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Non-basal dislocations should be accounted for in simulating ice mass flow

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Abstract

Prediction of ice mass flow and associated dynamics is pivotal at a time of climate change. Ice flow is dominantly accommodated by the motion of crystal defects - the dislocations. In the specific case of ice, their observation is not always accessible by means of the classical tools such as X-ray diffraction or transmission electron microscopy (TEM). Part of the dislocation population, the geometrically necessary dislocations (GNDs) can nevertheless be constrained using crystal orientation measurements via electron backscattering diffraction (EBSD) associated with appropriate analyses based on the Nye (1950) approach. The present study uses the Weighted Burgers Vectors, a reduced formulation of the Nye theory that enables the characterization of GNDs. Applied to ice, this method documents, for the first time, the presence of dislocations with non-basal $[c]$ or $\langle c+a \rangle$ Burgers vectors. These $[c]$ or $\langle c+a \rangle$ dislocations represent up to 35% of the GNDs observed in laboratory-deformed ice samples. Our findings offer a more complex and comprehensive picture of the key plasticity processes responsible for polycrystalline ice creep and provide better constraints on the constitutive mechanical laws implemented in ice sheet flow models used to predict the response of Earth ice masses to climate change.

Keywords:

Non-basal dislocations in ice, Weighted Burgers Vectors, cryo-EBSD, crystal plasticity

1. Introduction

Understanding the deformation behavior of ice crystals is essential for modeling the flow of glaciers and ice sheets. Ice on Earth, ice Ih, has an hexagonal crystalline structure. It has a strong viscoplastic anisotropy, since deformation occurs almost exclusively by dislocation glide on the basal plane (Duval et al., 1983). This crystal-scale anisotropy results in strong textures (crystallographic orientations) and, hence, in large-scale texture-induced anisotropy. This anisotropy has crucial effects on large-scale ice flow (e.g. Durand et al. (2007)). It is responsible, for instance, for abrupt changes in rheology between the ice sheet and the ice

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shelf (Ma et al., 2010) and for basal folding (Bons et al., 2016). The viscoplastic anisotropy of ice crystals also results in strong strain and stress heterogeneity (Grennerat et al., 2012), leading to dynamic recrystallization (Duval et al., 1983; Chauve et al., 2015), a process that is essentially controlled by the dislocation behavior and interactions (Chauve et al., 2017). Ice is therefore a good analogue to study the behaviour of materials with high viscoplastic anisotropy deforming at high temperature ($T/T_{melt} > 0.9$), such as the Earth lower crust and mantle, where the dominant rock-forming minerals (e.g. feldspar, quartz, olivine, pyroxenes, micas) are highly anisotropic.

However, the difficulty in observing dislocations by TEM or X-ray diffraction results in a lack of knowledge on the activity of other slip systems or of mechanisms such as climb or cross-slip that may complement basal glide. The lack of constraints on the activity of the non-basal slip systems in ice limits the ability of micro-macro crystal plasticity methods to simulate the mechanical behaviour of ice and its evolution (see Montagnat et al. (2014) for a review). To approach a realistic mechanical behaviour, which can be used to model the flow of glaciers and polar ice sheets, strong assumptions have been made (see Castelnau et al. (1997); Kennedy et al. (2013) for instance). In particular, in all models based on crystal plasticity, four to five independent slip systems are required to maintain strain compatibility (Hutchinson, 1977), hence for ice, glide on non-basal slip systems is allowed. Castelnau et al. (1997) imposed a non basal activity 70 times harder than basal activity, while Llorens et al. (2016) lowered this ratio to 20, enabling a significant contribution of non-basal systems to deformation, without any experimental evidence to stand on.

Most observed dislocations in ice so far have one of the three equivalent $1/3 \langle 2\bar{1}\bar{1}0 \rangle$ Burgers vectors and are constrained to glide in the basal plane (0001) owing to their tendency to dissociate into partial dislocations (Higashi, 1988; Hondoh, 2000). Rare $1/3 \langle 2\bar{1}\bar{1}0 \rangle$ dislocations have been observed to glide on prismatic planes by X-ray diffraction in low strain conditions where very few dislocations were activated (Shearwood and Withworth, 1989), and when crystals were oriented to minimize the resolved shear stress in the basal plane (Liu and Baker, 1995). Indirect evidence of double cross-slip of basal dislocations was obtained from X-ray diffraction observations on single crystal deformed in torsion (Montagnat et al., 2006). Dislocation Dynamic simulations estimated the local stress necessary to activate this mechanism (Chevy et al., 2012).

So far, direct observations (via X-ray diffraction) of dislocations with Burgers vector $[c] = [0001]$ or $\langle c + a \rangle = 1/3 \langle 11\bar{2}3 \rangle$ are limited to very specific conditions such as peripheral dislocations of stacking faults formed during crystal growth or under cooling (Higashi, 1988). The formation of stacking faults under cooling is assumed to result from climb of the basal component of dislocation loops with $\langle c + a \rangle$ Burgers vector, induced by the precipitation of excess point defects generated by cooling. Dislocation loops with $[c]$ -component Burgers vectors were also observed to form due to tiny inclusions (water droplets for pure ice, or solute pockets for NH_3 -doped ice) formed during crystallization and due to thermal stress imposed in the crystal growing apparatus (Oguro and Higashi, 1971). To our knowledge, there are no other direct observations of dislocations with a $[c]$ -component Burgers vector for pure or natural ice.

Weikusat et al. (2011b) indirectly inferred $[c]$ or $\langle c + a \rangle$ dislocations as necessary to explain some subgrain boundary structures observed in ice core samples. The techniques used (surface sublimation to extract subgrain boundaries and discrete X-ray Laue diffraction analyses

83 to obtain local orientations along profiles) did not provide full constraints on the nature of
84 the subgrain boundaries. Nevertheless, by assuming that the subgrain boundaries were per-
85 pendicular to the surface, some could be interpreted as tilt boundaries composed of $[c]$ or
86 $\langle c + a \rangle$ dislocations.

87 Dislocations are nucleated and contribute to plastic deformation by gliding. The dislocations
88 can be stored in the microstructure by two modes; as trapped dislocations due to dislocation
89 interaction, called Statistically Stored Dislocations (SSDs) and as Geometrically Necessary
90 Dislocations (GNDs) (Fleck et al., 1994). GNDs are intimately associated with lattice cur-
91 vature, and hence contribute to local strain that can be detected by EBSD as misorientation
92 gradients. They contribute to heterogeneous plastic strain, such as bending or twisting but
93 they can develop even though the experimental conditions allows the possibility of a homo-
94 geneous deformation (Van der Giessen and Needleman, 2003). It is generally acknowledged
95 that density of GNDs is significantly higher than density of SSDs (Kubin and Mortensen,
96 2003).

