximately  
694 normal with a mean of one, higher  $A$ -values lead to a frequency peak below the  
695 mean and a "heavy tail" of high strain rate values. Inset shows the same data, but  
696 with a linear vertical scale.

697

698

699 **Table caption**

700

701 **Table 1.** Summary of method, deformation and properties of the models  
702 described in the text. All models were run using the ELLE platform.

703

704

705



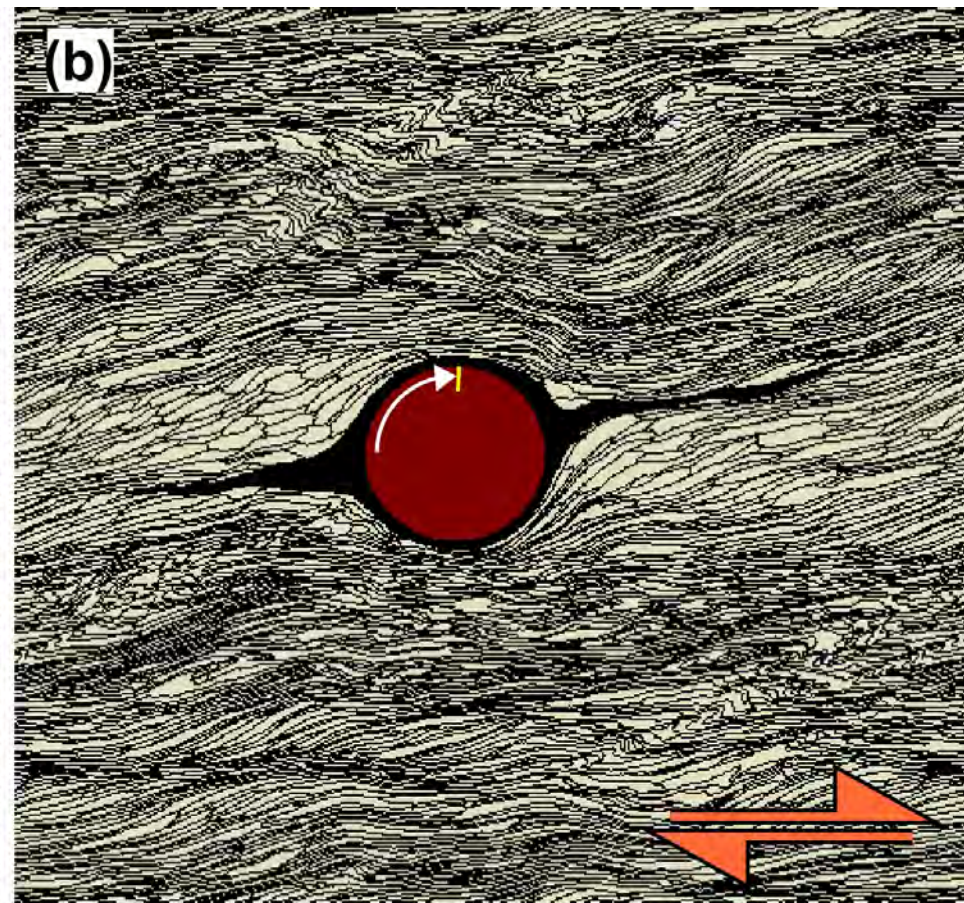
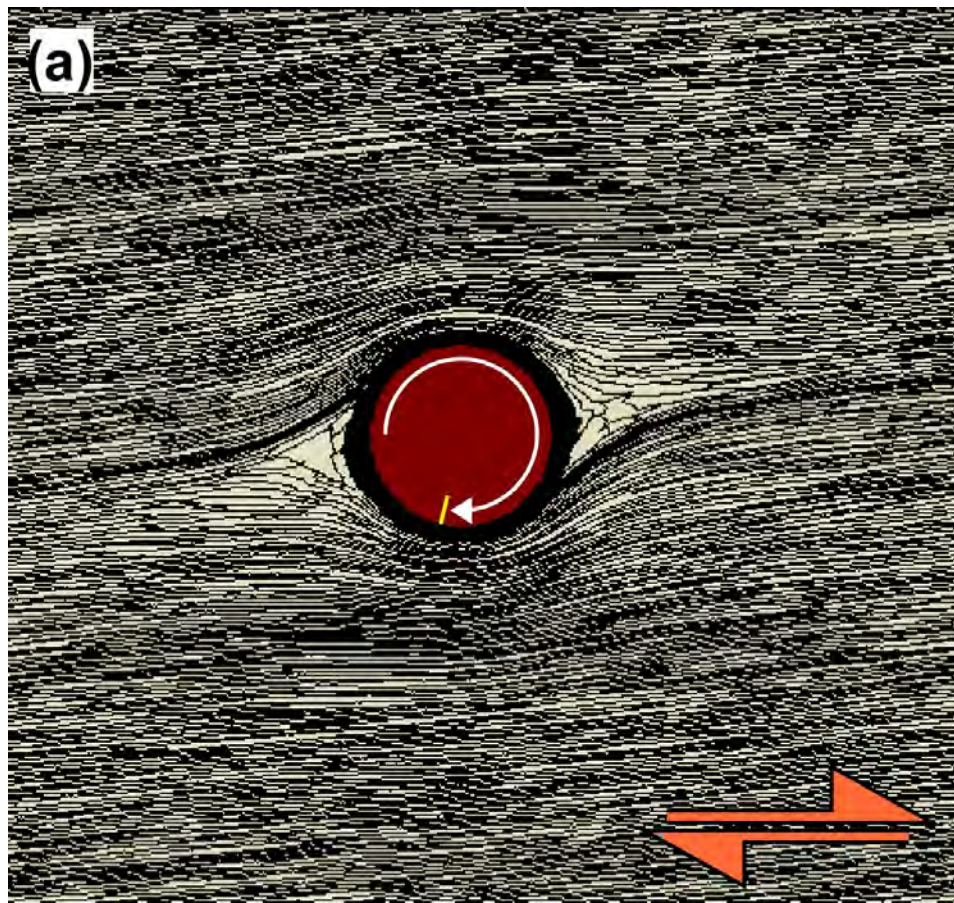


