

1 **The role of strain hardening in the transition from dislocation-mediated to frictional**
2 **deformation of marbles within the Karakoram Fault Zone, NW India**

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8 **Keywords**

9 Calcite; Schmid factor; resolved shear stress; strain hardening; seismogenesis; Karakoram
10 Fault Zone

11 **Abstract**

12 The onset of frictional failure and potentially seismogenic deformation in carbonate
13 rocks undergoing exhumation within fault zones depends on hardening processes that reduce
14 the efficiency of aseismic dislocation-mediated deformation as temperature decreases.
15 However, few techniques are available for quantitative analysis of dislocation slip system
16 activity and hardening in natural tectonites. Electron backscatter diffraction maps of crystal
17 orientations offer one such approach *via* determination of Schmid factors, if the palaeostress
18 conditions can be inferred and the critical resolved shear stresses of slip systems are
19 constrained. We analyse calcite marbles deformed in simple shear within the Karakoram Fault
20 Zone, NW India, to quantify changes in slip system activity as the rocks cooled during
21 exhumation. Microstructural evidence demonstrates that between ~300°C and 200–250°C the
22 dominant deformation mechanisms transitioned from dislocation-mediated flow to twinning

23 and frictional failure. However, Schmid factor analysis, considering critical resolved shear
24 stresses for yield of undeformed single crystals, indicates that the fraction of grains with
25 sufficient resolved shear stress for glide apparently increased with decreasing temperature.
26 Misorientation analysis and previous experimental data indicate that strain-dependent work
27 hardening is responsible for this apparent inconsistency and promoted the transition from
28 dislocation-mediated flow to frictional, and potentially seismogenic, deformation.

29 **1. Introduction**

30 Calcite exhibits marked velocity-weakening behaviour, which may promote nucleation
31 of unstable earthquake ruptures (Han *et al.*, 2010; Verberne *et al.*, 2015; Cowie *et al.*, 2017).
32 Faults hosted in calcite-rich lithologies are therefore major sources of seismic hazard in zones
33 of active continental deformation (Smith *et al.*, 2011). The depth extent of earthquake
34 nucleation in such faults broadly corresponds to the depth at which the activity of temperature-
35 dependent aseismic creep processes can prevent unstable frictional failure under interseismic
36 strain rate conditions (Scholz, 1988; Verberne *et al.*, 2015). Dislocation-mediated deformation
37 mechanisms (potentially including contributions from dislocation creep, low-temperature
38 plasticity, and/or dislocation-accommodated grain boundary sliding) are commonly inferred to
39 have operated in calcite-rich shear zones exhumed from mid-crustal depths and in which the
40 grain size and/or conditions were unfavourable for efficient diffusion creep (e.g. Bestmann *et*
41 *al.*, 2006; Rutter *et al.*, 2007; Wallis *et al.*, 2013; Parsons *et al.*, 2016). Therefore, competition
42 between dislocation-mediated flow and frictional failure may exert an important control on the
43 depth limit of earthquake nucleation. However, the precise microphysical processes that control
44 this transition in natural fault zones remain poorly constrained, particularly in situations where
45 rocks are progressively exhumed during deformation, resulting in a transition from aseismic
46 flow to potentially seismogenic frictional failure within the exhuming rock mass (Handy *et al.*,

47 2007). The strength of rocks undergoing dislocation-mediated deformation is a function of the
48 stresses required to activate dislocation glide on particular crystallographic slip systems, which
49 may depend on both environmental conditions (e.g. temperature, pressure, and strain rate) and
50 other state variables (e.g. composition, dislocation density and distribution) (e.g., Hobbs *et al.*,
51 1972; de Bresser and Spiers, 1997). However, it is challenging to determine the strength and
52 activity of slip systems during dislocation-mediated deformation in natural tectonites, and
53 relatively few techniques are available to do so. As a result, the precise controls on the transition
54 from aseismic creep to frictional failure and potentially seismogenic behaviour in natural fault
55 zones remain poorly constrained.

56 The most common approach to assess the relative activity of different slip systems in
57 natural tectonites is to interpret the slip system(s) most likely to have generated an observed
58 crystallographic preferred orientation (CPO); for example, by determining the slip system
59 inferred to have most readily rotated into orientations with high resolved shear stress (e.g., Toy
60 *et al.*, 2008). However, such analysis is often limited to qualitative interpretations and
61 comparisons. More quantitative information can be gleaned by comparing natural and
62 experimental CPOs to results from simulations of polycrystal plasticity (e.g. Wenk *et al.*,
63 1987). However, this approach tends to place relatively loose constraints on slip system activity
64 due to the large parameter space that needs to be searched (i.e., typically many combinations
65 of slip system strengths and deformation geometries have to be tested) and challenges in
66 comparing natural and simulated CPO geometries quantitatively.

67 Another approach is to analyse crystallographic misorientations resulting from the
68 presence of dislocations within grains (Lloyd *et al.*, 1997; Bestmann and Prior, 2003; Wheeler
69 *et al.*, 2009). However, due to the limited angular resolution of commonly available
70 measurement techniques (e.g. $\sim 0.2^\circ$ for misorientation angles from conventional electron

71 backscatter diffraction, EBSD) such analysis can only sample the fraction of the dislocation
72 population that is arranged into relatively high misorientation substructures such as subgrain
73 boundaries (Prior, 1999). As such, ‘free’ dislocations that are not in subgrain boundaries can
74 be difficult to detect and generally require higher precision and more computationally
75 expensive techniques such as high-angular resolution electron backscatter diffraction (Wallis
76 *et al.*, 2016a, 2017). Moreover, it is unclear to what extent the measured dislocation content
77 was glissile or sessile during deformation. This ambiguity also often applies to direct
78 observation of dislocations, by transmission-electron imaging, chemical etching, or decoration
79 by oxidation.

80 In this contribution, we exploit advances in EBSD (Prior *et al.*, 1999, 2009; Bachmann
81 *et al.*, 2010; Mainprice *et al.*, 2011) to develop a method of slip system analysis based on
82 determination of Schmid factors (Schmid, 1928; Schmid and Boas, 1950; Farla *et al.*, 2011;
83 Hansen *et al.*, 2011). The Schmid factor of a slip system quantitatively describes the relation
84 between resolved shear stress and applied stress state (the higher the Schmid factor, the greater
85 the resolved shear stress on the slip system). This orientation relationship is typically
86 qualitatively inferred when interpreting slip systems that contribute to CPO development (e.g.
87 Toy *et al.*, 2008). However, the Schmid factor not only quantifies this relationship, but also
88 allows for calculation of resolved shear stresses on each slip system, and enables mapping of
89 grains that are (un)favourably oriented for dislocation glide. Relatively few geological studies
90 have utilised detailed Schmid factor analysis. Most of these focussed on stress states associated
91 with radially-symmetric shortening or extension (e.g. Ralser *et al.*, 1991; Farla *et al.*, 2011;
92 Hansen *et al.*, 2011), and to our knowledge, only two have considered simple shear, both
93 focussed on quartz (Law *et al.*, 1990; Toy *et al.*, 2008).

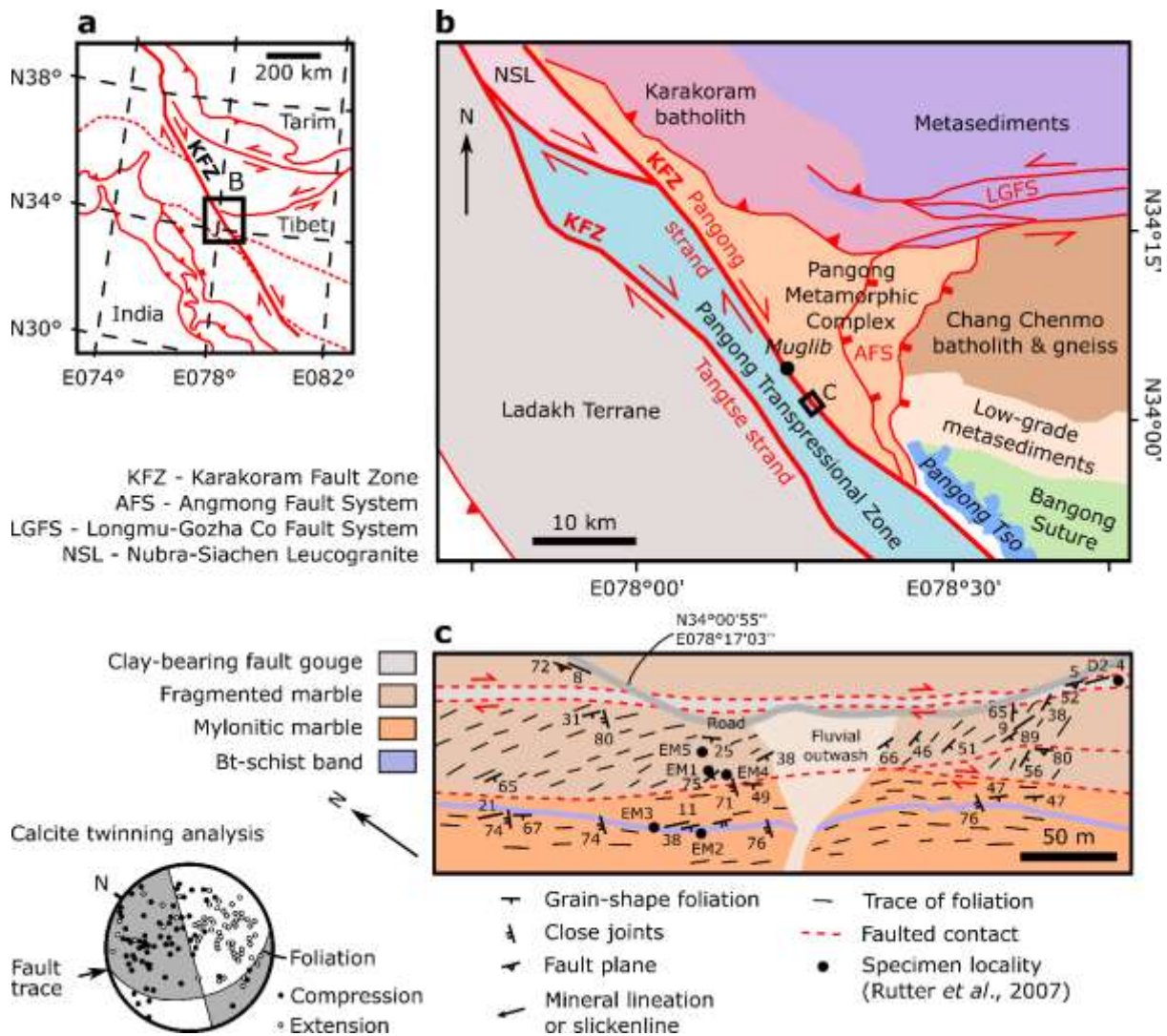
94 To explore the capabilities of this approach, we conduct a detailed Schmid factor