97 EBSD analyses of ice were recently made possible thanks to cryo-stages able to maintain
98 samples at very cold temperatures (-100 to -150°C), under low vacuum. This technique gives
99 access to full crystal orientations over reasonably large polycrystalline samples (few cm²),
100 with a good spatial resolution (down to 0.1 μm). The first applications of EBSD on ice
101 were oriented towards full crystal orientation measurements at the grain level (Obbard et al.,
102 2006). High spatial resolution crystal misorientations within grains were recently used to
103 characterize dislocation substructures (Piazolo et al., 2008; Montagnat et al., 2011; Weikusat
104 et al., 2011a; Montagnat et al., 2015; Chauve et al., 2017). EBSD observations performed in
105 the above mentioned studies are post-mortem and therefore record the effects of the GNDs
106 remaining after relaxation of the internal stress field through anelastic deformation.

107 Since conventional EBSD maps are 2D, they do not give access to the full dislocation (Nye)
108 tensor α but only to five components ($\alpha_{12}, \alpha_{21}, \alpha_{13}, \alpha_{23}, \alpha_{33}$) where the subscript 3 refers to
109 the normal to the EBSD surface. By this mean, EBSD observations provide lower bounds
110 of GND density (Pantleon, 2008). Recently, Wheeler et al. (2009) proposed a method of
111 characterization of the GNDs called the “weighted Burgers vector” (WBV) (see Appendix A
112 for a detailed description). It corresponds to the projection of the Nye tensor on the EBSD
113 surface and can be expressed as $\mathbf{WBV} = (\alpha_{13}, \alpha_{23}, \alpha_{33})$. The WBV tool does not aim at ap-
114 proaching the full dislocation density tensor (as attempted by Pantleon (2008) for instance),
115 but does not require the third dimension to provide meaningful information about the GND
116 population. Its amplitude gives a lower bound for the density of GNDs and its direction
117 refers to the Burgers vector of the sampled GNDs. One important point is that although the
118 WBV does not record all the GNDs present, it cannot contain phantom directions. If it has
119 a significant $[c]$ -component then at least some of the Burgers vectors of the GNDs must have
120 a $[c]$ -component though this does not mean they have to be parallel to $[c]$.

121 As for the Nye tensor, the WBV analysis only reflects the GND contribution to the dislo-
122 cation density. Without further assumptions, this contribution cannot be directly related to
123 the mobile dislocations responsible for most of the plastic deformation.

124 Cryo-EBSD associated with the WBV analysis was recently shown to be very efficient to
125 characterize the nature of GNDs in ice (Piazolo et al., 2015). Although restricted to small
126 areas, this previous study revealed a contribution of dislocations with $[c]$ - or $\langle c + a \rangle$ -
127 component. These observations encouraged us to perform new EBSD observations on ice

128 polycrystals deformed in the laboratory, with a higher spatial resolution and over larger ar-
 129 eas than in the preliminary study of Piazzolo et al. (2015).

130 The present work aims therefore at (i) documenting the presence of dislocations with Burg-
 131 ers vectors comprising a component along $[c]$, (ii) estimating quantitatively the significance
 132 of these dislocations within the observed GNDs, and (iii) discussing the implication of this
 133 observation for the micro-macro modeling of ice mechanical behaviour, up to the scale of
 134 glaciers and polar ice flow.

135 2. Material and Methods

136 Large ice polycrystalline samples were deformed in torsion and uniaxial unconfined com-
 137 pression under constant imposed load at high homologous temperature ($T/T_{melt} \sim 0.98$, in a
 138 cold room). The samples deformed by compression had a columnar initial grain shape with
 139 large grain size (1 to 4 cm^2) (see Grennerat et al. (2012); Chauve et al. (2017) for details)
 140 and were deformed under a constant load of 0.5 MPa applied in the plane perpendicular to
 141 the column directions, up to a macroscopic strain of about 3%. Torsion tests were performed
 142 on solid cylinders (radius \times height = 18 $mm \times 60 mm$) of granular ice (millimetre grain
 143 size), under a maximum applied shear stress at the outer radius between 0.5 and 0.6 MPa
 144 (experimental conditions similar to the ones in Bouchez and Duval (1982); Montagnat et al.
 145 (2006)). Several tests enabled to cover a range of maximum shear strain between 0.01 and
 146 2. These two experimental conditions are complementary. The compression tests enable to
 147 follow the first step of deformation in a model microstructure invariant in the third dimension
 148 (parallel to the columns) that is close to a 2.5D configuration, where surface observations are
 149 a good proxy to the bulk mechanisms (Grennerat et al., 2012). The torsion experiments give
 150 access to large strain levels on an initially isotropic microstructure and texture. A summary
 151 of the experimental conditions of the tests used in this study is given in table 1.

Id	Sample	Mechanical test	T °C	Stress	ϵ_{max}	γ_{max}
CI01	Columnar ice	Uniaxial comp.	-7	0.5 MPa	0.03	
TGI01	Granular ice	Torsion	-7	0.46 MPa	0.006	0.012
TGI02	Granular ice	Torsion	-7	0.49 MPa	0.1	0.2
TGI03	Granular ice	Torsion	-7	0.59 MPa	0.21	0.42
TGI04	Granular ice	Torsion	-7	0.63 MPa	0.87	1.96

Table 1: Summary of the experimental conditions for the tests used in the study. Compression tests were performed under constant applied load, and torsion test under constant applied torque (the corresponding maximum shear stress is given here).

152 Samples ($20 \times 10 \times 3 mm^3$) were extracted from the deformed blocks for cryo-EBSD obser-
 153 vations (angular resolution of 0.7° , spatial resolution of 5 and 20 μm for this study). The
 154 torsion samples were cut perpendicular to the radius, as close as possible to the external
 155 side of the cylinder. Appropriate adjustment of the vacuum and temperature (1 Pa and
 156 $-100^\circ C$) to reduce sublimation was made following Montagnat et al. (2015). This allowed
 157 EBSD mapping of the entire selected areas with indexation rates higher than 85%.