Figure 2



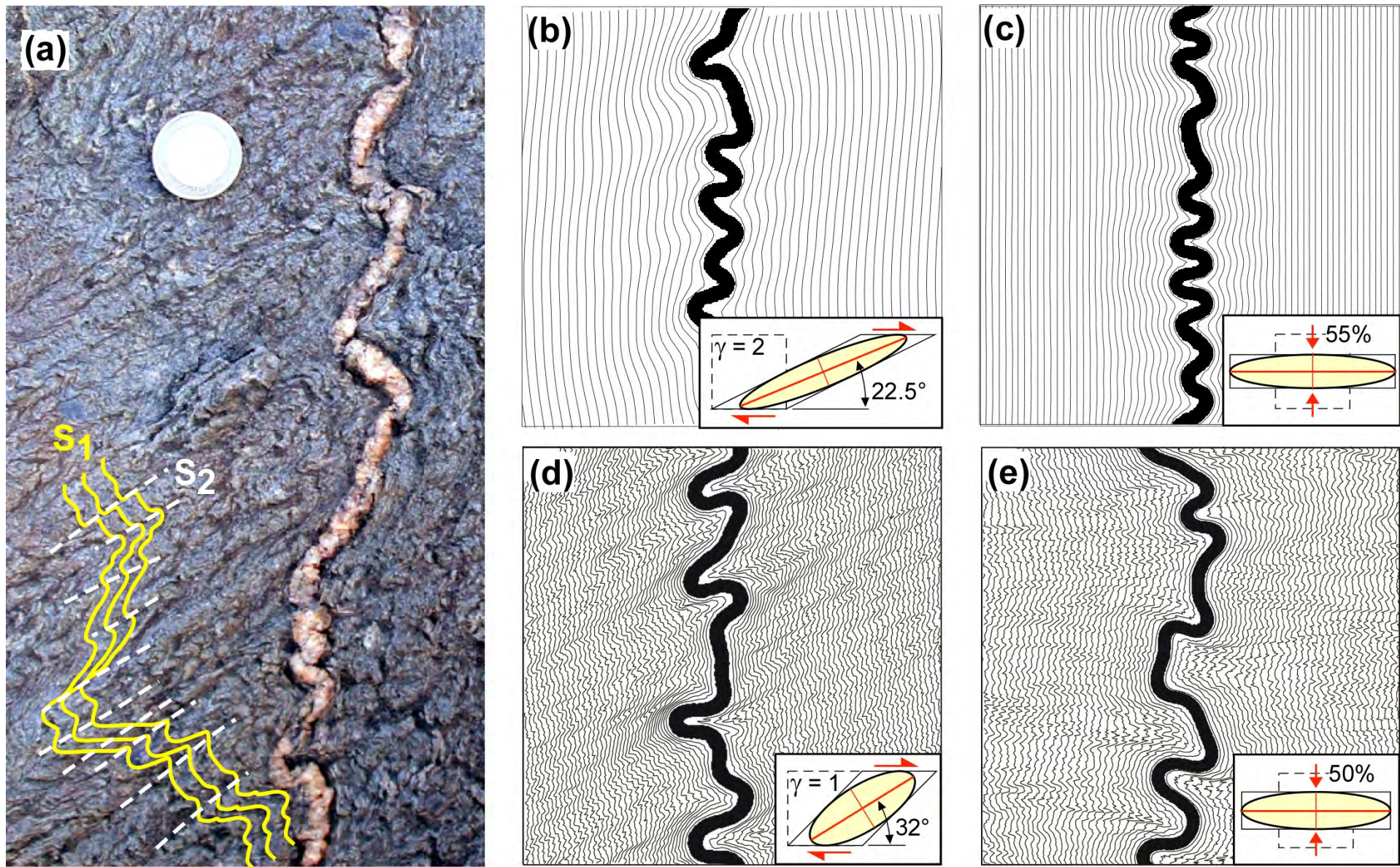


Figure 1