95 analysis of calcite in marbles deformed within a shear zone of the Karakoram Fault Zone
96 (KFZ), NW India (Figure 1). Calcite is particularly well suited for Schmid factor analysis
97 because: (1) techniques are well established to infer palaeostress magnitudes and orientations
98 (Turner, 1953; Rowe and Rutter, 1990) as well as metamorphic and deformation temperatures
99 (Covey-Crump and Rutter, 1989; Burkhard, 1993) from calcite microstructures; (2) the critical
100 resolved shear stresses (CRSSs) of calcite slip systems are experimentally constrained (De
101 Bresser and Spiers, 1997); and (3) these CRSSs and the post-yield behaviour exhibit low strain
102 rate sensitivity (stress exponents in the ranges 5.3–42.6 and 9.3–15.5, respectively) indicating
103 near plastic (as opposed to strain rate-sensitive viscous) behaviour when deformed at
104 differential stresses greater than approximately 30 MPa (Wang *et al.*, 1996; De Bresser and
105 Spiers, 1997). The marbles that we investigate have undergone a protracted deformation history
106 during exhumation and cooling from upper amphibolite-grade conditions to near surface depths
107 and occur in a fault zone that exhibits geomorphological evidence for M_w 7+ earthquakes
108 during the Quaternary (Brown *et al.*, 2002; Rutter *et al.*, 2007; Wallis *et al.*, 2013). We
109 investigate the latter part of this history as the rocks were exhumed and cooled through the
110 frictional-viscous transition zone (Wallis *et al.*, 2013, 2015) and underwent a transition from
111 aseismic flow to potentially seismogenic frictional failure (Rutter *et al.*, 2007). In particular,
112 we use Schmid factor analysis combined with other microstructural observations to test: (1)
113 the manner in which slip system activity potentially varied under evolving temperature and
114 stress conditions during exhumation, (2) the impact of strain hardening on slip system activity,
115 and (3) how these factors affected the transition from crystal plastic to frictional and potentially
116 seismogenic styles of deformation.

117 **2. Geological Setting**

118 The KFZ is a > 800 km long fault zone that strikes NW-SE and delineates the western
119 margin of the Tibetan plateau, accommodating dextral displacement resulting from the India-

120 Asia collision (Figure 1). Along the central KFZ in NW India structures formed at and below
 121 lower amphibolite grade are unequivocally attributable to deformation within the KFZ, and
 122 record a sequence of fault rocks formed at progressively lower temperature due to ongoing
 123 deformation during exhumation (Phillips and Searle, 2007; Wallis *et al.*, 2013, 2015). We
 124 investigate marbles deformed within the Pangong strand of the KFZ, adjacent to the Pangong
 125 Transpressional Zone (PTZ) (Figure 1).



126

127 **Figure 1**

128 *Simplified structural maps of the studied outcrop in the KFZ and wider tectonic context. (a)*
 129 *and (b) are drawn following Phillips and Searle (2007) and Van Buer *et al.*, (2015). (c) is*

130 *modified from Rutter et al. (2007) and includes their specimen localities and the results of their*
131 *calcite twinning analysis.*

132 Between Muglib and Pangong Tso, the Pangong strand deforms rocks of the Pangong
133 Metamorphic Complex (PMC) and juxtaposes them with the PTZ (Figure 1). The PMC consists
134 of banded marbles, amphibolites, and pelites that underwent regional metamorphism under
135 kyanite grade (up to $736 \pm 47^\circ\text{C}$ and 1059 ± 219 MPa, Wallis *et al.*, 2014) and sillimanite grade
136 conditions (Streule *et al.*, 2009), followed by retrograde metamorphism and KFZ deformation
137 under lower amphibolite to sub-greenschist conditions (Rutter *et al.*, 2007; Streule *et al.*, 2009;
138 Wallis *et al.*, 2014; Van Buer *et al.*, 2015).

139 Rutter *et al.* (2007) studied in detail an outcrop of deformed marble near Muglib
140 ($\text{N}34^\circ00'55''$ $\text{E}078^\circ17'03''$), providing the context for this study (Figure 1). Here we
141 summarise the most relevant findings of their study. Grain-shape foliation at this locality dips
142 moderately SW and mineral stretching lineations plunge gently both NW and SE, consistent
143 with the wider KFZ kinematics. Rutter *et al.* (2007) investigated seven marble samples
144 exhibiting microstructures that record mylonitic fabrics evident as varying degrees of dynamic
145 recrystallisation. From the reconstructed grain size of weakly recrystallised host grains, they
146 estimated metamorphic temperatures in the range $300 \pm 20^\circ\text{C}$ to $480 +130/-30^\circ\text{C}$, using the
147 grain size-temperature relationship of Covey-Crump and Rutter (1989). These data place an
148 upper limit on the temperature of overprinting deformation in each sample. The grain size of
149 dynamically recrystallised neoblasts indicates flow stresses in the range of 40 ± 20 MPa to 110
150 ± 40 MPa according to the calibration of Rutter (1995) based on dynamic recrystallisation by
151 grain boundary migration. The choice of this calibration, rather than an alternative based on
152 dynamic recrystallisation by subgrain rotation (Rutter, 1995), is supported by our
153 microstructural analysis in the following sections, which reveals irregular grain boundary
154 morphologies but limited subgrain development, consistent with microstructures reported by

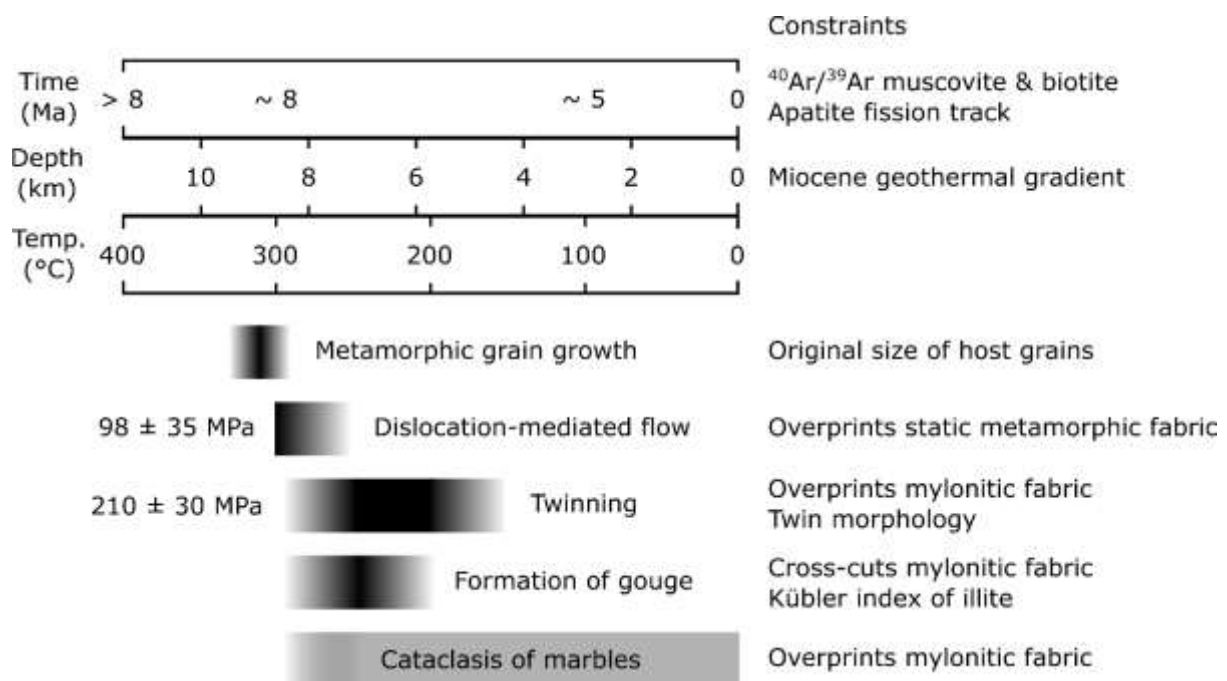
155 Rutter *et al.* (2007). Twin incidence (the percentage of grains, in a given grain size class
 156 interval, that contain optically visible twin lamellae) indicates differential stresses in the range
 157 of 160 ± 30 MPa to 250 ± 30 MPa according to the calibration of Rowe and Rutter (1990).
 158 Thick twins exhibit straight, or curved and tapered boundaries indicating temperatures of 200–
 159 250°C (Burkhard, 1993). These constraints, along with observations that the mylonitic fabric
 160 is cross-cut by calcite veins that are twinned but not mylonitised, suggest that twinning
 161 postdates dynamic recrystallisation (Rutter *et al.*, 2007). Dynamic analysis of calcite twins,
 162 using the method of Turner (1953), indicates a palaeostress state that exerted N-S compression
 163 and E-W extension, consistent with transpressional motion on the NW-SE-trending fault trace,
 164 foliation and lineations (Figure 1).

165 **Table 1** *Microstructural data from calcite in EM1 and inferred deformation conditions*
 166 *experienced by sample EM1, from Rutter et al. (2007)*

Parameter	Value	Notes
Host grain size (μm)	240 ± 11	Measured from weakly recrystallised grains where the original grain outline could be established.
Dynamically recrystallised grain size (μm)	40 ± 9	Measured from digital maps of several hundred grains following Rutter (1995).
Overall (host and recrystallised) grain size (μm)	48 ± 10	Measured from digital maps of several hundred grains following Rutter (1995).
Temperature ($^{\circ}\text{C}$)	310 ± 20	From grain size-temperature relationship of marbles on Naxos, Greece, based on Covey-Crump and Rutter (1989). Taken as an approximate upper-bound for the deformation temperature.
Flow stress (differential) (MPa)	98 ± 35	From dynamically recrystallised grain size using the calibration of Rutter (1995).
Twinning stress (differential) (MPa)	210 ± 30	From the twinning incidence piezometric relationship of Rowe and Rutter (1990).

167

168 The marbles at the Muglib locality are locally overprinted by bands of cataclasite and
 169 are cross-cut by a ~10 m thick zone of clay-bearing fault gouge that displays P foliations and
 170 R₁ Riedel shears consistent with dextral KFZ deformation (Figures 1 and 2). The Kübler index
 171 for authigenic illite in the gouge indicates gouge formation at the anchizone-epizone transition,
 172 tentatively taken to be ~300°C (Figure 2; Rutter *et al.*, 2007). The overprinting of mylonitic
 173 textures by cataclastic textures records the transition from crystal plastic deformation of the
 174 marbles to frictional and potentially seismogenic deformation within the marble cataclasite and
 175 clay-rich gouge zone.