158 At the compression and shear strains reached, dynamic recrystallization mechanisms such
 159 as nucleation at triple junctions, highly misoriented subgrain boundaries and kink bands are

160 observed as in Chauve et al. (2017). In the compression sample analyses we focused on grain
 161 boundaries and triple junction areas. “Typical” dislocation substructures are presented in
 162 figures 1 and 2. Similar features were observed in the torsion samples. In these samples,
 163 we analyzed larger areas in order to obtain statistical information about the nature of the
 164 dislocations involved in the observed substructures.

165
 166 In order to characterize the dislocations involved in the formation of subgrain boundaries,
 167 we used WBV analyses following Wheeler et al. (2009) (see Appendix A for a detailed de-
 168 scription). The WBV represents the sum over different dislocation types of the product of
 169 [(density of intersections of dislocation lines within a selected area of the map) \times (Burgers
 170 vector)]. Each dislocation line crossing the EBSD surface contributes to the WBV but the
 171 weight of this contribution depends of the angle between the dislocation line and the EBSD
 172 surface. It is one (zero) if the dislocation line is perpendicular to (within) the EBSD surface.
 173 The WBV analysis gives a vector which can be expressed in the crystal or sample reference
 174 frame.

175 The WBV analyses were performed as (i) a point by point analysis that enables to plot
 176 the WBV direction and magnitude along the dislocation substructures and (ii) an integral
 177 WBV calculation of the net Burgers vector content of dislocations intersecting a given area
 178 of a map by an integration around the edge of this area. The integral WBV calculated over
 179 a given area is projected over the four non-independent lattice components of the hexago-
 180 nal symmetry ($[11\bar{2}0]$, $[\bar{2}110]$, $[1\bar{2}10]$ and $[0001]$ noted WBV_{a1} , WBV_{a2} , WBV_{a3} , WBV_c). This
 181 integral WBV analysis complements the point-by-point WBV calculations and, due to the
 182 integration over an area, reduces the noise level in the analysis (see Appendix A). In special
 183 cases the integration also induces a loss of information. For instance, in the case of an integral
 184 calculation over an area containing a perfect kink band, the resulting integral WBV will be
 185 null if the two opposite tilt bands have similar misorientation angles.

186 The proportion of dislocations with a $[c]$ -component Burgers vector (that includes dislocations
 187 with $[c]$ and $\langle c + a \rangle$ Burgers vectors, thereafter referred to as $[c]$ -component dislocations)
 188 in the subgrain boundaries is estimated as the ratio between the WBV_c component over
 189 the Euclidian norm of the WBV ($|WBV_c|/||\mathbf{WBV}||$), thereafter called $rWBV_c$. For the
 190 pixel-scale calculations, a cut-off value was defined in such a way to restrict the analysis to
 191 sub-structures with a misorientation higher than 0.9° , to remain slightly above the EBSD
 192 resolution. This cut-off value transposed to the WBV norm depends on the EBSD step-size
 193 since the WBV is calculated per unit length ($1.4 \times 10^{-3} \mu m^{-1}$ for $5 \mu m$ EBSD step size
 194 and $3.5 \times 10^{-4} \mu m^{-1}$ for $20 \mu m$ EBSD step size). Subgrain boundaries are distinguished by
 195 selecting the pixels for which the norm of the WBV is higher than this threshold and lower
 196 that the upper bound for a subgrain boundary set at 7° of misorientation (Chauve et al.,
 197 2017). The cut-off value is coherent with the limit of accuracy of EBSD data and leads
 198 to a good agreement with the subgrain boundary segmentation defined based on the local
 199 misorientation only. By doing so, less that 1% of pixels are selected as “sub-structures” in
 200 the non deformed sample and the corresponding values of $|WBV_c|/||\mathbf{WBV}||$ are uniformly
 201 distributed.

202 The WBV analyses are associated with classical measurements of the rotation axis of the
 203 misorientation induced by the subgrain boundary (by making use of absolute orientations
 204 from EBSD data) together with the orientation of the boundary trace. From this method

205 known as “boundary trace analysis” (Mainprice et al., 1993; Lloyd et al., 1997; Prior et al.,
206 2002; Piazzolo et al., 2008), the boundary plane can be inferred. These information are used
207 as a visualisation tool in figure 2.

208 Finally, statistical analyses were performed by using a probability density function that rep-
209 resents the ratio between the number of pixels with a WBV norm higher than the threshold
210 (defined above) over the total number of pixels. It can be seen, for instance in figure 4,
211 that this ratio is small for the low torsion strain experiment. The pixels with a WBV norm
212 higher than the threshold are also separated as a function of the nature of the WBV, meaning
213 mostly composed of $[c]$ -component dislocations, mostly composed of $\langle a \rangle$ dislocations, or
214 composed of a similar amount of both types of dislocations.

215 3. Experimental observations

216 We present first detailed observations of a few subgrain boundaries that illustrate the
217 techniques used to distinguish $\langle a \rangle$ from $[c]$ -component Burgers vectors on GND sub-
218 structures, and then a global analysis performed over large-scale EBSD maps containing
219 hundreds of grains (from the torsion test samples), which aims at evaluating the statistical
220 significance of the dislocations with $[c]$ -component Burgers vectors within the substructures.
221 Frequently observed subgrain structures in ice deformed by plasticity include “closed” shaped
222 subgrain boundaries (SGBs) formed in the vicinity of serrated grain boundaries (Fig. 1), in
223 areas where the microstructure is very heterogeneous. These “closed” shaped SGBs were
224 shown in (Chauve et al., 2017) to act as precursor of nucleation by strain induced boundary
225 migration (SIBM) and bulging. The superposition of the WBV data (projection of the WBV
226 on the sample plane and relative contribution of $[c]$ -component dislocations, $rWBV_c$) to the
227 trace of the SGBs (Fig. 1) highlights the complexity of the dislocation sub-structures and
228 the variability of the contribution of $[c]$ -component Burgers vector dislocations (from almost
229 null to almost 1) in the different subgrain boundary segments.

230 The “closed loop” substructure on the left side of figure 1 has been selected for a detailed
231 characterization (Fig. 2 and Table 2). It can be separated into three domains with distinct
232 WBV orientations. Two of them, domains 1 and 3, have WBV orientations pointing in two
233 opposite $\langle m \rangle$ ($\langle 1\bar{1}00 \rangle$) axis directions. These two subgrains accommodate a rotation
234 around an axis parallel to the boundary plane (along $\langle a \rangle$ axes) but with opposite rotation
235 directions. Such a configuration, characteristic of two tilt-bands with opposite signs, forming
236 a kink band, is frequently observed in ice (Montagnat et al., 2011; Piazzolo et al., 2015).

