

Quantifying the intensity of crystallographic preferred orientation (CPO): some practical considerations and recommended practices

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Abstract

Crystallographic preferred orientations (CPOs) commonly develop during the crystal-plastic deformation of rocks and minerals, and are widely used to infer strain intensity and geometry, reconstruct deformation conditions, and estimate material anisotropy. Although CPO intensity is often quantified using scalar metrics that reduce the full orientation distribution to a single value, these measures can be highly sensitive to their calculation parameters and input data quality. Here, we examine the performance of two widely used metrics—the J-index and the M-index—using orientation data from a diverse suite of simulated, natural, and experimental specimens. We show that ODF-based measures of CPO intensity such as the J-index (and the ODF-derived variant of the M-index) can vary markedly with kernel halfwidth and ODF construction method. However, when the ODF is constructed using an automatically selected optimal halfwidth, the ODF-derived M-index closely reproduces the M-index calculated in its original form using random-pair misorientation angle histograms. Nevertheless, this original formulation requires no kernel or ODF construction step, and is largely insensitive to its single free parameter—the histogram bin width—leaving far fewer opportunities for user choice to bias the result. Monte Carlo resampling shows that the M-index can be accurately estimated

using ~1,000 independent orientation measurements for moderate-to-strong CPOs ($M \geq 0.3$), whereas weak CPOs ($M \approx 0.1$) may require up to ~3,900 measurements. We further examine several other controls on measured CPO intensity, including the number of measurements taken per grain, as well as the quality and construction parameters of the orientation map. Because the maximum attainable value of the M-index depends on CPO type, we also propose a normalisation scheme that, within a defined set of end-member textures, allows for more direct comparison among specimens of differing type. Together, these results highlight the inherent limitations of reducing complex orientation distributions to one-dimensional metrics, and underscore the importance of consistent methodology, adequate sampling, and transparent reporting. We therefore set out a series of practical guidelines intended to improve the robustness and comparability of CPO intensity estimates among studies.

1. Introduction

At elevated pressures and temperatures, crystalline materials—including rocks and minerals—often deform via crystal-plastic mechanisms that produce a rotation and/or alignment of their constituent crystals. For instance, when deformation is mediated by dislocation motion, grains will rotate into orientations that maximise dislocation glide and the shear stresses resolved on their weakest crystal lattice planes (Andrade & Roscoe, 1937), producing a crystallographic preferred orientation (CPO) defined by the alignment of certain crystal axes relative to the bulk kinematic flow. The resulting CPO geometry depends on the imposed kinematics. In simple shear, the dominant glide plane and glide direction (i.e., the Burgers vector) tend to rotate towards parallelism with the macroscopic shear plane and shear direction, respectively, whereas

46 in axial compression the glide-plane normal tends to rotate toward the shortening axis. Thus,
47 CPO geometry commonly reflects the symmetry and orientation of the imposed deformation
48 field.

49

50 Although CPO development is often attributed to deformation via dislocation creep (e.g., Tullis,
51 1979; Karato, 1988; Fliervoet et al., 1999), there is also a growing body of literature
52 demonstrating that modest CPOs may develop during dislocation-accommodated grain
53 boundary sliding (disGBS) in olivine (Hansen et al., 2011; Précigout & Hirth, 2014), quartz (Cross
54 et al., 2017a; Tokle et al., 2019), calcite (Rutter et al., 1994; Pozzi et al., 2019; Demurtas et al.,
55 2019), and plagioclase (Miranda et al., 2016). In contrast, deformation via diffusive mass transfer
56 is often found to systematically weaken, or perhaps even entirely randomise, a pre-existing CPO
57 (Boullier & Gueguen, 1975; Zhang et al., 1994; Wheeler, 2009; Cross & Skemer, 2017), although
58 several exceptions to this have also been identified (Bons & den Brok, 2000; Barreiro et al., 2007;
59 Sundberg & Cooper, 2008; Miyazaki et al., 2013; Soda et al., 2019). Various other processes may
60 also form or modify CPO, including deformation twinning (e.g., Tullis, 1970; Barber & Wenk,
61 1979), cataclasis (Demurtas et al., 2019), metamorphic reactions (Gillgannon et al., 2024), and
62 polymorphic phase transitions (Goddard et al., 2025).