176
 177 **Figure 2** Summary of constraints on the deformation and exhumation histories of the
 178 investigated marble sample EMI (metamorphic grain growth, dislocation-mediated flow, and
 179 twinning) and the surrounding rocks (formation of gouge and cataclasis). Constraints on
 180 temperatures of deformation and metamorphic processes, along with differential stresses, are
 181 obtained or inferred from Rutter *et al.* (2007). The Miocene geothermal gradient within the
 182 Pangong Transpressional Zone was estimated by Wallis *et al.* (2014) to be ~35°C/km based on
 183 geothermobarometry of migmatites formed at ~17 Ma. Time constraints are derived from

184 $^{40}\text{Ar}/^{39}\text{Ar}$ and apatite fission track thermochronology (Boutonnet *et al.*, 2012; Wallis *et al.*,
185 2016b).

186 Thermochronological data from biotite $^{40}\text{Ar}/^{39}\text{Ar}$ (Boutonnet *et al.*, 2012) and apatite fission
187 track (Wallis *et al.*, 2016b) indicate that the Pangong strand and PTZ cooled from $\sim 320^\circ\text{C}$ to
188 $\sim 120^\circ\text{C}$ between ~ 9 Ma to ~ 5 Ma (Figure 2). Dynamic recrystallisation of the marbles therefore
189 likely occurred at 7–9 Ma, and deformation twinning at ~ 6 –7 Ma (Figure 2). Offset geological
190 markers indicate long-term average slip rates of 2.7–10.2 mm/yr since ~ 15 Ma (Phillips *et al.*,
191 2004).

192 Quaternary deformation on the Pangong strand is recorded by offset debris flows and
193 alluvial fans, which indicate an average slip rate of 4 ± 1 mm/yr since 11–14 ka (Brown *et al.*,
194 2002). These landforms are offset by several metres, indicating the occurrence of earthquakes
195 of $> 7 M_w$, with probable recurrence intervals of ~ 500 –1000 years based on both the ages of
196 the landforms and earthquake scaling relationships (Brown *et al.*, 2002; Wallis *et al.*, 2013).
197 Brown *et al.* (2002) inferred that a 7 M_w earthquake has occurred on the Pangong strand since
198 1–2 ka.

199 For this study we focus on mylonitic marble sample EM1 of Rutter *et al.* (2007), for
200 which the deformation conditions are particularly well constrained (Table 1, Figure 2).
201 Notably, this is one of the lowest temperature samples studied by Rutter *et al.* (2007), with the
202 size of host grains placing an upper limit of $310 \pm 20^\circ\text{C}$ on the temperature of formation of the
203 mylonitic fabric (Table 2). This temperature is similar to the temperature of $\sim 300^\circ\text{C}$ estimated
204 for formation of the gouge layer. Therefore, EM1 records mylonitic deformation shortly
205 preceding, or broadly coincident with, the onset of frictional deformation at this structural level.
206 The results derived from detailed analysis of this sample are interpreted in the well-constrained
207 context, outlined above, of evolving deformation processes and conditions as the marbles and

208 surrounding units were exhumed.

209 3. Methods

210 A section of sample EM1 of Rutter *et al.* (2007) was cut parallel to the lineation and
211 perpendicular to the foliation. This section was polished with successively decreasing grit sizes
212 down to 0.25 μm diamond grit, followed by 0.03 μm colloidal silica. Electron backscatter
213 diffraction (EBSD) data were collected on a band of fine-grained matrix calcite using an FEI
214 Quanta 650 FEG E-SEM in the Department of Earth Sciences, University of Oxford. The
215 system is equipped with an Oxford Instruments NordlysNano EBSD camera and
216 AZtec/Channel5 software. Data were collected by automated mapping and consist of 1003 x
217 692 points with a step size of 1 μm . 96.9% of the map area was indexed as calcite, and the
218 majority of points that were not indexed were due to the presence of other phases with rare
219 occurrence, such as quartz. The data were processed to remove individual mis-indexed pixels
220 that had $> 10^\circ$ misorientation from all their neighbours. Next, non-indexed pixels with ≥ 7
221 neighbours belonging to the same grain were filled with the average orientation of their
222 neighbours. Maps of crystal orientation and local misorientation within a 3x3 pixel kernel were
223 produced using Channel5. Pole figures and Schmid factor analyses were computed and plotted
224 using the MATLAB® toolbox MTEX 4.5 (Bachmann *et al.*, 2010; Mainprice *et al.*, 2011).
225 Analysis in MTEX utilised the built-in *SchmidFactor* function to operate on *slipSystem* and
226 stress *tensor* MTEX objects (Supplementary Material). These objects were specified as the
227 relevant slip systems for calcite and stress tensor for the natural deformation as described
228 below.

229 The Schmid factor of a slip/twin system describes the fraction of the applied stress that
230 is resolved onto a particular slip/twin plane in the slip/twin direction, and can be described
231 either as a scalar value (Schmid, 1928; Schmid and Boas, 1950) or as a second rank tensor (e.g.

232 Pokharel *et al.*, 2014). In the conventional definition, originally formulated for uniaxial tension
 233 (Schmid, 1928; Schmid and Boas, 1950), the Schmid factor (m^s) of a slip/twin system (s) is
 234 computed as

$$m^s = \cos\phi\cos\lambda, \quad (1)$$

235 where ϕ and λ are the angles between the maximum principal stress direction and the slip/twin
 236 plane normal and slip/twin direction, respectively. This scalar Schmid factor then relates the
 237 applied differential stress (σ_{diff} , i.e., the difference between the maximum and minimum
 238 principal stresses) to the shear stress resolved on the slip/twin system (τ^s) by

$$\tau^s = m^s\sigma_{\text{diff}}. \quad (2)$$

239 The maximum fraction of the differential stress (σ_{diff}) that can be resolved onto a slip/twin plane
 240 in the slip/twin direction is 0.5. This corresponds to the maximum value of m^s .

241 An alternative approach, which allows analysis of varied stress states, is to employ the
 242 Schmid tensor. The symmetric Schmid tensor (\mathbf{m}^s) describes the projection of the deviatoric
 243 stress tensor ($\boldsymbol{\sigma}$, i.e., with the mean stress subtracted from each normal stress) onto a slip/twin
 244 system (s), defined by unit vectors describing a slip/twin direction (\mathbf{b}^s) and slip/twin plane
 245 normal (\mathbf{n}^s), by

$$\tau^s = \frac{1}{2}(\mathbf{b}^s \otimes \mathbf{n}^s + \mathbf{n}^s \otimes \mathbf{b}^s) : \boldsymbol{\sigma} = \mathbf{m}^s : \boldsymbol{\sigma}, \quad (3)$$

246 which yields the shear stress resolved on that slip system (τ^s) (for a recent review, see Pokharel
 247 *et al.*, 2014). In other words, the components of \mathbf{m}^s determine the fraction of each component
 248 in the deviatoric stress tensor that is resolved onto the slip/twin plane in the slip/twin direction.
 249 In plastically deforming crystals, dislocation glide or twinning can only occur when τ^s exceeds
 250 a threshold value, that is, the critical resolved shear stress (τ_c^s) (Schmid, 1928; Schmid and
 251 Boas, 1950). The value of τ_c varies with slip/twinning system, material, and environmental
 252 conditions, primarily temperature (e.g. De Bresser and Spiers, 1997; Morales *et al.*, 2014).

253 To calculate Schmid factors for past deformations, constraints on the palaeo-stress state
 254 are required. Differential stresses applied to sample EM1 have been estimated from
 255 palaeopiezometric analyses (Table 1; Rutter *et al.*, 2007), but the shape of the stress tensor also
 256 needs to be determined. Based on the macroscopic kinematics of the Pangong strand, along
 257 with asymmetric deformation microstructures and distributions of foliations, lineations, and
 258 palaeostress orientations reported by Rutter *et al.* (2007) (Figure 1), we infer that the
 259 deformation history of EM1 was dominated by simple shear. To further test the hypothesis that
 260 deformation was dominantly simple shear, we apply the approach of Michels *et al.* (2015) to
 261 determine the macroscopic vorticity axis from crystallographic orientation data. This method
 262 uses principal geodesic analysis of intragranular orientation dispersion to fit a single
 263 ‘crystallographic vorticity axis’ (CVA) to each grain. For samples in which dislocation activity
 264 accommodated significant strain, CVAs averaged over many grains may record the vorticity
 265 axis of deformation.

266 Values of the scalar Schmid factor, m^s , can be computed by entering a normalised stress
 267 tensor, $\hat{\sigma}$, in the right hand side of Equation 3 to give

$$m^s = \mathbf{m}^s : \hat{\sigma}. \quad (4)$$

268 Assuming macroscopic simple shear deformation within the Pangong strand, and defining $\hat{\sigma}$ as

$$\hat{\sigma} = \boldsymbol{\sigma} / \sigma_{\text{diff}}, \quad (5)$$

269 gives

270

$$\hat{\sigma} = \begin{bmatrix} 0 & 1/2 & 0 \\ 1/2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \quad (6)$$

271 This formulation denotes that the maximum possible value of the shear stress components is
 272 half the magnitude of the applied differential stress. This approach is equivalent to that of Law
 273 *et al.* (1990), except that they normalised the shear stress components by their maximum

274 possible magnitude, which leads to non-zero terms in $\hat{\sigma}$ having a value of one and m with values
275 in the range 0–1. In contrast, by normalising the shear stress components by the magnitude of
276 the differential stress, we obtain values of m in the conventional range 0–0.5, which can be
277 used more directly in conjunction with differential stress magnitudes from palaeopiezometry.
278 If crystal orientations can be mapped across the microstructure and the differential stress
279 measured or inferred, then the scalars τ^s and m^s can be mapped across the microstructure.

280 To determine which of the calcite slip systems could potentially be activated by the
281 palaeostresses, we transform the normalised stress tensor, $\hat{\sigma}$, in Equation 6, into the crystal
282 coordinate system of each measured orientation and compute m^s for each slip system. This
283 stress tensor, $\hat{\sigma}$, and Schmid tensor, m^s , allow calculation of m^s by Equation 4. Values of m^s are
284 multiplied by σ_{diff} to calculate the corresponding shear stress, τ^s , resolved on each slip system
285 according to Equation 2. In crystals with multiple symmetrically equivalent variants of each
286 slip/twin system, such as calcite, the variant with the highest value of m^s will slip/twin at the
287 lowest applied stresses.