237 The subgrain boundary in domain 2 is characterized by a boundary plane that is perpen-
238 dicular to the ones of the SGBs from domains 1 and 3. However its rotation axis is also
239 parallel to an $\langle a \rangle$ axis and it is contained within the subgrain boundary plane. Subgrain
240 segment 3 is therefore also a tilt boundary. The WBVs are, this time, aligned along the $[c]$
241 axis and perpendicular to the rotation axis. This configuration cannot be explained without
242 an important contribution of edge dislocations with a $[c]$ -component Burgers vectors. This
243 interpretation is confirmed quantitatively by the estimation of the integral WBV in the three
244 areas of interest (table 2). The relative contribution of the $[c]$ -component dislocations, which
245 is estimated as the ratio $rWBV_c$ is shown to dominate in domain 2.

246

247 The torsion experiments provide samples deformed in simple shear in the range $\gamma = 0.012$

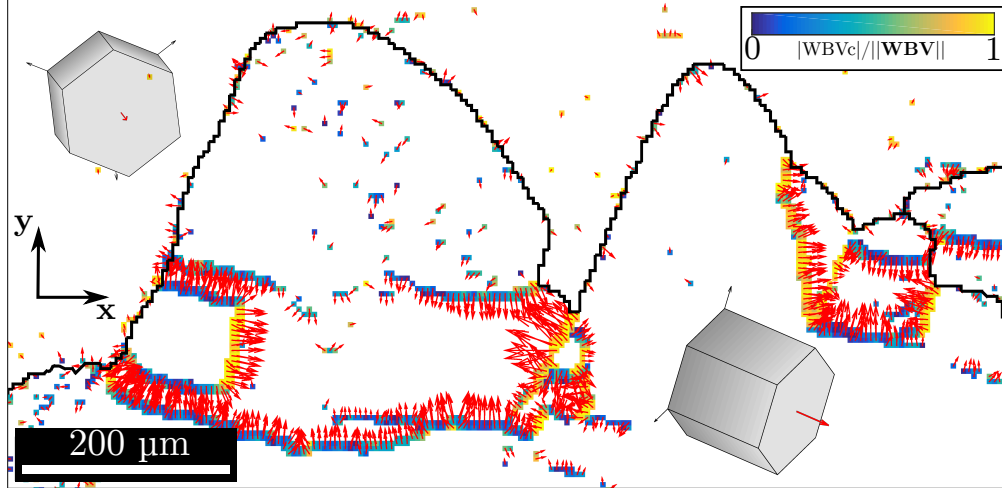


Figure 1: Serrated grain boundary observed in sample CI01. The ratio $\frac{|WBV_c|}{||WBV||}$ (see text) and the WBVs are plotted for the pixels where $||WBV||$ is higher than $1.4 \times 10^{-3} \mu m^{-1}$. The red arrows show the in-plane projections of the WBV direction (above a threshold of $1.4 \times 10^{-3} \mu m^{-1}$, EBSD step size $5 \mu m$).

Analyzed area	Integral WBV μm^{-2}				
	WBV_{a1}	WBV_{a2}	WBV_{a3}	WBV_c	$ WBV_c / WBV $
1	-2.77	1.14	1.64	-0.12	0.03
2	-0.60	0.47	0.13	2.65	0.94
3	1.84	-1.02	-0.82	-0.16	0.06

Table 2: Integral WBV projections over the four non-independent axes of the hexagonal crystal symmetry and the ratio $rWBV_c$ (see Materials and Methods), calculated for the areas of sample CI01 selected in figure 2.

248 to 1.94, for which EBSD observations reveal a high density of subgrain boundaries (Fig.
 249 3). For each sample, the local WBV analysis was performed over the entire mapped surface
 250 (about $20 \times 10 \text{ mm}^2$). In figure 3a, data for the most deformed sample are plotted as a function
 251 of the relative amount of $[c]$ -component dislocations, $rWBV_c$. This analysis highlights the
 252 high frequency of subgrain boundaries with a high proportion of $[c]$ -component dislocations
 253 (yellow pixels in figure 3). The $[c]$ -component dislocations are not confined to grain bound-
 254 ary areas, as some subgrain boundaries in the central part of grains display non-negligible
 255 contribution of $[c]$ -component dislocations (Fig. 3c).

256 Similar analyses were performed on samples deformed up to different finite shear strains.
 257 The resulting evolution of the relative occurrence of GNDs composed of $[c]$ -component dis-
 258 locations with finite strain is presented in figure 4. Although the overall number of pixels with
 259 a significant WBV magnitude increases significantly with strain, the ratio of substructure
 260 composed of $[c]$ -component dislocations remains stable. Except for the almost non-deformed
 261 sample, which shows a higher proportion of $[c]$ -component dislocations, about 65% of the
 262 pixels belonging to substructures are made of $\langle a \rangle$ dislocations, whereas the substructures
 263 containing $[c]$ -component dislocations represent a non-negligible contribution of about 35%
 264 (substructures with clear $[c]$ -component dislocation dominant are 13%, those including simi-
 265 lar proportion of $\langle a \rangle$ and $[c]$ -component dislocations, 22%)