63

64 Regardless of the precise mechanisms responsible for their development, CPOs exert a major
65 influence over the mechanical properties and geophysical signatures of deformed rocks. Given
66 that CPOs often arise from the alignment of easy-slip crystal lattice planes during deformation,
67 the presence of a strong CPO can impart significant viscous anisotropy, whereby a material flows
68 more readily along certain crystal orientations than others. Polycrystalline olivine, for instance,

is up to ~15 times weaker when deformed in an orientation that maximises shear stress on the (010)[100] slip system, versus in an orientation normal to that slip system (Hansen et al., 2012). Similarly, “enhancement” factors of up to 17 have been found for polycrystalline ice deforming via basal (0001) slip (Shoji & Langway Jr., 1988). Thus, CPO development is widely thought to impart progressive weakening—and influence strain localisation—during the viscous flow of Earth’s lithosphere (e.g., Bystricky et al., 2000; Skemer et al., 2013) and cryosphere (e.g., Azuma, 1994; Fan et al., 2021a). Meanwhile, CPOs also produce elastic anisotropy that gives rise to seismic anisotropy: a common means for inferring the magnitude and direction of viscous flow in ice sheets (e.g., Smith et al., 2017), the lower crust (e.g., Mainprice & Nicolas, 1989) and the upper mantle (see Karato et al., 2008; Skemer & Hansen, 2016).

79

80 **2. Scalar CPO intensity metrics: The *J*- and *M*-index**

Given the rheological, structural, and geophysical importance of mineral anisotropy, there has long been interest in quantifying CPO intensity, and its evolution, in exhumed natural shear zones and in experimental specimens. Although a population of crystal orientations can most accurately be described using a continuous, harmonic, probability density function—the orientation density function (ODF)—it is often desirable to represent CPO strength using a single, scalar value. Arguably the most widely used of these metrics is the *J*-index, defined as the L^2 -norm of the ODF or, in plainer terms, as the sum of the squared orientation density over the ODF (Bunge, 1982):

90

$$J_{\text{ODF}} = \|f\|_{L^2}^2 = \int |f(g)|^2 dg$$

89

(1)

91

92 where $f(g)$ represents the ODF for a population of orientations, g .

93

94 The J -index ranges from 1 for a uniform orientation distribution to infinity for a single
 95 orientation, and can therefore be ambiguous in terms of what qualifies as a “strong” or “weak”
 96 CPO. Furthermore, because the ODF is defined over the symmetry-reduced fundamental region
 97 of SO(3) orientation space—which occupies a larger volume for low-symmetry crystal systems—
 98 phases with lower symmetry (e.g., triclinic) will naturally exhibit larger J values than high-
 99 symmetry phases (e.g., cubic) for comparable orientation concentration. This difference is an
 100 inherent expression of crystal symmetry, rather than a deficiency of the J -index. Nevertheless, J
 101 may be rescaled to account for the difference in SO(3) volume, if desired (e.g., Mainprice et al.,
 102 2015).

103

104 As an alternative, Skemer et al. (2005) proposed the misorientation index, M -index, defined as
 105 the difference between the random-pair (uncorrelated) misorientation-angle distribution (MAD)
 106 expected for a random orientation population of a given crystal symmetry class, R^0 , and the
 107 random-pair MAD measured for a given sample, R^T :

108

$$110 \quad M = \frac{1}{2} \int |R^T(\theta) - R^0(\theta)| d\theta$$

109

(2)

111

where θ is misorientation angle. As a reminder, the random-pair MAD is obtained by calculating the misorientation angle between every possible pair of orientations in a particular population—though in practice a subset of orientation pairs is typically sampled for computational efficiency—as opposed to the neighbour-pair MAD, which uses the misorientation angle only between orientation pairs measured adjacent to one another in Cartesian (sample coordinate) space. Thus, as CPO develops and grains become more strongly aligned, their random-pair MAD will progressively deviate from the theoretical MAD by migrating towards smaller misorientation angles (Wheeler et al., 2001). The M -index varies from 0 for a randomly oriented aggregate (i.e., with complete overlap between R^0 and R^T) to 1 for a single orientation (i.e., with no overlap between R^0 and R^T).