288 Once the Schmid factor and resolved shear stress for each slip system have been
289 calculated, it is necessary to assess whether the applied stress was sufficient to activate
290 dislocation glide, i.e., whether $\tau^s > \tau_c^s$. The experimental work on calcite single crystals and
291 data compilation of De Bresser and Spiers (1993, 1997) established the operative calcite slip
292 and twinning systems and their absolute CRSSs over the temperature range 20–800°C.
293 Therefore, we take the values of τ_c for $\{e\}$ -twinning and dislocation slip on the $\{r\}$ - and $\{f\}$ -
294 planes, for temperatures of 200°C and 300°C, from De Bresser and Spiers (1997) (Table 2).
295 These temperatures approximately correspond to the lower- and upper-bounds for temperature
296 constrained by the geological context (Section 2), for the occurrence of twinning and dynamic
297 recrystallisation respectively in sample EM1. We use values of τ_c for the variant of the $\{f\}$ slip
298 system active at $\leq 300^\circ\text{C}$ (i.e., $\{-1012\}\langle 2-201\rangle$), rather than the variant active at $\geq 500^\circ\text{C}$ (i.e.,

299 $\{-1012\}\langle -101-1\rangle$ in the experiments of De Bresser and Spiers (1997). These experiments
 300 demonstrated that values of τ_c for calcite slip systems depend little on strain rate (stress
 301 exponents in the range 5.3–42.6), which reduces the uncertainty associated with applying them
 302 to analyse deformation that occurred at lower strain rates than the deformation experiments.
 303 The range of values of τ_c for slip on the $\{r\}$ system at 300°C, reported by De Bresser and Spiers
 304 (1997), is on the order of 20 MPa. As this range is smaller than the uncertainties of the
 305 palaeopiezometric stress estimates for the nature samples (30–35 MPa, Table 1, Rutter *et al.*,
 306 2007), we consider only the best-fit values of τ_c at each temperature, interpolated from the fits
 307 reported by De Bresser and Spiers (1997), to make simple first-order comparisons. From the
 308 critical resolved shear stresses constrained by experiments (De Bresser and Spiers, 1997) and
 309 from the applied differential stresses constrained by palaeopiezometry (Rutter *et al.*, 2007), we
 310 compute the minimum value of m^s (i.e. m_{\min}) necessary to initiate twinning or dislocation glide
 311 on each system by

$$m_{\min} = \tau_c / \sigma_{\text{diff}}, \quad (7)$$

312 (Table 2).

313 **Table 2** Summary of slip system information for EMI

Deformation temperature (°C)	Slip system	τ_c (MPa)	Applied differential stress (MPa)	Minimum m for twinning/dislocation glide
300	$\{e\}$ -twinning $\{-1018\}\langle 40-41\rangle$	2	98 ± 35	0.02
300	$\{r\}$ -slip $\{10-14\}\langle -2021\rangle$	22	98 ± 35	0.22
300	$\{f\}$ -slip $\{-1012\}\langle 2-201\rangle$	52	98 ± 35	0.53
200	$\{e\}$ -twinning $\{-1018\}\langle 40-41\rangle$	3	210 ± 30	0.01
200	$\{r\}$ -slip	41	210 ± 30	0.20

	{10-14}<-2021>			
200	{f}-slip	77	210 ± 30	0.37
	{-1012}<2-201>			

314

315 By computing maps of m^s , we are able to determine which grains have $m > m_{\min}$ (and
316 $\tau^s > \tau_c^s$) and therefore estimate the area fraction of grains that can deform by each deformation
317 mode under the applied palaeostress conditions. We also perform this analysis for applied
318 stresses throughout the range 1–250 MPa to explore the effects of increasing stress acting on
319 the mapped microstructure at 300°C and 200°C. An MTEX script to carry out these procedures
320 is included as Supplementary Material.

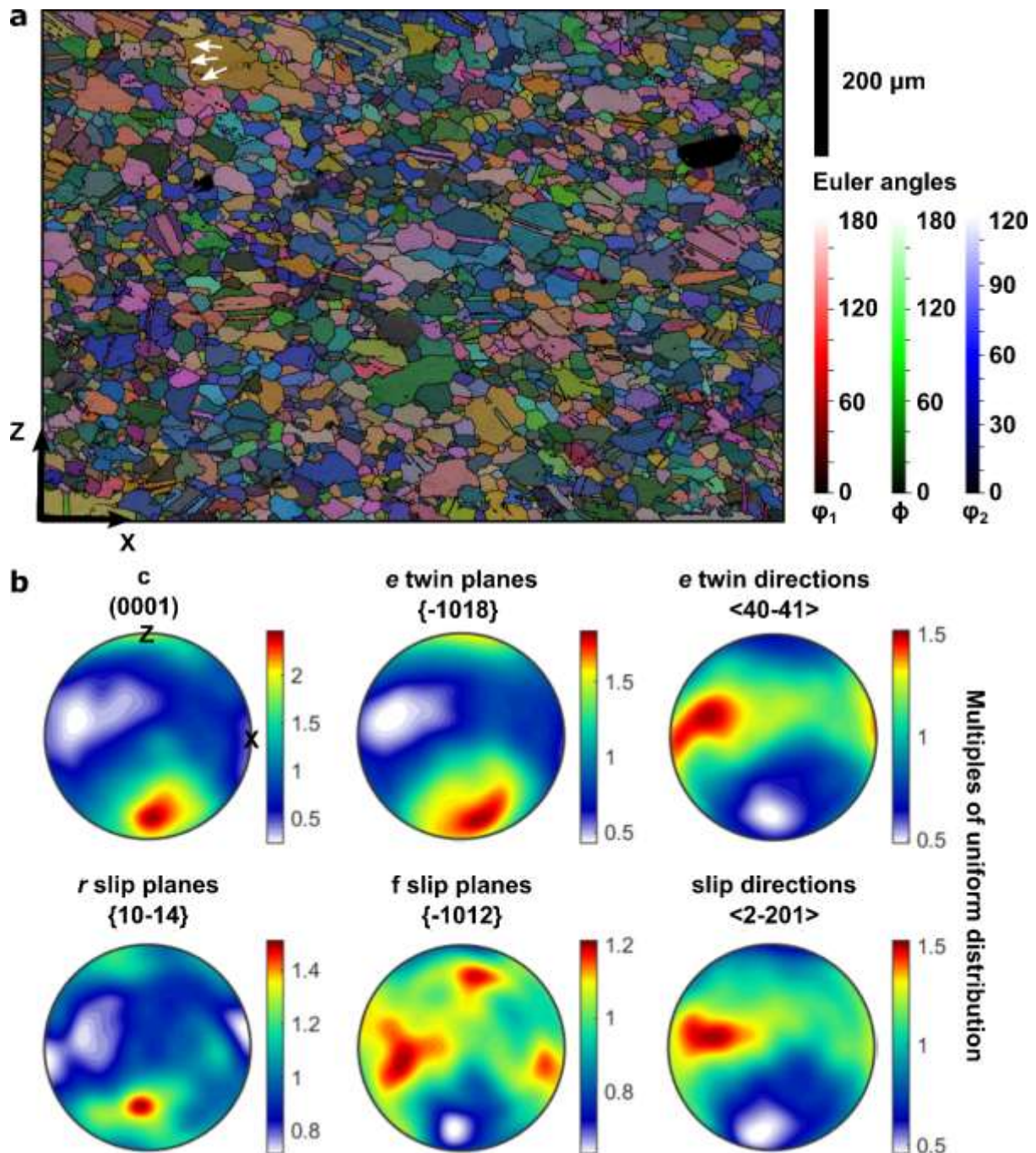
321 An important caveat to the analysis described here is that the stress state would need to
322 be homogeneous throughout the material for the point-by-point Schmid factors to be reliably
323 accurate. However, micromechanical models of viscoplastic deformation that explicitly
324 account for detailed microstructures suggest that stress and strain vary significantly among
325 grains and are even distributed heterogeneously within grains (e.g. Pokharel *et al.*, 2014).
326 Heterogeneous distributions of stress and strain arise due to the elastic and plastic anisotropy
327 of individual grains and local grain-grain interactions. Such heterogeneities have been recently
328 observed in experimentally deformed Carrara marble (Quintanilla-Terminel and Evans, 2016).
329 Thus, rather than interpreting the behaviour of specific individual points or grains, we take the
330 approach of considering the distribution of Schmid factors and predicted slip/twin system
331 activity over ~2500 grains, providing an averaged estimate of the slip system activity across
332 the bulk material. We suggest that these averaged values of slip system activity are more
333 reliable than the results for individual grains displayed in the maps because the stress states
334 averaged throughout the rock volume must equal the macroscopic applied stress state. The
335 Schmid factor approach offers a simple method to consider a larger number of grains than

336 would be possible using more advanced computational techniques that include stress
337 heterogeneity.

338 During progressive deformation, Schmid factors define only an instantaneous
339 relationship between stress and crystal orientation, as ongoing crystal rotations continuously
340 modify the Schmid factors for each slip system in aggregates deforming by dislocation glide.
341 Therefore, Schmid factors calculated from the microstructure of an exhumed rock indicate
342 which slip systems would have been well aligned for dislocation glide during the *next*
343 increment of slip (which *ipso facto* never occurred). In contrast, use of mapped Schmid factors
344 to interpret prior deformation that led to formation of the observed microstructure is more
345 complex and requires additional assumptions/constraints regarding microstructural evolution
346 (particularly grain rotations) or steady state. Therefore, Schmid factor analysis is well suited to
347 our application, in which the mylonitic microstructure records a snapshot formed at ~300°C as
348 the dislocation-mediated processes that formed it ceased to operate, and in which our aim is to
349 investigate the controls on the *subsequent* evolution of deformation processes.

350 **4. Results**

351 The measured CPO is consistent with the inference of simple shear deformation. Calcite
352 {*c*}, {*e*} and {*r*} poles are clustered in point maxima near the foliation normal, whereas the
353 twin and slip directions are weakly girdled with superimposed point maxima close to the
354 lineation direction (Figure 3). The CPO of {*f*} planes is weak, with three low intensity maxima
355 (Figure 3b).