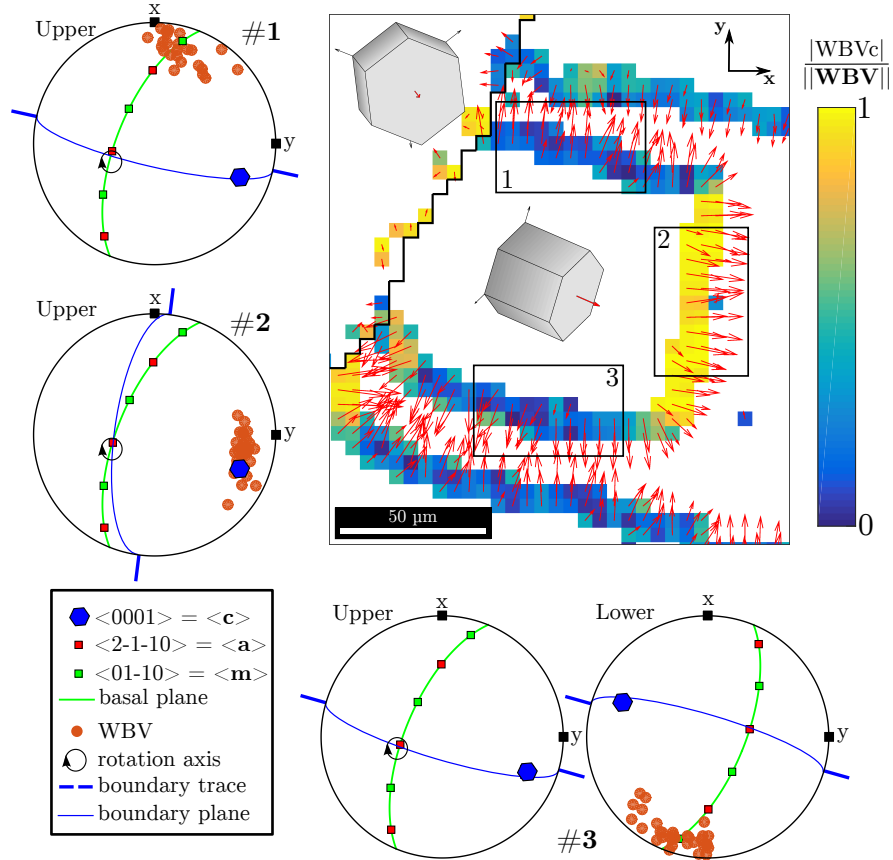


Figure 2: Weighted Burgers Vectors plotted over a zoomed area from the left side of figure 1, sample CI01. The colorscale gives the relative magnitude of $[c]$ -component dislocations, $rWBV_c$, and the red arrows show the in-plane projection of the WBV directions (above a threshold of $1.4 \times 10^{-3} \mu m^{-1}$, EBSD step size of $5 \mu m$). "Boundary plane" refers to "inferred" boundary plane, see text. Rectangular areas mark the domains selected for integral WBV calculations (table 2).

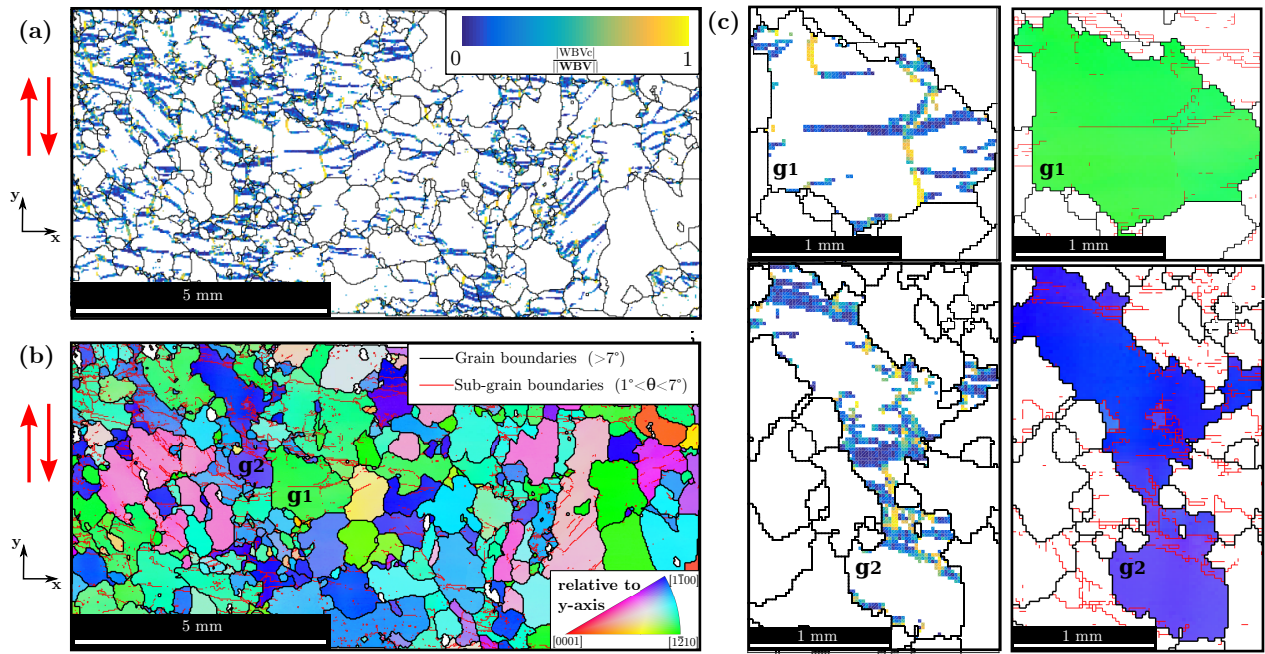


Figure 3: a) Ratio between the WBV_c component over the norm of the full WBV ($rWBV_c$) calculated at the pixel scale on sample TGI04 deformed in torsion up to $\gamma = 1.94$. As EBSD step size is $20 \mu m$, a cut-off value of $3.5 \times 10^{-4} \mu m^{-1}$ was taken for $||WBV||$ below which pixels are not considered in the calculation. b) Inverse Pole Figure color-coded EBSD image of the microstructure showing subgrain boundaries (in red) and grain boundaries (in black). c) Four small images to provide a focus on two illustrative cases, with the legend of respectively a) (left) and b) (right).

Another important observation is that at first sight, the presence of dislocations with a $[c]$ -

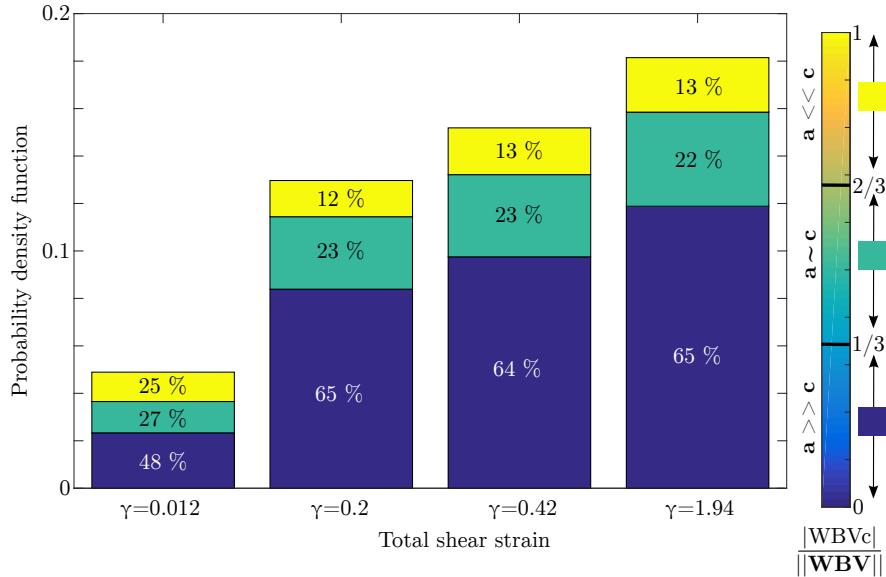


Figure 4: Distribution of pixels with a $\|\mathbf{WBV}\|$ higher than a threshold of $(3.5 \times 10^{-4} \mu m^{-1})$, EBSD step size of $20 \mu m$). Evolution with torsion strain of the relative $[c]$ and $\langle a \rangle$ components over the norm of the full WBV ($\|\mathbf{WBV}_c\|/\|\mathbf{WBV}\|$) for four distinct torsion creep tests.