In its original form, the M -index was calculated using a histogram of the random-pair MAD—that is, with measurements discretised into bins of a finite width, typically 1° (Skemer et al., 2005):

$$M_{\text{MAD}} = \frac{\theta_{\text{max}}}{2n} \sum_{i=1}^n |R_i^T - R_i^0| \quad (3)$$

where θ_{max} is the maximum misorientation angle for a given crystal symmetry class, and n is the number of bins. While Skemer *et al.* demonstrated that the M -index is insensitive to bin width up to (and including) a bin size of 40° , Mainprice et al. (2015) proposed an alternative, continuous variant of the M -index, M_{ODF} :

$$M_{\text{ODF}} = \frac{1}{2} \int |f^U(\theta) - f^M(\theta)| d\theta$$

(4)

which is calculated from the measured and uniform ODFs, $f^M(\theta)$ and $f^U(\theta)$, respectively.

3. Limitations and critiques of scalar CPO intensity metrics

Although scalar CPO metrics are often treated—implicitly or explicitly—as quantitative measures of an intrinsic material property (e.g., seismic anisotropy, viscous anisotropy, etc.), it is important to recognise that any such metric represents a severe dimensional reduction of the underlying orientation distribution. In the most complete sense, CPO represents a three-dimensional probability density function defined over orientation space, $SO(3)$, whereas scalar indices collapse that information down to a single value by integrating, differentiating, or otherwise projecting the distribution onto a one-dimensional measure. Inevitably, this process discards information about the shape, symmetry, and topology of the ODF, meaning that distinct orientation distributions may yield identical scalar intensities. For example, note that a perfect [100]-fibre texture in the orthorhombic (“mmm”) crystal system can produce an M-index value no greater than 0.436—a value that would otherwise correspond to a unimodal ODF of relatively modest strength. This limitation is not unique to the M-index: scalar CPO metrics in general, including the J-index, depend on *how* orientation density is distributed in $SO(3)$, not solely on the *degree* of crystallographic alignment. Scalar CPO metrics should therefore be understood not as complete mathematical descriptors of orientation distributions, but as heuristic quantities

155 that facilitate comparison among similar datasets, provided that their limitations and sensitivities
156 are explicitly acknowledged.

157

158 It is precisely this unavoidable loss of information that underlies a long-standing debate over
159 how CPO intensity should be quantified in practice. To date, two broad schools of thought have
160 emerged: one emphasising statistical rigour, and the other prioritising practical utility. Notably,
161 Skemer et al. (2005) previously argued that ODF-based measures such as the J -index can be
162 highly sensitive to data population size and numerical choices associated with ODF construction
163 (e.g., bandwidth, Gaussian halfwidth), motivating the development of the M -index as an
164 ostensibly more robust, parameter-insensitive alternative. However, in a subsequent
165 commentary, Schaeben (2007) countered that *all* scalar measures of CPO intensity—including
166 the M -index—are intrinsically limited in their own ways for the reasons described above.

167

168 Responding to the specific criticism that J systematically decreases as a function of n , the number
169 of orientation measurements, Schaeben (2007) emphasised that this bias is a natural
170 consequence of estimation variance within a finite population rather than a conceptual flaw of
171 the J -index itself. As an extreme example, consider the case in which we have a uniform
172 distribution of N orientations. If we were to construct an ODF for just $n = 1$ measurement taken
173 at random, that ODF would effectively exhibit a monodisperse (i.e., single-crystal) distribution,
174 with $J \rightarrow \infty$. More generally, an ODF constructed from a limited number of measurements will
175 naturally feature a low signal-to-noise ratio, producing spurious ODF peaks that, when squared
176 and summed (Equation 1), will yield an artificially large value of J . As n increases and the
177 orientation distribution is sampled more comprehensively, the signal-to-noise ratio will improve,

178 allowing a more coherent signal to emerge that is dominated by genuine features of the
179 underlying orientation distribution. This effect, termed the $1/n$ law, is examined in detail by
180 Matthies & Wagner (1996), who show that sufficient sampling of the orientation distribution
181 produces approximately linear behaviour over a broad range of J versus $1/n$. By extrapolating
182 this relationship to $1/n = 0$ (i.e., $n = \infty$), it is thus possible to obtain the “true” value of J .
183 Furthermore, Schaeben (2007) argues that while the variance of J can be rigorously estimated
184 using (geo)statistical approaches that account for spatial correlation among orientations (e.g.,
185 Boogaart, 2001), similar evaluation for the M-index is less straightforward because it is based on
186 a reduced representation of the data (i.e., the misorientation angle distribution).