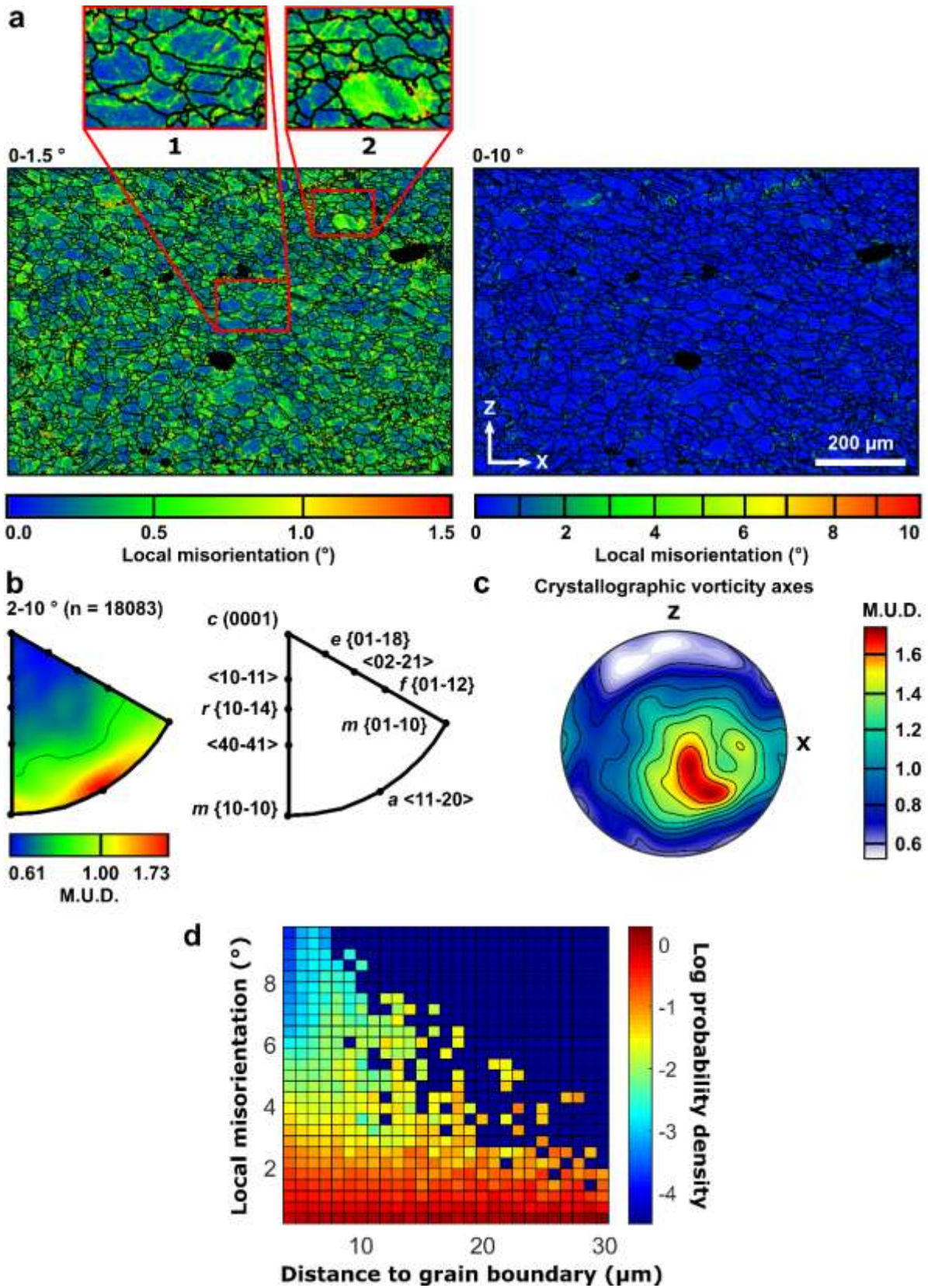


356

357 **Figure 3** Crystal orientation data from EBSD analysis of sample EM1. (a) Map of crystal
 358 orientations colour-coded using Euler angles in the convention of Bunge (1982), superimposed
 359 on a grey-scale map of diffraction pattern band contrast. Black lines mark boundaries of $\geq 10^\circ$
 360 misorientation between adjacent pixels. White arrows indicate an example of a lobate and
 361 irregular grain boundary. (b) Lower hemisphere pole figures of crystal planes and directions

362 *relevant to the calcite slip and twin systems considered. X indicates the lineation and Z the*
363 *foliation normal. Shear sense is top-to-right.*

364 Crystallographic misorientation data indicate that relatively few subgrain boundaries
365 with misorientations in the range 1–10° are present (Figure 4a), but the inverse pole figure of
366 misorientation axes demonstrates that those subgrain boundaries that are present have rotation
367 axes parallel to the $a\langle 11-20 \rangle$ directions (Figure 4b). The map of local misorientations scaled
368 from 0–1.5° reveals the presence of abundant low-angle misorientations of ~1° (Figure 4a).
369 These misorientations are arranged in networks of low-angle subgrain boundaries and regions
370 of more distributed lattice curvature. The portions of grains close to grain boundaries have
371 greater local misorientation relative to the interior, representing higher dislocation densities,
372 than grain interiors (Figure 4a,d). The visible microstructure indicates that the measurements
373 are generally above the background noise level, despite the small misorientation angles.
374 Crystallographic vorticity axes are generally aligned sub-perpendicular to both the lineation
375 and foliation normal, consistent with dominantly simple shear (Figure 4c; Michels *et al.*, 2015).
376 This observation provides independent support for our choice of stress state (i.e. Equation 6)
377 used for Schmid factor analysis.

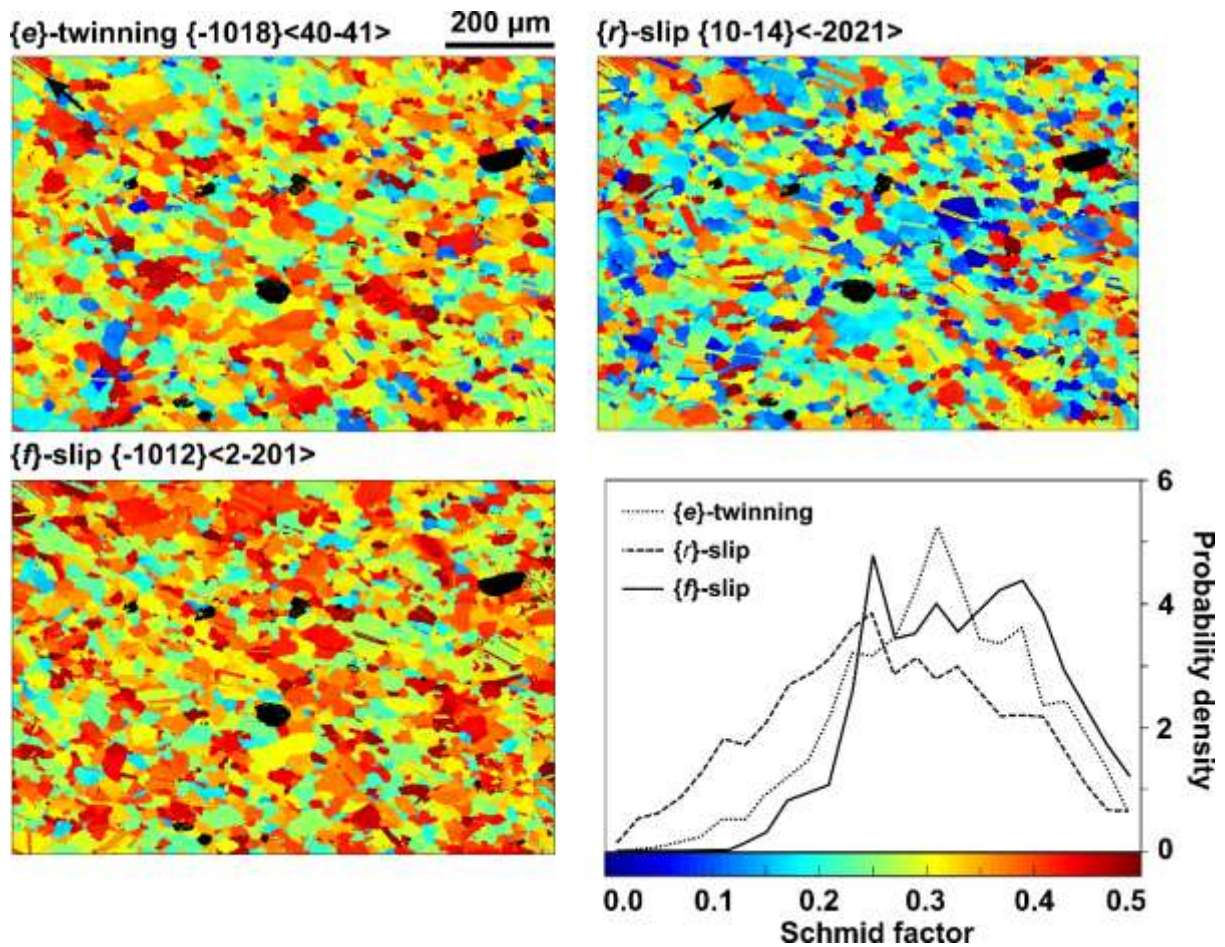


378

379 **Figure 4** Misorientation analysis of EM1. (a) Maps of local misorientation within 3x3 pixel
 380 kernels, scaled for two ranges of misorientation angle. Grain and twin boundaries are overlaid

381 as black lines. Region 1 exhibits higher values of misorientation concentrated near grain
382 boundaries. Region 2 shows both subgrain boundaries (top left) and more widespread
383 misorientation (lower right). (b) Inverse pole figure presents the orientation of misorientation
384 axes of subgrain boundaries in the crystal reference frame. (c) Stereoplot illustrating
385 contoured crystallographic vorticity axes (one axis per grain), determined using the method of
386 principal geodesic analysis of intragranular dispersion (Michels et al., 2015). X indicates the
387 lineation and Z the foliation normal. (d) Probability density functions (PDFs) of local
388 misorientation in 1 μm bins of Euclidean distance to grain boundary (including twin
389 boundaries) within the 2-D EBSD map plane, i.e. each column is a different PDF. This plotting
390 approach addresses the bias of having different numbers of points at each distance by allowing
391 PDFs to be compared between different distances. Local misorientation was calculated within
392 a 3x3 pixel kernel. Only points at distances $> 3 \mu\text{m}$ from a grain boundary are plotted to avoid
393 processing artefacts in kernels that include boundaries. Grain boundaries were defined as
394 $>10^\circ$ misorientation.

395 Maps of Schmid factor show grain-by-grain variations in the maximum Schmid factor
396 of each family of slip systems (Figure 5). Each family of slip systems exhibits a wide range of
397 Schmid factors within the map area (Figure 5). The probability densities of Schmid factors
398 exhibit similar general form between each slip system, being skewed towards high Schmid
399 factors. The distribution describing Schmid factors for slip on $\{f\}$ -planes is most heavily
400 skewed towards high values (Figure 5). Schmid factors vary between twins and host grains,
401 evident as stripes of different Schmid factor. More subtle variations in Schmid factor are
402 apparent across subgrain boundaries.