266

267 component Burgers vector does not seem to be correlated with the orientation of the crystal.
 268 To further test this point, orientation data at the pixel scale were correlated with the relative
 269 amplitude of the WBV components. To do so, we selected data from the sample deformed
 270 by torsion at $\gamma = 0.42$ (TGI03), since at this rather low shear strain the macroscopic texture
 271 remains reasonably weak to provide a wide enough orientation range (Fig. 5).

272 As performed in (Grennerat et al., 2012), an adapted Schmid factor, that does not account for
 273 slip direction, is used to describe the pixel orientation relative to the imposed stress configura-
 274 tion ($S = \sqrt{|\boldsymbol{\sigma} \cdot \mathbf{c}|^2 - (\mathbf{c} \cdot \boldsymbol{\sigma} \cdot \mathbf{c})^2}$, where $\boldsymbol{\sigma}$ is the stress tensor and \mathbf{c} is the c-axis orientation).

275 The distribution of this Schmid factor (Fig. 5) reveals a slight under representation of orienta-
 276 tion with low Schmid factors, which may slightly bias the statistics. With this limitation in

277 mind, figure 5 gives an overview of the relative contributions of the different components of
 278 the WBV as a function of the Schmid factor, and therefore as a function of the orientation of

279 the pixel. First, the density of substructures (evaluated by the density of pixels with a WBV
 280 norm higher than the threshold) is similar independently of the crystallographic orientation.

281 The slight increase with Schmid factor must result from a statistical bias due to different
 282 number of pixels analysed for each orientation range (see top of Fig. 5). Second, dislocations

283 with a $[c]$ -component occur within similar proportions for every orientation. This statistical
 284 analysis confirms that there is no clear relationship either between local orientation and the

285 density of GNDs, or between local orientation and the type of dislocations involved in the
 286 GND substructures.

287

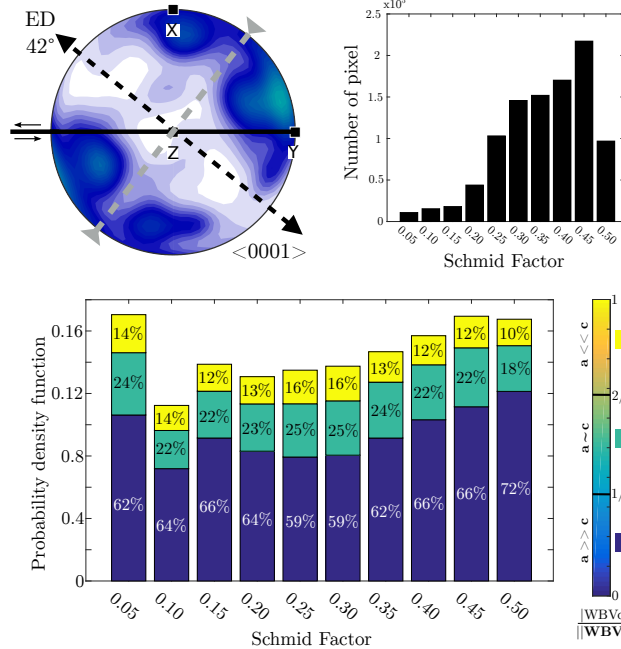


Figure 5: Distribution of the WBV dominant component as a function of the pixel orientation characterised by its adapted Schmid factor ($S = \sqrt{|\boldsymbol{\sigma} \cdot \mathbf{c}|^2 - (\mathbf{c} \cdot \boldsymbol{\sigma} \cdot \mathbf{c})^2}$, where $\boldsymbol{\sigma}$ is the stress tensor and \mathbf{c} is the axis orientation), from the sample TGI03 deformed in torsion up to $\gamma = 0.42$. *Top*: \mathbf{c} -axis pole figure and distribution of Schmid factors. *Bottom*: Ratio of pixels with $\|\mathbf{WBV}\|$ higher than $3.5 \times 10^{-4} \mu\text{m}^{-1}$ (EBSD step size of $20 \mu\text{m}$). Each ratio is decomposed in 3 parts showing the dominant component of the WBV.

288 4. Discussion

289 From these results, one important observation can be emphasized. Dislocations in ice,
 290 more specifically here GNDs, are clearly not composed solely by dislocations with $\langle a \rangle$
 291 Burgers vectors. A non negligible amount of dislocations with a $[c]$ component in their Burg-
 292 ers vectors contributes to the formation of subgrain boundaries in various configurations
 293 (boundary conditions, strain levels...) under laboratory conditions.
 294 Dislocations with a $[c]$ component Burgers vector are theoretically energetically unfavourable,
 295 and possess a Peierls barrier up to 10 times the one of $\langle a \rangle$ dislocations (Hondoh, 2000).
 296 They require therefore a higher level of resolved shear stress to be activated. Previous work
 297 on ice highlighted the link between local subgrain boundary development and local strain
 298 and/or stress concentrations based on misorientation measurements associated with full-field
 299 modeling approach (Montagnat et al., 2011; Piazzolo et al., 2015), on direct comparison be-
 300 tween strain field estimation by Digital Image Correlation and microstructure observations
 301 (Chauve et al., 2015) and full-field modeling predictions (Grennerat et al., 2012). Based on
 302 these recent works, we can assume that the combined effect of local redistribution of stress
 303 due to strain incompatibilities between grains (Duval et al., 1983; Montagnat et al., 2011;
 304 Piazzolo et al., 2015) and the built up of dislocation fields and their associated internal stress
 305 field (Chevy et al., 2012; Richeton et al., 2017) may produce local stresses that allow the
 306 activation of non-basal slip systems or the glide of non-basal dislocations, and in particular
 307 $[c]$ -component dislocations as observed here. The assumed link between local stress con-
 308 centrations and formation of GNDs is consistent with high-resolution EBSD measurements