187

188 In addressing Schaeben’s (2007) criticisms, Skemer & Karato (2007) clarified that the M-index
189 was not designed to replace the J-index but, rather, to provide a complementary measure of
190 CPO intensity that is more practical for Earth-science applications, both by requiring fewer
191 corrections to account for undersampling (c.f., Matthies & Wagner, 1996) and by giving a more
192 stable result for limited numbers of measurements, albeit at the cost of strict mathematical
193 rigour. For example, unless an impractically large number of grains are measured ($n = 181,584$
194 for complete sampling of a uniform orientation distribution at 5° ODF resolution; Wenk, 2002),
195 the orientation distribution must be faithfully interpolated using a smoothing (e.g., Gaussian)
196 function, the ideal halfwidth of which is not known *a priori*, and which will depend on CPO
197 intensity, CPO type/symmetry, and the measured number of orientations. Whereas a typical 46
198 $\times 27$ mm polished thin section might contain only $\sim 6,000$ individual grains of 0.5 -mm diameter,
199 that same specimen would yield ~ 18 million random-pair misorientations even if only one
200 orientation measurement per grain were to be considered. Furthermore, while the M-index also

201 exhibits a $1/n$ -type variance, Skemer et al. (2005) report that a stable value is obtained for as few
202 as 150–600 independent orientation measurements (although, as we shall see later, this is valid
203 only for relatively strong CPOs under the stricter convergence criterion adopted here).

204

205 **4. Objectives**

206 Despite—or perhaps because of—the debate outlined above, no standardised practices for
207 measuring or reporting CPO intensity have emerged within the Earth-science community. In the
208 absence of such standards, methodological choices are often guided more by convention or
209 convenience than by a clear understanding of the various sensitivities and limitations involved.
210 Consequently, substantial (apparent) variability may arise among otherwise comparable
211 datasets, complicating efforts to interpret the microphysical processes responsible for CPO
212 development and modification. Although important foundations for rigorously quantifying CPO
213 intensity have already been laid (e.g., Matthies & Wagner, 1996; Wenk, 2002; Skemer et al., 2005;
214 Schaeben, 2007), these issues have so far only been addressed in a limited or fragmented
215 manner, often focusing on single metrics, specific crystal symmetry classes, and/or isolated
216 datasets. Here, we test many of the sensitivities raised in that exchange directly—including
217 dependence on population size, ODF construction method, and grain reconstruction—using a
218 common set of simulated, natural, and experimental datasets spanning a range of crystal
219 symmetries and CPO types. We also address several practical considerations not examined
220 previously, namely the choice between all-points and one-point-per-grain data, and the
221 dependence of M on CPO type.

222

223 The primary objectives of this contribution are, thus, threefold. First, to demonstrate the
224 sensitivity of common CPO intensity metrics to their calculation parameters. Second, to
225 determine the number of measurements required to obtain a stable, robust value of CPO
226 intensity for a broad spectrum of simulated, experimental, and natural specimens. Finally, to
227 establish some guiding principles and best practices for quantifying and reporting CPO intensity.

228

229 Although the present study relies heavily on orientation data collected using EBSD, the findings
230 should, in principle, be applicable to orientation data obtained using any microanalytical or
231 numerical method from which the complete crystal orientation is derived (e.g., excluding
232 polarised-light analyses from which only the optic-axis orientation is provided). Likewise,
233 although we shall focus on the J - and M -index as these are by far the most widely used CPO-
234 intensity metrics within the Earth-science community, similar principles should apply to other
235 scalar metrics derived from the complete ODF; for example, those based on ODF entropy
236 (Schaeben, 1988) or component volume (e.g., ball volume, fibre volume; Hielscher et al., 2010).