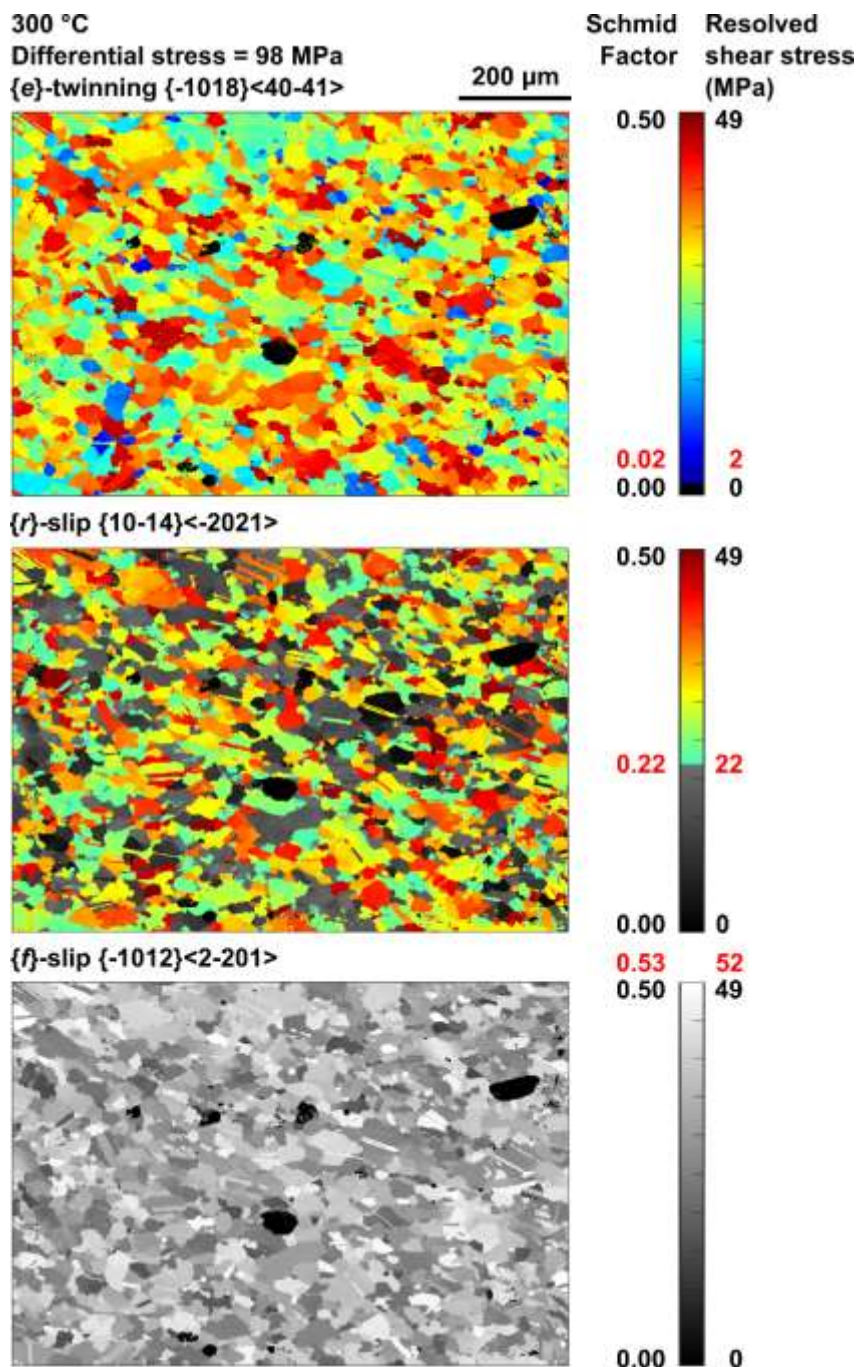


403

404 **Figure 5** Maps and probability density plots of Schmid factor for each calcite slip/twin system.
 405 Probability densities were calculated for bins of 0.02 width. The black arrow in the upper-left
 406 of the map of Schmid factor for {e}-twinning indicates an example of changes in Schmid factor
 407 across twin boundaries. The black arrow in the upper-left of the map of Schmid factor for {r}-
 408 slip indicates an example of changes in Schmid factor across a subgrain boundary.

409 The apparent proportions of grains that can deform by each slip/twin system vary across
 410 the temperature and stress ranges within which deformation is inferred to have taken place
 411 (figures 6–8). At 300°C and a piezometric stress of 98 MPa, none of the grains can deform by
 412 {f}-slip because τ_c (52 MPa) is greater than 0.5 of the applied stress (figures 6 and 8a, Table
 413 2). However, within the upper-bound uncertainty of the stress estimate, up to 29% of the
 414 microstructure can deform by {f}-slip (Figure 8a). Within the stress uncertainty, 63 +18/-39%

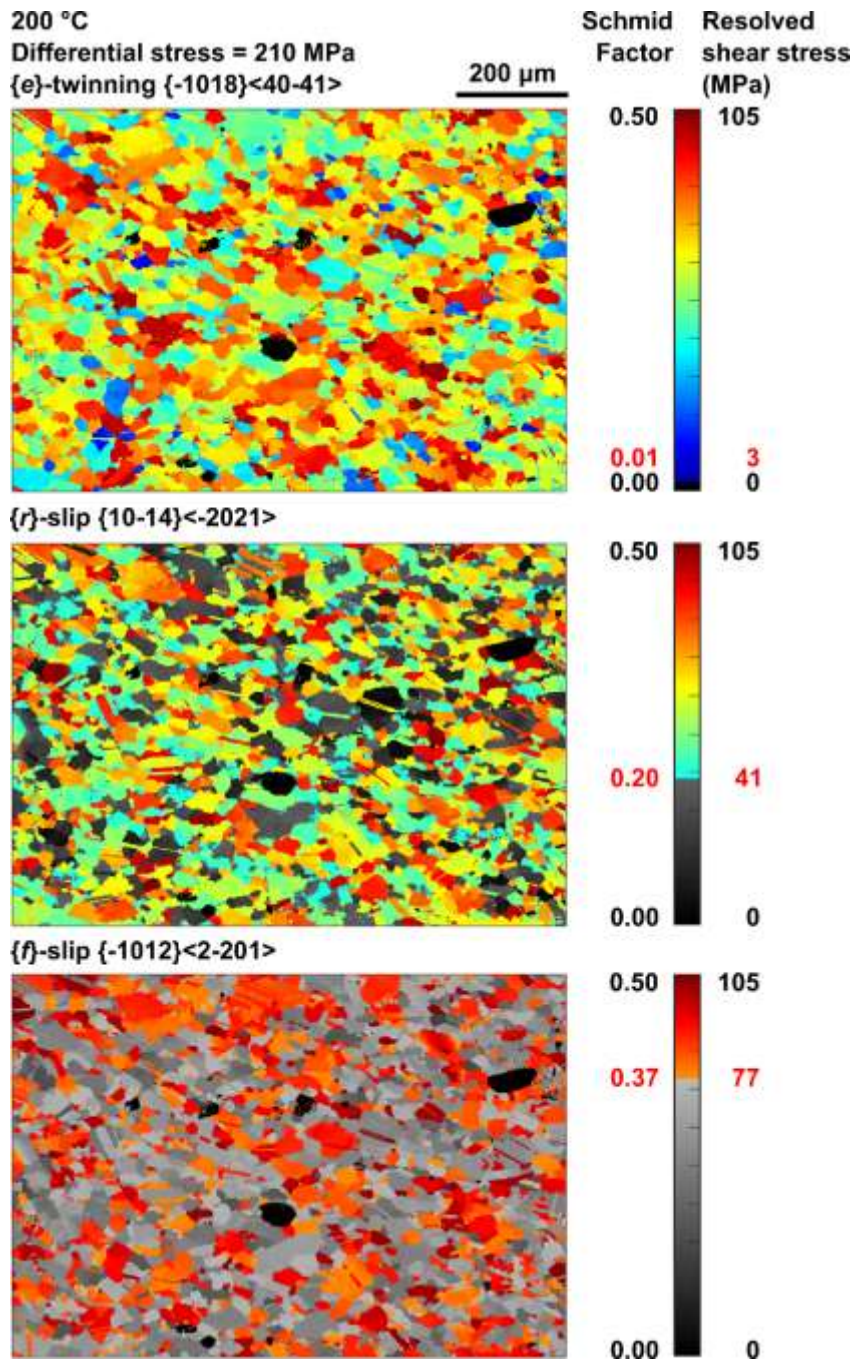
415 can deform by $\{r\}$ -slip and 100% can deform by $\{e\}$ -twinning (figures 6 and 8a). At 200°C
 416 and the higher stress conditions estimated from twinning incidence, 39 +17/-25% should be
 417 able to deform by $\{f\}$ -slip and 72 +7/-10% should be able to deform by $\{r\}$ -slip (figures 7 and
 418 8b). Again 100% of the grain area exceeds the critical resolved shear stress for $\{e\}$ -twinning
 419 (Figures 7 and 8b).



420

421 **Figure 6** Maps of grains that exceed the minimum Schmid factor necessary to initiate twinning

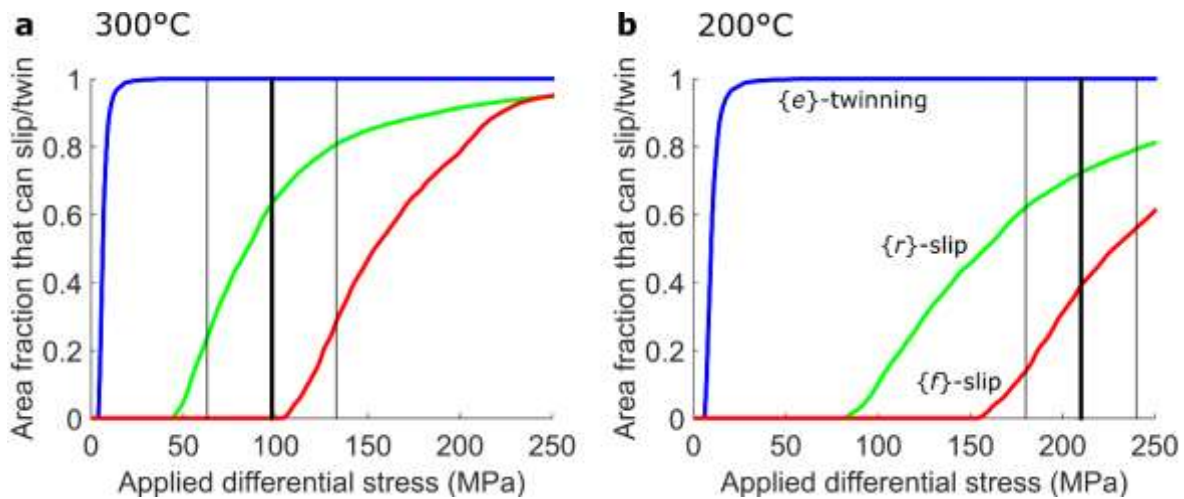
422 or dislocation glide at 300°C and the stress determined from dynamically recrystallised grain
 423 size. The minimum Schmid factor and corresponding critical resolved shear stress are marked
 424 in red beside the colour bar. Areas above and below this threshold are represented by colour-
 425 scale and grey-scale respectively.