309 recently performed on copper which show a correlation between high GND density and high
310 intragranular residual stresses, directly inferred from HR-EBSD (Jiang et al., 2015).
311 WBVs only capture part of the GNDs, which are, in turn, a fraction of the total disloca-
312 tion population. The total contribution of $[c]$ -component dislocations may therefore differ
313 from the present estimations. Moreover, the GNDs populations observed on post-mortem 2D
314 cryo-EBSD data might not be proportional to the population of glissile dislocations, that is,
315 representative of the relative activity of the slip systems, which are responsible for deforma-
316 tion. However they are responsible for the accommodation of stress heterogeneities through
317 their contribution to the formation of the subgrain boundaries. By the association of strain
318 measurements by DIC and microstructural observations, Chauve et al. (2015) demonstrated
319 that the formation of subgrain boundaries lead to a marked strain redistribution within a
320 polycrystal, which in the case of kink bands resulted in shear along the newly formed bound-
321 aries. GNDs act significantly during dynamic recrystallization by controlling nucleation by
322 SIBM for instance (Piazolo et al., 2015; Chauve et al., 2015). Last but not least, the internal
323 stress fields resulting from dislocation fields (Varadhan et al., 2006) can induce the activation
324 of mechanisms such as climb and cross-slip (Montagnat et al., 2006).. We therefore expect
325 GNDs to play a significant role during deformation at local and large scales.

326

327 All micro-macro modelling approaches applied to ice are so far based on drastic assump-
328 tions concerning the activated slip systems and on the mechanisms accommodating strain.
329 These assumptions are directly projected on the plasticity (or visco-plasticity) laws describ-
330 ing the dislocation glide and interactions during deformation. In most homogenization ap-
331 proaches (mean or full-field), plasticity is assumed to occur only through dislocation slip
332 on at least four independent slip systems, and their interactions are taken into account by
333 the critical resolved shear stresses which control the relative activities of the various slip
334 systems, and their evolution laws. These laws are generally adjusted based on compari-
335 son of the modelled macroscopic mechanical response with experimental results (Castelnau
336 et al., 1996, 2008; Suquet et al., 2012). These assumptions led to an unavoidable minimal
337 activation of non-basal slip which compensates for the lack of knowledge of accommodating
338 mechanisms (climb and cross-slip for instance), and the inability of the models to represent
339 them, except for a few attempts (Lebensohn et al., 2010, 2012). The non-basal activity, and
340 more specifically the fact that a minimum of pyramidal slip-system activity associated with
341 $[c]$ dislocations is always necessary was, until now, not justified by any observations. Most
342 of these empirically adjusted parameters were used in further applications with, sometimes,
343 limited validation tests (Lebensohn et al., 2009; Montagnat et al., 2011; Grennerat et al.,
344 2012; Llorens et al., 2016).

345 The fact that we have observed for the first time a non-negligible contribution of $[c]$ -component
346 dislocations to the GNDs population in ice polycrystals deformed in the laboratory provides
347 new constraints for modeling the deformation of ice. First, it gives a first order justification
348 for the introduction of the activity of pyramidal slip that requires $[c]$ -component dislocations
349 into crystal plasticity laws. Indeed, Castelnau et al. (2008) and Suquet et al. (2012) both
350 highlighted the necessity of a minimum amount of pyramidal slip to correctly simulate the
351 behavior of ice polycrystals during transient creep by mean of full-field approaches. Secondly,
352 the present observations open the possibility for a direct comparison between model predic-
353 tions based on Dislocation Dynamics (Devincre et al., 2008) or Dislocation Field approaches

354 (Taupin et al., 2007, 2008; Richeton et al., 2017) and the actual distribution of $\langle a \rangle$ and $[c]$ -
355 component dislocations in experimentally and naturally deformed ice samples as performed
356 in Richeton et al. (2017). Finally, it suggests the necessity to introduce secondary mecha-
357 nisms such as climb and cross-slip in the micro-macro approaches just mentioned, that is,
358 of simulating the complexity of dislocation interactions and assessing its impact on the me-
359 chanical behaviour.

360 Only recently attempts have been made to consider the long-range internal stress field asso-
361 ciated with dislocation substructures in crystal plasticity models (Taupin et al., 2007, 2008;
362 Richeton et al., 2017). These approaches, based on the elastic theory of continuously dis-
363 tributed dislocations account for the build up of GNDs and their transport during plasticity
364 but they are limited to multi-crystals with few grains (~ 20) because of numerical costs.
365 The validation of these approaches could strongly benefit from an accurate description of the
366 nature of GNDs such as the one presented here. They could, in turn, provide constraints on
367 the internal stress field favorable for the activation of $[c]$ -component dislocations.

368
369 Coupling detailed analyses of dislocation substructures, like the one presented here, with
370 such models, will produce a new generation of crystal plasticity laws which, when imple-
371 mented in micro-macro approaches coupled with large-scale flow models, will provide more
372 accurate estimations of the mechanical response of ice in the extreme conditions encountered
373 in natural environments. These large-scale models will be able to accurately represent the
374 texture evolution with strain and, hence, to take into account the mechanical anisotropy
375 associated with the texture evolution with deformation in ice sheets (Gillet-Chaulet et al.,
376 2006). These new plasticity laws will also be able to tackle complex boundary conditions as
377 the cyclic loading encountered in extraterrestrial bodies submitted to tidal forcing, as the
378 saturnian satellite Enceladus (Shoji et al., 2013).

379

380 5. Conclusions

381 The present study reveals for the first time the presence of a non-negligible (between 13%
382 and 35%) proportion of dislocations with $[c]$ -component Burgers vector within dislocation
383 substructures in pure ice deformed in the laboratory at close to the melting temperature.
384 The characterization was made possible by the use of Weighted Burgers Vectors (WBV)
385 analyses that estimate the nature of geometrically necessary dislocations (GNDs) from "rou-
386 tine" EBSD measurements. This method is an alternative to classical techniques (X-ray
387 diffraction, TEM) to identify the Burgers vector components of the GNDs, which has proven
388 to be well adapted to the characterization of large, strongly deformed and recrystallized ice
389 samples.

390 The fraction of dislocations with $[c]$ -component Burgers vector in substructures is similar for
391 various strain geometries and levels (compression or torsion creep, low to high strain). As
392 $[c]$ -component dislocations are energetically less favourable and possess higher Peierls bar-
393 riers than $\langle a \rangle$ dislocations, they are expected in areas submitted to high local stresses.
394 Hence they should play an important role on the dislocation interactions during deforma-
395 tion (responsible for local hardening, internal stress field evolution), but also in the dynamic
396 recrystallization processes (nucleation and grain boundary migration) that strongly impact

397 microstructure and texture evolution in ice sheets. The present experimental evidence for
398 activation of $[c]$ -component dislocations in ice is a first, but essential step for perfecting the
399 current crystal plasticity models and constraining the simulation of the role of these disloca-
400 tions on the mechanical response of ice. To be able to represent this complexity in the chain
401 of modeling tools that leads to the prediction of ice sheet and shelf flow is a step further
402 toward an accurate prediction of their evolution in the frame of global climate changes.