237 Although component volumes offer an intuitive physical interpretation—giving the fraction of
238 crystals within a given angular distance of a specified orientation—and have been applied in a
239 small number of geoscience studies (Kilian & Heilbronner, 2017; Kuehn et al., 2024), they require
240 a component centre to be identified, which presupposes knowledge of the texture geometry,
241 and a reference radius, which is typically chosen arbitrarily. Furthermore, when calculated from
242 the ODF, these methods are also susceptible to the kernel sensitivities examined below for the
243 J -index and M_{ODF} . Finally, certain other metrics shall be omitted entirely—specifically, those
244 based on maximum pole figure intensity or eigenvalue-based shape parameters (Woodcock,
245 1977; Vollmer, 1990), as those methods must be calculated for individual crystal axes rather than

for the ODF as a whole and, as such, provide an incomplete view of CPO intensity. Indeed, Larson et al. (2023) recently showed that eigenvalue-based metrics are sensitive to the opening angle of cross-girdled quartz CPOs, demonstrating that such metrics conflate CPO geometry with CPO intensity.

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251

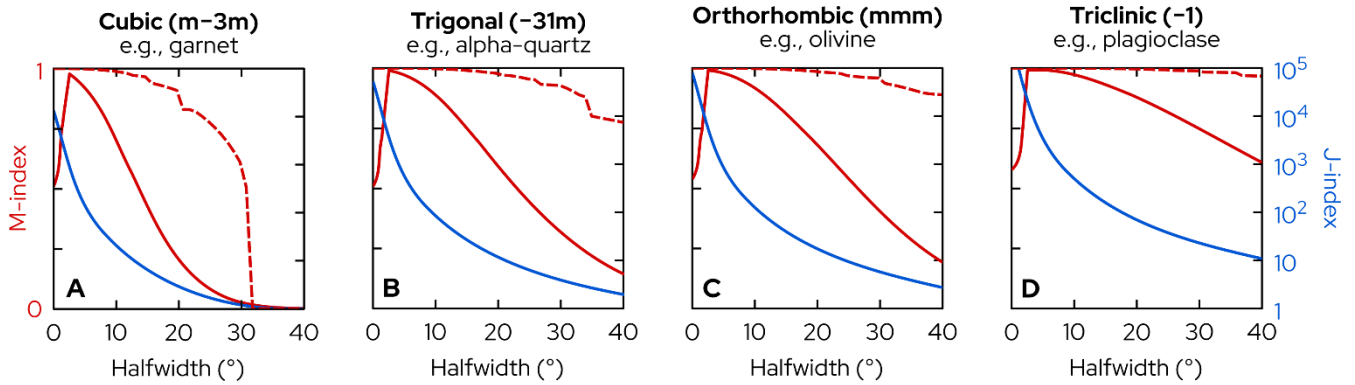
5. Performance of the J- and M-indices for synthetic data

5.1 Single crystals

As a starting point, we can examine how the *J*-index and *M*-index respond to the end-member case of a monodisperse (i.e., single-crystal) orientation distribution. Figure 1 shows J_{ODF} and M_{ODF} as a function of ODF halfwidth for several crystal-symmetry classes. The halfwidth—defined as the half-width at half-height of the kernel function used to construct the ODF—controls the "sharpness" of the resulting distribution. Larger halfwidths emphasise broad, long-wavelength features, whereas smaller halfwidths resolve increasingly fine-scale orientation structure. Because the harmonic bandwidth required to accurately represent the ODF depends on its sharpness, the bandwidth was selected automatically for each halfwidth. At halfwidths below 1°, the bandwidth required to faithfully represent the ODF may exceed 200 harmonic components, whereas fewer than 20 components are sufficient at halfwidths greater than 20°. Example pole figures corresponding to a range of ODF halfwidths are shown in Supplementary Figure S1. Note that the range of halfwidths examined here (1–40°) is intentionally broad. In practice, most geological CPOs can be reasonably represented using halfwidths of ~5–15°; however, considerably larger values have been used in some widely cited studies (e.g., 40° in Jung &

268 Karato, 2001; 30° in Katayama et al., 2004), and the halfwidth is frequently not reported at all.
 269 The range examined here therefore spans the values that may be encountered in the published
 270 literature, rather than those recommended for routine analysis.