426

427 **Figure 7** Maps of grains that exceed the minimum Schmid factor necessary to initiate twinning
 428 or dislocation glide at 200°C and the stress determined from twinning incidence. The minimum

429 Schmid factor and corresponding critical resolved shear stress are marked in red beside the
 430 colour bar. Areas above and below this threshold are represented by colour-scale and grey-
 431 scale respectively.



432

433 **Figure 8** Area fraction of grains in mapped microstructure that can deform by
 434 twinning/dislocation glide at (a) 300°C and (b) 200°C, under applied differential stresses
 435 ranging from 0–250 MPa. The stress estimates are determined from (a) dynamically
 436 recrystallised grain size (at ~300°C) and (b) twinning incidence (at 200–250°C) and are
 437 marked by vertical bold black lines with uncertainties marked by fine black lines.

438 5. Discussion

439 5.1. Effects of changing temperature and stress on slip system activity

440 This study constitutes a detailed examination of the microstructure of a single sample
 441 of marble, EM1, deformed by dislocation glide and twinning whilst the Pangong Metamorphic
 442 Complex, within which it was situated, was exhumed through the frictional-viscous transition
 443 zone at temperatures of approximately 200–300°C around 7–8 Ma (Rutter *et al.*, 2007; Wallis
 444 *et al.*, 2013, 2016b). Although this sample represents only a small volume of the fault zone
 445 material, the surrounding rocks, which include a wide range of fault rock types formed under

446 varied conditions, provide a well-documented context (Rutter *et al.*, 2007) in which to interpret
447 the changing styles of deformation in both sample EM1 and the unit as a whole (Figures 1 and
448 2). In particular, the frictional fault rocks, i.e. marble cataclasites and clay-rich gouge, are more
449 spatially localised than the mylonitic marbles that they overprint (Figure 1; Rutter *et al.*, 2007).
450 Therefore, microstructural evidence for earlier deformation mechanisms and processes, such
451 as the recrystallised microstructure indicative of dislocation-mediated deformation in EM1,
452 remains preserved and available for analysis, whilst the subsequent switch to frictional failure
453 of the adjacent rocks can be inferred from the locally overprinting frictional fault rock types.
454 The Kübler index of illite in the clay-rich gouge layer suggests that it formed at up to
455 approximately 300°C and therefore closely post-dated mylonitisation, which ceased at
456 approximately 300°C (Figure 2; Rutter *et al.*, 2007). As such, formation of the gouge was
457 broadly coincident with twinning in the mylonitic marbles, which occurred at approximately
458 200–250°C (Figure 2, Burkhard, 1993). Similarly, the mylonitic marbles are fragmented and
459 overprinted by cataclasites in a zone tens of metres wide adjacent to the gouge layer (Figure 1;
460 Rutter *et al.*, 2007). The fragmented marbles contain relict microstructures indicative of partial
461 dynamic recrystallisation by grain boundary migration prior to cataclasis (Rutter *et al.*, 2007).
462 Therefore, cataclasis must also have occurred after mylonitisation and been broadly coincident
463 with, or more recent than, formation of the gouge layer and twinning in the mylonites (Figure
464 2). As the mylonitic fabric of EM1 formed at temperatures similar to or only slightly above
465 those at which frictional deformation commenced in the adjacent rocks, we infer that the
466 mylonitic microstructure of the sample remained largely unmodified during subsequent
467 exhumation. We also note that EM1 is located close to the boundary between the mylonitic and
468 fragmented marbles and therefore is well suited (in both spatial location and timing of
469 formation of its deformation fabric) to recording the transition between dislocation-mediated
470 and frictional deformation. These relationships allow us to examine one sample in detail whilst

471 also considering the significance of the deformation processes in the evolution of the rock unit
472 more widely.

473 The predicted changes in slip system activity in EM1 (Figure 8) reflect the combined
474 influence of changing stress and temperature conditions as the rock was exhumed. The decrease
475 in temperature from 300°C to 200°C increases values of τ_c by factors of 1.5–1.9 (Table 2),
476 acting to inhibit dislocation glide. However, palaeopiezometric estimates suggest that, at the
477 same time, the applied stress increased by a factor of ~ 2.1 (Rutter *et al.*, 2007). As a result, a
478 greater fraction of the microstructure appears to have potential to deform by dislocation glide
479 at 200°C and 210 ± 30 MPa than at 300°C and 98 ± 35 MPa (Figures 6–8). This effect is
480 particularly pronounced for $\{f\}$ -slip, which has the highest τ_c . The 98 ± 35 MPa applied stress
481 at 300°C is generally insufficient for slip on $\{f\}$ -planes, whereas, at 200°C and 210 ± 30 MPa,
482 $39 +17/-25\%$ of the microstructure exceeds τ_c for $\{f\}$ -slip (Figure 8). However, these findings
483 are superficially at odds with other microstructural and structural features that indicate
484 dislocation activity was greater at higher temperature. Within the sample, dynamically
485 recrystallised grains formed under the lower stress, higher temperature conditions, and were
486 not overprinted by further dynamic recrystallisation under the subsequent higher stress, lower
487 temperature conditions (Figure 2; Rutter *et al.*, 2007). More widely in the rock unit, the
488 mylonitic textures formed at the higher temperatures are overprinted by cataclasites and gouges
489 formed at similar and lower temperatures (Figure 2; Rutter *et al.*, 2007). One possible
490 explanation for the discrepancy between the predictions of slip system activity (Figure 8) and
491 the observed (micro)structural evolution is that the stresses predicted from twinning incidence
492 by the palaeopiezometer of Rowe and Rutter (1990) are inaccurate. This method for estimating
493 past stresses is fully empirical and lacks a detailed microphysical basis often used to support
494 application of laboratory-derived relationships to natural contexts. However, the predicted
495 stresses would have to be in error by approximately a factor of two, or approximately 100 MPa,

496 to preclude slip on the $\{r\}$ system in well oriented grains (Figure 8). Therefore, in the following
497 section, we discuss in more detail the evolution of deformation processes as the rock cooled
498 during exhumation to explore the possibility that microphysical processes are responsible for
499 lack of significant dislocation glide under the low temperature and high stress conditions.

500 **5.2. Evolution of deformation mechanisms during exhumation through the frictional-** 501 **viscous transition zone**

502 Calcite microstructures in EM1 (this study) and the other samples reported by Rutter *et*
503 *al.* (2007) include lobate grain boundaries (Figures 3 and 4), porphyroclasts with fine grained
504 mantles (Rutter *et al.*, 2007), and subgrain boundaries (Figure 4). These microstructural
505 observations indicate deformation by dislocation motion, accompanied by dynamic
506 recrystallisation due to grain boundary migration and (to a lesser extent) subgrain rotation
507 (Figures 3 and 4; Rutter *et al.*, 2007). Crosscutting relationships and contrasting
508 palaeopiezometric estimates indicate that these microstructures formed close to the upper
509 bound temperature of $310 \pm 20^\circ\text{C}$ for EM1, constrained by the (now partially overprinted)
510 equilibrium grainsize (Figure 2; Rutter *et al.*, 2007).

511 The general scarcity of subgrain boundaries with misorientations of several degrees or
512 more (Figure 4) indicates that dislocation climb was limited at these temperatures and/or that
513 recovery of intracrystalline strain occurred by other processes, such as cross-slip, dislocation
514 annihilation or climb into high-angle grain boundaries and grain-boundary migration (de
515 Bresser and Spiers, 1990; Liu and Evans, 1997). Misorientation analysis of the few subgrain
516 boundaries that are present indicates that they mostly involve lattice rotations around axes
517 parallel to $a\langle 11-20 \rangle$. Bestmann and Prior (2003) demonstrated that misorientation axes parallel
518 to $\langle a \rangle$ in calcite cannot represent twist boundaries due to the lack of appropriate screw
519 dislocation types in calcite. They also suggested that a precisely defined misorientation axis

520 could result from coupled activity of glide in two co-planar directions, but that this is unlikely
521 in general as it requires an equal contribution from both slip directions. Rather, the
522 misorientation axes are consistent with tilt boundaries constructed of edge dislocations on the
523 $r\{10\text{-}14\}\langle\text{-}2021\rangle$ or $f\{-1012\}\langle10\text{-}11\rangle$ slip systems (Bestmann and Prior, 2003). However, as
524 $f\{-1012\}\langle10\text{-}11\rangle$ is the high temperature form of $\{f\}$ -slip, active above 500°C in the
525 experiments of De Bresser and Spiers (1997), dislocations on this slip system are unlikely to
526 have formed the subgrain boundaries in EM1. Edge dislocations on the low temperature $\{f\}$ -
527 slip system, $f\{-1012\}\langle2\text{-}201\rangle$, which we have analysed here, do not generate lattice rotations
528 around $\langle a \rangle$ and therefore also cannot form the subgrain boundaries in EM1. We infer therefore
529 that the subgrain boundaries are constructed of edge dislocations on the $r\{10\text{-}14\}\langle\text{-}2021\rangle$ slip
530 system. This interpretation is consistent with the estimate that ~63–72% of the microstructure
531 had sufficient resolved shear stress for slip on $r\{10\text{-}14\}\langle\text{-}2021\rangle$ across the range of conditions
532 investigated (Figure 8). These conclusions are similar to those reached by Bestmann and Prior
533 (2003), who investigated calcite deformed at temperatures in the range ~300–350°C.

534 The marble mylonites are sequentially overprinted by more localised marble cataclasite
535 and the clay-bearing gouge zone (Figures 1 and 2; Rutter *et al.*, 2007). These cross-cutting
536 relationships and associated microstructures indicate that, as temperature decreased during
537 exhumation, stress increased sufficiently that the frictional failure strength of the rock was
538 exceeded. This onset of frictional deformation occurred after mylonitisation at ~300°C and
539 before, or broadly coincident with, development of the preserved set of twins in the marble
540 (200–250°C, Figure 2; Rutter *et al.*, 2007). We provide additional insight through our Schmid
541 factor analysis, which demonstrates that the calcite would still have had sufficient resolved
542 shear stress for dislocation glide in most crystal orientations *if* CRSS values taken from the
543 yield points in single crystal experiments are applicable to the natural microstructure. The
544 resolved shear stress appears sufficient for considerable dislocation glide even at the lower

545 temperatures of 200–250°C (Figures 7 and 8) at which only twinning and frictional failure
546 occurred (Rutter *et al.*, 2007). In fact, the predictions of slip system activity (Figure 8) indicate
547 that the applied shear stress would have to have been approximately half of the value measured
548 by twinning incidence to de-activate $\{r\}$ -slip in a significant portion of the microstructure.