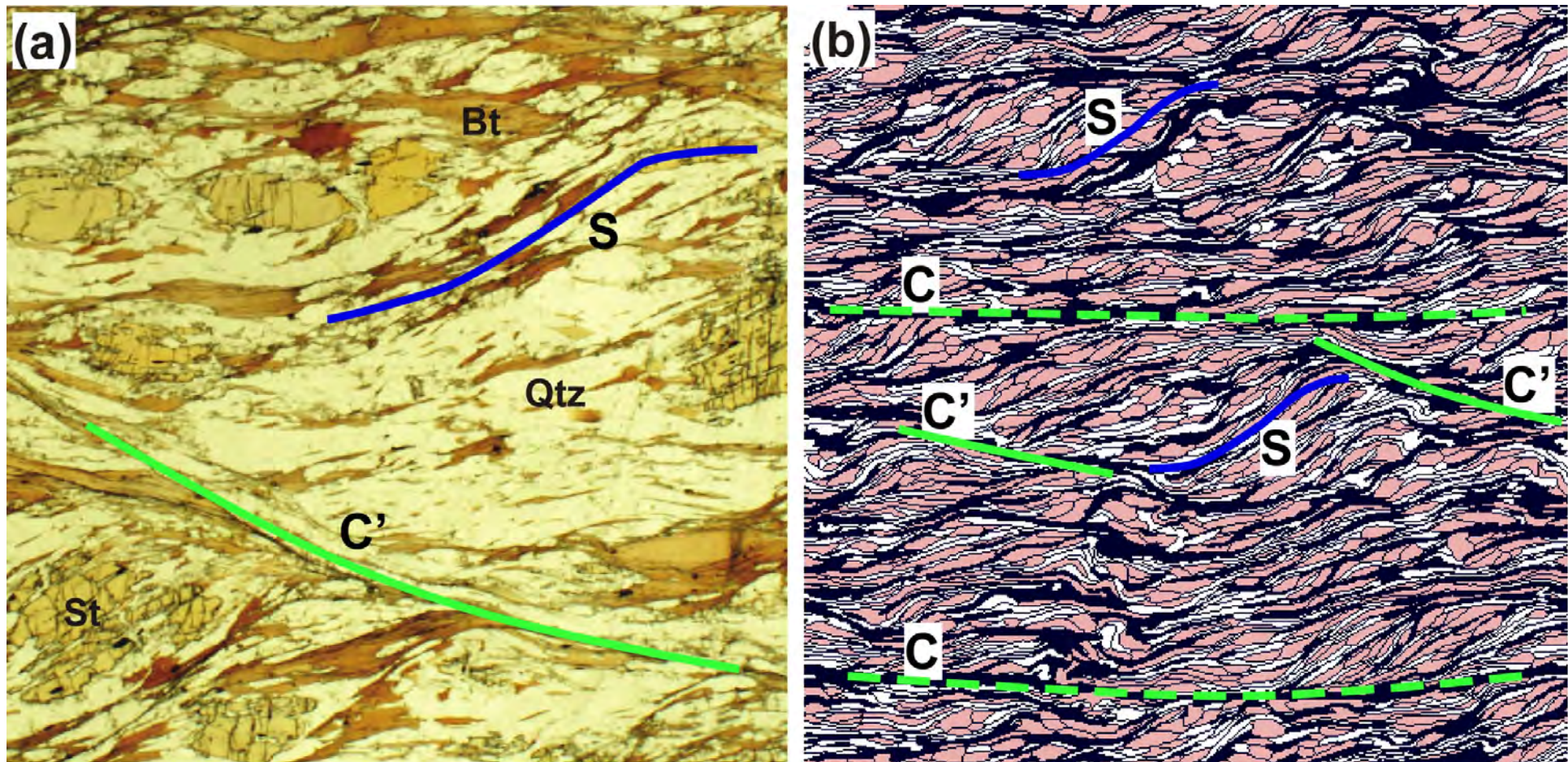


Figure 3