271



272

273

274 **Figure 1:** J_{ODF} (solid blue curves; Equation 1) and M_{ODF} (solid red curves; Equation 4) as a function of ODF
 275 halfwidth for a single orientation of A) cubic, B) trigonal, C) orthorhombic, and D) triclinic crystal
 276 symmetries. All ODFs were constructed in MTEX (version 6.1.0) using the default de la Vallée Poussin
 277 kernel (Schaeben, 1997). M -index values were also calculated using the original, discrete method of
 278 Skemer et al. (2005; Equation 3), and are plotted as red dashed lines—for these values, the x-axis
 279 corresponds to the bin width of the misorientation angle histogram, rather than the ODF halfwidth.

280

281 As highlighted by Skemer et al. (2005), J_{ODF} is highly sensitive to the ODF halfwidth (Figure 1,
 282 blue curves). At large halfwidth values (20–40°), J_{ODF} approaches unity; that is, the value expected
 283 for a random orientation distribution (recall that these calculations are for monodisperse, single-
 284 crystal CPOs where J should approach infinity). However, as halfwidth decreases to 2°, J_{ODF}
 285 increases over several orders of magnitude. The maximum magnitude of J_{ODF} also increases as
 286 crystal symmetry decreases, from 10^4 for cubic crystals to 10^5 for triclinic crystals, highlighting
 287 that CPO intensity cannot easily be compared among phases belonging to different crystal
 288 systems unless extra care is taken to normalise the results (e.g., Mainprice et al., 2015).

290 Marked differences are also observed between M_{ODF} and M_{MAD} , with M_{ODF} being similarly
291 sensitive to ODF halfwidth, particularly with increasing crystal symmetry—note that M_{ODF}
292 becomes severely underestimated and approaches 0 as ODF halfwidth exceeds 20° for the cubic
293 case (Figure 1A, solid red curve). Even for more typical ODF halfwidths of $5\text{--}15^\circ$, M_{ODF} falls 7–
294 56% below the true value of $M = 1$ for cubic crystals, and 2–24% below $M = 1$ for orthorhombic
295 and trigonal crystals. Values close to $M_{\text{ODF}} = 1$ are obtained only as the ODF halfwidth
296 approaches 2° , yet drop off precipitously at smaller halfwidth values. In contrast, we find that
297 the original, discrete formulation of the M -index (Equation 3) is relatively stable, providing M_{MAD}
298 ≈ 1 so long as the MAD bin width does not exceed 10° (Figure 1, dashed red curves).

299

300 Given the strong sensitivity of J_{ODF} , M_{ODF} , and other such properties to ODF halfwidth, substantial
301 effort has been devoted to developing objective, data-driven approaches for selecting an
302 “optimal” kernel halfwidth for a given orientation distribution, with the aim of reducing
303 subjective parameter selection and ensuring reproducibility. For example, the default method
304 currently implemented within MTEX relies on a Kullback-Leibler cross-validation approach
305 (Bowman, 1984) whereby candidate halfwidths are evaluated by minimising the discrepancy
306 between an estimated ODF and a set of withheld orientation data.

307

308 5.2 Numerical polycrystals

309 To produce more broadly applicable results, we can now examine CPO intensity for a
310 polycrystalline aggregate featuring varying degrees of crystallographic alignment. Figures 2 and
311 3 show how J and M evolve with increasing strain in numerical aggregates of olivine (Figure 2)