549 It is important to note that the τ_c values upon which this analysis is based were
550 experimentally determined for relatively low strains of just a few percent ($\leq 4.3\%$, De Bresser
551 and Spiers, 1997). De Bresser and Spiers (1997) recognized significant strain hardening in their
552 experiments, such that the CRSS obtained from yield point stresses effectively places a
553 minimum bound on the resolved shear stress required for further dislocation glide on the
554 corresponding slip system at higher strains. This observation led De Bresser and Spiers (1997)
555 to suggest that strain hardening on the first slip system to activate (i.e., $\{r\}$ -slip) could lead to
556 a strain-induced transition to a different dominant slip system (e.g., $\{f\}$ -slip).

557 Strain hardening in calcite during cooling is likely the result of a reduction in the
558 efficiency of thermally activated intracrystalline strain recovery processes such as cross slip or
559 dislocation climb into either static or migrating twin, subgrain, and grain boundaries (Rutter,
560 1974; De Bresser and Spiers, 1990; Kennedy and White, 2001). As a result, dislocation
561 interactions and long-range stress fields associated with accumulations of blocked dislocations
562 would have inhibited further dislocation glide (Fleck *et al.*, 1994; Renner *et al.*, 2002). Two
563 lines of microstructural evidence support this interpretation. The widespread occurrence of
564 subgrain boundaries with low misorientation angles of approximately 0.5–1.0° (Figure 4)
565 suggests that significant dislocation content is present but that dislocations could not organise
566 into lower-energy structures. Similarly, misorientation angles, and hence dislocation content,
567 generally increase towards grain boundaries (Figure 4) suggesting that dislocation climb into
568 boundaries and grain-boundary migration were relatively inefficient compared to the rate of

569 dislocation accumulation.

570 Renner *et al.* (2002) suggested that calcite commonly exhibits a Hall-Petch relationship
571 whereby strength increases with decreasing grain size because back-stresses from dislocations
572 accumulated near grain boundaries inhibit further dislocation glide. This model is consistent
573 with the microstructural observations (orientation gradients generally increasing towards grain
574 boundaries) and mechanical inferences (occurrence of strain hardening) of this study. Kennedy
575 and White (2001) reached similar conclusions based on observations of calcite naturally
576 deformed at relatively low temperatures of 150–250°C. Microstructures in their samples
577 indicated that coarse-grained vein calcite that crystallised with low dislocation densities was
578 able to deform by dislocation glide, whereas finer-grained mylonitic matrix exhibited high
579 densities of tangled dislocations and was interpreted to have strain-hardened. We suggest
580 therefore that the transition from dislocation-mediated flow to frictional failure was promoted
581 by work hardening due to low efficiency of recovery processes, particularly slow climb into
582 grain boundaries, rather than simply the temperature-dependency of critical resolved shear
583 stresses, as the rocks cooled during exhumation. This inference is consistent with experimental
584 observations that strain hardening is more pronounced at lower temperatures for both single
585 crystals (de Bresser and Spiers, 1993, 1997) and aggregates (Rutter, 1974). The predictions of
586 slip system activity (Figure 8) suggest that strain hardening must have imposed additional
587 resistance to glide of at least tens of MPa to prevent large fractions of the microstructure
588 deforming by $\{r\}$ -slip.

589 Microstructures indicative of frictional deformation are preserved within both the
590 cataclastic marbles and the phyllosilicate-rich gouge band (Figure 1; Rutter *et al.*, 2007). As
591 Quaternary earthquakes of magnitude 7+ are recorded by offset alluvial fans and debris flows
592 within 2 km of the sample site (Brown *et al.*, 2002; Rutter *et al.*, 2007), it is pertinent to consider

593 the extent to which the exhumed cataclastic fault rocks record seismogenic processes as an
594 analogue for those occurring at depth. Phyllosilicate-rich gouges typically exhibit velocity-
595 strengthening behaviour and therefore are unfavourable in general for nucleation of earthquake
596 ruptures (Ikari *et al.*, 2011). However, carbonate rocks exhibit strong velocity weakening (Han
597 *et al.*, 2010), and therefore the fragmented marble band was likely capable of nucleating
598 unstable earthquake ruptures whilst at depth. In this case, one important consequence of strain
599 hardening may be to result in the onset of seismogenic deformation at the structural levels at
600 which rocks are exhumed and cooled from $\sim 300^{\circ}\text{C}$ to $\sim 200\text{--}250^{\circ}\text{C}$. We suggest that the
601 processes recorded in the presently exposed fault rocks of the Pangong strand are likely
602 analogous to those occurring at depth, where similar rocks of the PMC continue to be exhumed
603 through the frictional-viscous transition zone.

604 In the case of the KFZ, cooling through the frictional-viscous transition zone was due
605 to ongoing deformation during erosional exhumation (Wallis *et al.*, 2016b). However, the
606 processes documented in this study may also be important in controlling transitions in
607 deformation mechanism and the onset of seismogenic behaviour in other tectonic settings. In
608 particular, carbonate units are commonly dissected by extensive normal fault systems in which
609 tectonic exhumation of footwalls may contribute to cooling (Smith *et al.*, 2011; Cowie *et al.*,
610 2017). The processes of strain hardening leading to frictional failure may be important controls
611 on the depth of seismicity and strength of the extending mid-crust in such settings. An
612 implication of this finding is that the depth extent of the dominantly frictional upper crust,
613 where earthquakes typically nucleate, potentially varies in both space and time in response to
614 the evolving strain state of rocks in the mid-crust.

615 **5.3. Schmid factor analysis as a tool for analysing crystal plasticity**

616 Schmid-factor analysis provides several useful insights in addition to those that can be

617 gained from more commonly used methods of slip system analysis. Schmid factor maps
618 provide an extension of common CPO analysis by allowing populations of crystal orientations
619 to be readily related directly to specific microstructural elements (e.g. Figures 5–7). This
620 approach is similar to plotting EBSD maps colour-coded using inverse pole figures, except that
621 Schmid factor maps consider the complete crystallography (i.e. angular relationships involving
622 both the slip direction and slip plane normal) rather than individual crystal directions, and relate
623 this explicitly to a stress state of interest (which is often only implied in other approaches).

624 Schmid factor mapping is also the first step to more detailed quantitative analysis of
625 slip system activity, which requires a range of geological (e.g. stress and temperature) and
626 experimental (e.g. CRSS and strain rate sensitivity) constraints. In these respects, calcite is
627 ideal, whereas other common rock forming minerals may present additional challenges. For
628 example, the slip systems of quartz are relatively well constrained and quartz slip system
629 analysis is widely applied in studies of crustal deformation (e.g. Law *et al.*, 1990; Lloyd *et al.*,
630 1997; Morales *et al.*, 2014). However, single crystals of quartz exhibit complex yield
631 behaviour, with strength dependent not only on temperature but also strain rate and
632 intragranular water content (Hobbs *et al.*, 1972). Consequently, comprehensive measurements
633 of slip system strength, such as those available for calcite (de Bresser and Spiers, 1997), are
634 not currently available for quartz. As a result of these limitations, although it is possible to
635 calculate Schmid factors for quartz slip systems, it is not yet possible to infer which slip systems
636 have sufficient resolved shear stress for slip. Similar detailed considerations must be applied
637 to other common rock-forming minerals.

638 More generally, Schmid factor analysis can require a range of assumptions, depending
639 on the application, which must be critically evaluated. In the present work we are concerned
640 with why dislocation activity ceased at the time that the preserved mylonitic microstructure

641 was formed. In this respect, Schmid factor analysis is highly appropriate because it constrains
642 which slip systems were well aligned for dislocation glide during a hypothetical *future*
643 increment of dislocation-mediated strain. However, a common objective of other rock
644 deformation studies is to interpret how an observed microstructure formed in the first place.
645 Schmid factors calculated for specific points/grains in a mapped microstructure will generally
646 not equal those present during *prior* deformation that lead to formation of the observed
647 microstructure due to microstructural evolution (e.g., grain rotation, grain boundary migration).
648 In some instances, this limitation might be overcome by assuming that the microstructure had
649 ‘on average’ reached a steady state, in combination with analysing Schmid factor distributions
650 over a large portion of the microstructure. However, microstructural steady state, and in
651 particular steady-state CPO, can require shear strains of several hundred percent and can be
652 difficult to prove (Skemer and Hansen, 2016). Averaging over large portions of the
653 microstructure also provides the benefit of reducing the influence of inter- and intra-granular
654 stress heterogeneities. Such heterogeneities have been predicted by numerical modelling (e.g.,
655 Pokharel *et al.*, 2014; Lebensohn and Needleman, 2016) and documented in geological
656 crystalline aggregates, including calcite (Quintanilla-Terminel and Evans, 2016) and quartz
657 (Chen *et al.*, 2015), and even in single crystals of olivine (Wallis *et al.*, 2017). Therefore, it is
658 important to map Schmid factors over a sufficiently large portion of the microstructure that the
659 averaged internal stress state can be reasonably expected to have approached the macroscopic
660 externally applied stress state during deformation. Notwithstanding these caveats, the present
661 study demonstrates that Schmid factor analysis can provide geologically relevant information,
662 if used in conjunction with appropriate objectives and geological constraints.

663 **6. Conclusions**

664 Schmid factor analysis indicates that calc-mylonites in the Pangong strand of the KFZ
665 deformed primarily by dislocation glide on $r\{10-14\}\langle-2021\rangle$ at $\sim 300^\circ\text{C}$ and 98 ± 35 MPa

666 differential stress (Rutter *et al.*, 2007) and by $\{1018\}$ twinning at similar and lower
667 temperatures. In contrast, the critical resolved shear stress for dislocation glide on $\{1012\}$
668 201 precluded this slip system from activating in the majority of grains under the same
669 conditions. Deformation within the Karakoram Fault Zone continued as the rocks cooled during
670 exhumation, resulting in hardening of the calc-mylonites and thereby leading to a transition
671 from crystal plastic to frictional deformation mechanisms (Rutter *et al.*, 2007, Wallis *et al.*,
672 2013). One mechanism for such hardening is by the direct temperature effect of increasing
673 critical resolved shear stresses of the active slip and twin systems (De Bresser and Spiers,
674 1997). However, Schmid factor analysis indicates that this alone was insufficient to induce
675 frictional failure as a greater fraction of the microstructure apparently had sufficient resolved
676 shear stress for dislocation glide at 200°C than at 300°C. Instead, microstructural observations,
677 such as widespread low angle crystallographic misorientations, which increase towards grain
678 boundaries, indicate that intracrystalline strain recovery was inefficient. Strain hardening, due
679 to decreasing efficiency of recovery as temperature decreased, provides an additional
680 hardening mechanism, which we interpret as having led to the onset of frictional and potentially
681 seismogenic deformation in the rocks at this structural level. These findings highlight the
682 importance of detailed understanding of the interplay of strain hardening and recovery
683 processes for models of crystal plasticity, particularly at relatively low homologous
684 temperatures where they impact the transition to frictional and potentially seismogenic
685 deformation.

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