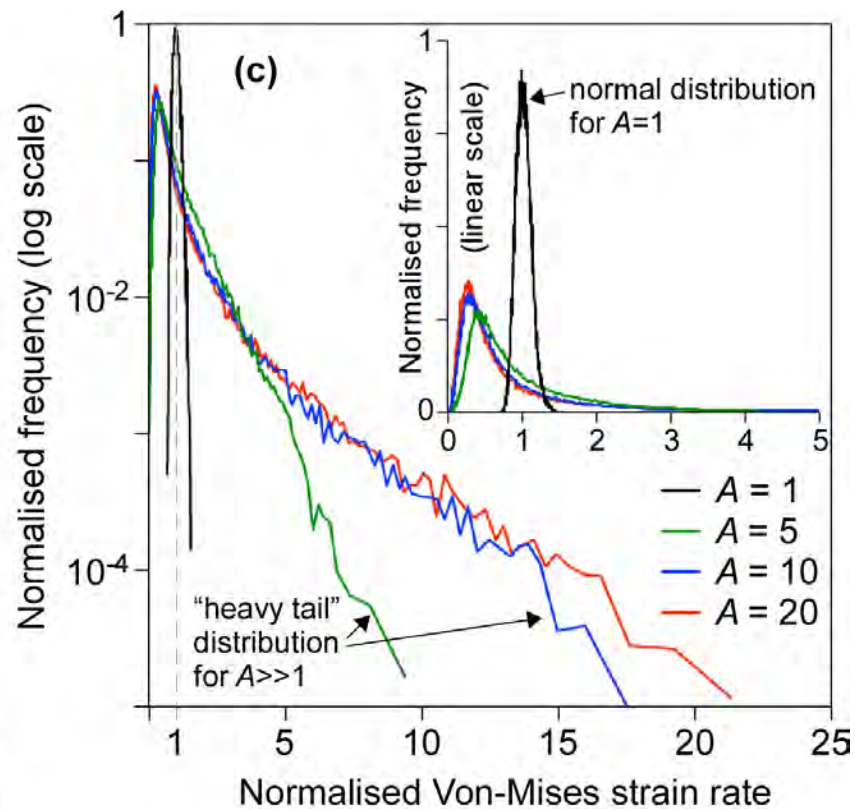
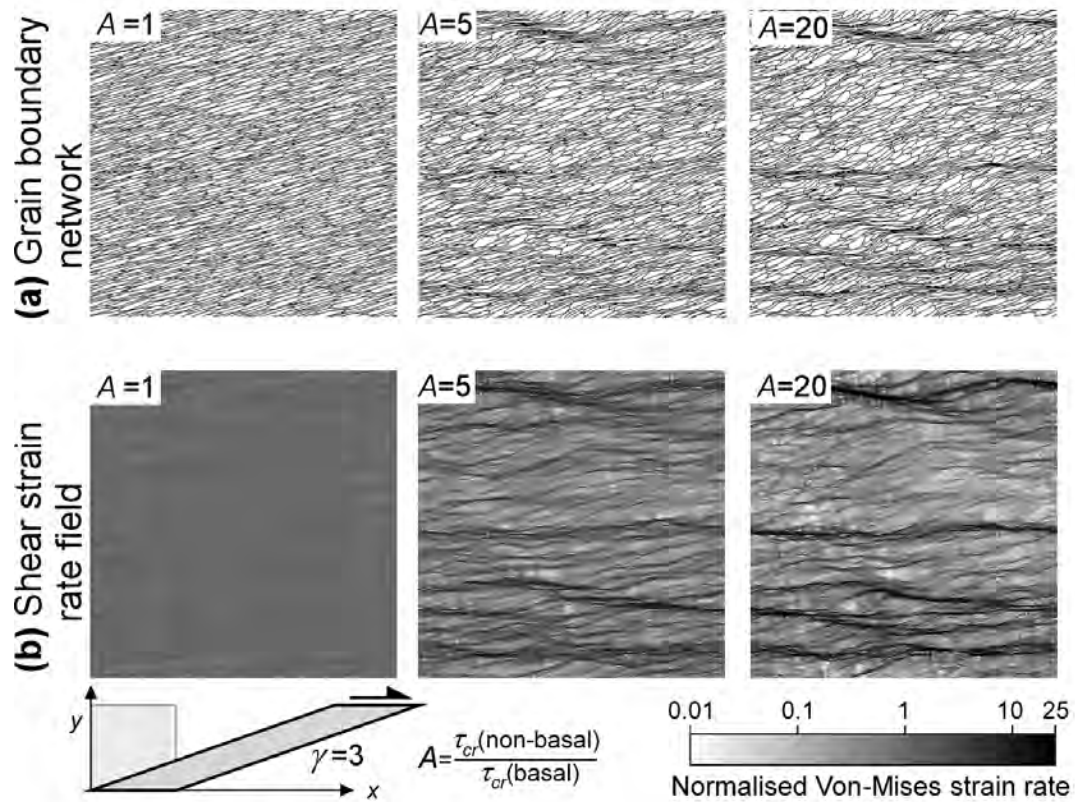