and ice (Figure 3) subjected to simple-shear deformation using the viscoplastic self-consistent (VPSC) model of Lebensohn & Tomé (1993). The goal of these models is not to produce a fully realistic simulation of CPO evolution—that has been achieved elsewhere using more sophisticated analyses (e.g., Boneh et al., 2015; Hansen et al., 2016; Rathmann et al., 2024)—but, rather, to produce CPOs that span the range from random ($M = 0$; $J = 1$) to strongly unimodal ($M \rightarrow 1$; $J \rightarrow \infty$). Slip systems and critical resolved shear stresses (CRSS) were chosen to promote the formation of a strong A-type (010)[100] CPO in olivine, and a strong basal- $\langle a \rangle$ (0001) $\langle \bar{1}2\bar{1}0 \rangle$ CPO in ice: both commonly observed in natural settings. Olivine CPO evolution was modelled using six slip systems chosen after Boneh et al. (2015) and Tommasi et al. (2000) to satisfy von Mises' criterion, with two other slip systems—{110}[110] and {031}[113]—added to strengthen the A-type CPO and enable model convergence at large strains. Ice CPO evolution was modelled using the same slip systems employed by Castelnau et al. (1996). The slip systems and their corresponding CRSS values are summarised in Table 1. VPSC simulations were conducted for 20,000 grains—far exceeding the population size needed to obtain a robust estimate of CPO intensity, as shown below—with no neighbour-grain interactions (i.e., co-rotation), and using tangent linearisation to validate the Eshelby-type VPSC inclusion scheme (Molinari et al., 1987). The data were subsequently analysed within the MTEX open-source toolbox for MATLAB (MTEX version 6.1.0; Bachmann et al., 2010).

331 **Table 1:** Slip systems and CRSS values used for olivine and ice VPSC simulations

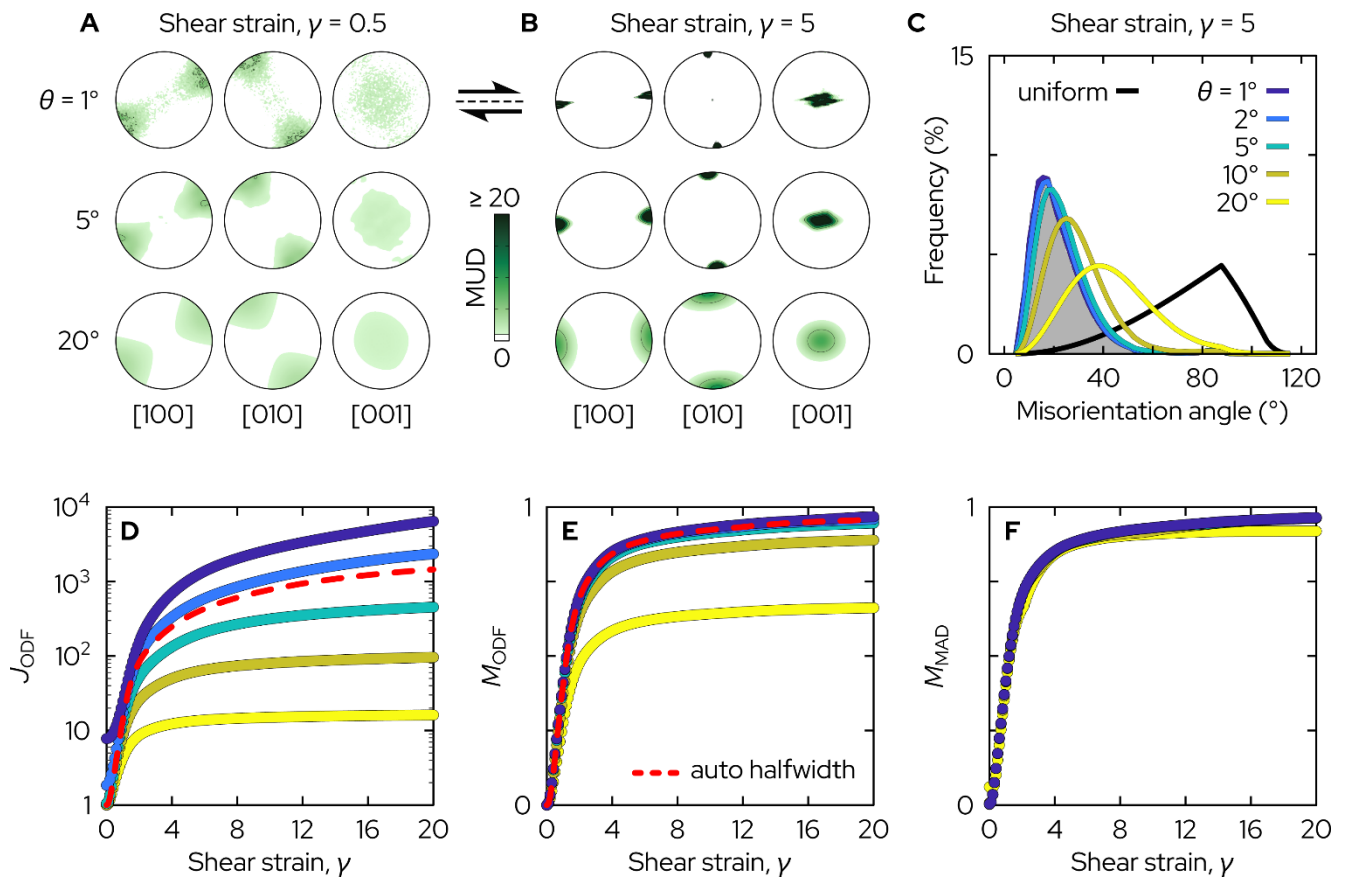
Slip system	CRSS
<i>Olivine</i>	
(010)[100]	1
(001)[100]	1
(010)[001]	2
(100)[001]	3
{021}[100]	6
{110}[001]	6
{110}[110]	10
{031}[113]	10
<i>Ice</i>	
(0001) $\langle\bar{1}2\bar{1}0\rangle$	1
$\{\bar{1}010\}\langle\bar{1}2\bar{1}0\rangle$	20
$\{11\bar{2}2\}\langle11\bar{2}\bar{3}\rangle$	200