403

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575 **Appendix A. The Weighted Burgers Vector tool**

Dislocations produce local distortions in crystal lattices. When dislocations of different signs are close together these distortions balance out and are not visible at the scale of microns. However when significant numbers of dislocations with the same signs are present, optically visible and (with EBSD) measurable variations of lattice orientation are a consequence the dislocations are then called geometrically necessary dislocations (GNDs). Crystalline materials generally have large elastic moduli meaning that lattice bending due to elastic stress is likely to be small; significant curvature generally relates to the presence of GNDs. Nye (1953) recognized that the lattice curvature can be described by a second rank tensor (now

named after him), in general non-symmetric so having 9 independent components, and that this can be directly linked to the densities of GNDs and their line vectors.

$$\alpha_{i\gamma} = \sum_N \rho^N b_i^N l_\gamma^N \quad (\text{A.1})$$

576 where (N) indicates the Nth type of dislocation line, and for each type ρ is the density
 577 (m^{-2}), b_i the Burgers vector in crystal coordinates (m) and l_γ the unit line vector in sample
 578 coordinates. As written the first index in α relates to the crystal reference frame and the
 579 second to sample reference frame and its units are m^{-1} .

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581 The idea is explained concisely in (Sutton and Balluffi, 1995). It provides in principle
 582 a powerful way of constraining possible GND types from lattice curvature, although there
 583 is not a unique way of deciding on dislocation types (lines and Burgers vectors) without
 584 further information or assumptions. Using EBSD data from 2D maps only 3 out of the 9
 585 components of the tensor can be unambiguously determined without further assumptions,
 586 but Wheeler et al. (2009) argued that even these three can provide valuable insights into
 587 possible dislocation types. Specifically the 3 components α_{i3} (where 3 indicates the sample
 588 coordinate direction perpendicular to the map) make up a vector related to the Burgers vec-
 589 tors of dislocations present. It is weighted with regard to the individual dislocation densities
 590 (through ρ) and the angles the dislocation lines make to the EBSD map (through l_3): hence
 591 Weighted Burgers Vector (WBV). For hexagonal phases such as ice the WBV can indicate
 592 the presence of vectors with a $[c]$ component. Although the WBV does not record all the
 593 GNDs present, it cannot contain phantom directions. If it has a significant $[c]$ component
 594 then at least some of the Burgers vectors of the GNDs must have a $[c]$ component though
 595 this does not mean they have to be parallel to $[c]$. Wheeler et al. (2009) give two versions of
 596 the calculation.

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1. In the differential form, local orientation gradients are used to calculate the WBV. Errors are likely to be significant because of error-prone small misorientations, although Wheeler et al. (2009) show how they may be mitigated by filtering out the shortest WBVs. Adjacent measurement points with misorientations above a threshold value are omitted from gradient calculations, so as to exclude high angle boundaries which lack organised dislocation substructures. The magnitude and direction of the WBV can be displayed on maps in a variety of ways. Given that the shortest WBVs are the most error prone, the display may be chosen to show only those above a particular magnitude (cf. Fig 3a).
2. In the integral form, contour integration round the edge of a region on an EBSD map gives the net dislocation content of that region, though the spatial distribution of dislocations (domains of high or low density) within the region are not constrained. The advantage is that errors are lower. This was asserted in (Wheeler et al., 2009) on the basis that numerical integration reduces the effects of noise, and has since been demonstrated using model EBSD maps for distorted lattices with added noise. The method rejects any regions with high angle boundaries intersecting the border, using the threshold value mentioned above. The integral and differential methods are complementary and are built on the same mathematical foundation (they are linked via Stokes theorem).

616 In this contribution we discuss subgrain boundaries (SGBs). As happens in many mate-
617 rials, GNDs have moved by recovery into discrete structures. As these are two dimensional
618 features, with zero volume, then strictly the dislocation density is infinite. However the inte-
619 gral method still gives a rigorous measure of the dislocation content within a region, if that
620 region includes a subgrain boundary: Sutton and Balluffi (1995) show how closely the anal-
621 ysis of SGBs relates to the analysis of smoothly curved lattices. Hence the direction of the
622 integral WBV still carries useful information related to the GNDs in SGBs. We show colour
623 coded maps of the magnitude of the differential form of the WBV. When this is calculated,
624 numerical differentiation is used. Suppose we have two measurement points with 2.5° differ-
625 ence in orientation separated by a $5 \mu\text{m}$ step size, then the calculated orientation gradient
626 will be $0.5^\circ / \mu\text{m}$. This may in reality be a smoothly curved lattice, or relate to a sharp
627 2.5° SGB passing between the two measurement points the method cannot distinguish such
628 possibilities. If it is an SGB then a smaller step size of $2.5 \mu\text{m}$ would give rise to an apparent
629 gradient of $1^\circ / \mu\text{m}$. Consequently around SGBs the magnitude of the WBV depends on
630 step size (and hence should be interpreted with caution) but the direction can still be used
631 to constrain GND types.

632 The disadvantages of the WBV approach are: it is less precise than calculations using high
633 (angular) resolution EBSD (Wallis et al. 2016), it is biased towards dislocation lines inter-
634 secting the EBSD map at a high angle, and it does not give a decomposition of the GND
635 population into different dislocation types. The latter can be attempted by making particu-
636 lar assumptions about the dislocation types present and then making a calculation assuming
637 total dislocation energy is minimised. As argued in Wheeler et al. (2009), though, minimis-
638 ing energy without taking into account elastic interactions between dislocations (which will
639 mean that line energies are not simply additive) may not be an appropriate procedure.

640 The advantages of the WBV are: it can be calculated from routinely collected EBSD data,
641 in a way free from assumptions except that the elastic strains be small. The integral form
642 reduces the propagation of errors inherent in Kikuchi pattern indexing, and can be used to
643 analyse both smoothly curved lattices and SGBs, without any assumptions about twist or
644 tilt nature. As this contribution shows the WBV approach is sufficient to test the hypothesis
645 that dislocations with $[c]$ component Burgers vectors in ice form a significant part of the
646 dislocation substructures.

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648 **References - Appendix**

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