Figure 4

**Table 1**

Figure	Method <sup>1</sup>	Deformation	Properties		
			Layer	Matrix	
Fig. 1b	FEM	simple shear	$B=50$	$B=1$	
Fig. 1c	FEM	pure shear	$B=50$	$B=1$	
Fig. 1d	VPFFT	simple shear	$\tau_{cr}(\text{all})=100$	$\tau_{cr}(\text{basal})=1$ $\tau_{cr}(\text{other})=20$	
Fig. 1e	VPFFT	pure shear	$\tau_{cr}(\text{all})=100$	$\tau_{cr}(\text{basal})=1$ $\tau_{cr}(\text{other})=20$	
			Core object	Mantle	Matrix
Fig. 2a	VPFFT	simple shear	$\tau_{cr}(\text{all})=50$	$\tau_{cr}(\text{all})=0.8$	$\tau_{cr}(\text{all})=1$
Fig. 2b	VPFFT	simple shear	$\tau_{cr}(\text{all})=50$	$\tau_{cr}(\text{all})=4$	$\tau_{cr}(\text{basal})=1$ $\tau_{cr}(\text{other})=10$
			Strong phase	Intermediate	Weak phase
Fig. 3b	VPFFT	simple shear	$\tau_{cr}(\text{all})=30$	$\tau_{cr}(\text{all})=15$	$\tau_{cr}(\text{basal})=1$ $\tau_{cr}(\text{other})=10$
			Whole model		
Fig. 4	VPFFT	simple shear	$\tau_{cr}(\text{basal})=1$ $\tau_{cr}(\text{other})=1, 5, 20$		

<sup>1</sup>FEM = finite element method with BASIL (Houseman et al., 2008). VPFFT= Viscoplastic Full-Field Transform method (Lebensohn, 2001), using 256x256 elements.