332

333

334 5.2.1. Halfwidth sensitivity

335 Figures 2 and 3 show many of the same trends discussed above. At any given strain, J_{ODF} and
336 M_{ODF} decrease with increasing ODF halfwidth (Figures 2D–E, 3D–3E) as the ODF increasingly fails
337 to capture short-wavelength (i.e., low misorientation angle) features (Figures 2C, 3C). In contrast,
338 M_{MAD} monotonically increases along the same trajectory for all MAD bin widths $\leq 10^\circ$, spanning
339 the expected range of $0 \rightarrow 1$. In general, M_{ODF} provides values very similar to M_{MAD} for ODF
340 halfwidths of $\leq 5^\circ$; however, M_{ODF} decreases significantly at ODF halfwidths greater than 5°
341 (Figures 2E, 3E). Encouragingly, kernel optimisation (i.e., automatic halfwidth, bandwidth
342 selection) via the Kullback-Leibler method yields $M_{\text{ODF}} \approx M_{\text{MAD}}$ (red line in Figures 2E, 3E), with
343 MTEX selecting an optimal halfwidth that decreases rapidly from $\sim 22^\circ$ to $\sim 2.5^\circ$ as strain and
344 CPO intensity increase (Supplementary Figure S2). However, note also that the optimal kernel
345 halfwidth depends on population size, decreasing as the number of orientation measurements
346 increases (Supplementary Figure S2)—see also Bozzolo et al. (2007).



348

349

Figure 2: CPO evolution in a numerical olivine aggregate undergoing simple shear deformation (see main text for details). (A–B) Contoured pole figures of the [100], [010], and [001] axes at shear strains of (A) $\gamma = 0.5$ and (B) $\gamma = 5.0$, produced using ODF kernel halfwidths of $\theta = 1^\circ, 5^\circ$, and 20° . (C) The random-pair misorientation angle distribution (MAD) at $\gamma = 5.0$ (grey histogram; 2° bin width), alongside misorientation angle distribution functions (MDFs) constructed from ODFs with halfwidths of $\theta = 1$ – 20° (coloured lines) and the theoretical uniform MDF (black line). Note that the ODF-derived MDFs provide a poor description of the MAD at $\theta \geq 10^\circ$. (D–F) The J -, M_{ODF} -, and M_{MAD} -indices as a function of strain for (D–E) ODF halfwidths of 1 – 20° and (F) MAD bin widths of 1 – 20° . The red dashed line in (D) and (E) shows J and M_{ODF} when the ODF kernel (halfwidth, bandwidth) is chosen automatically using the default MTEX Kullback-Leibler cross-validation approach.

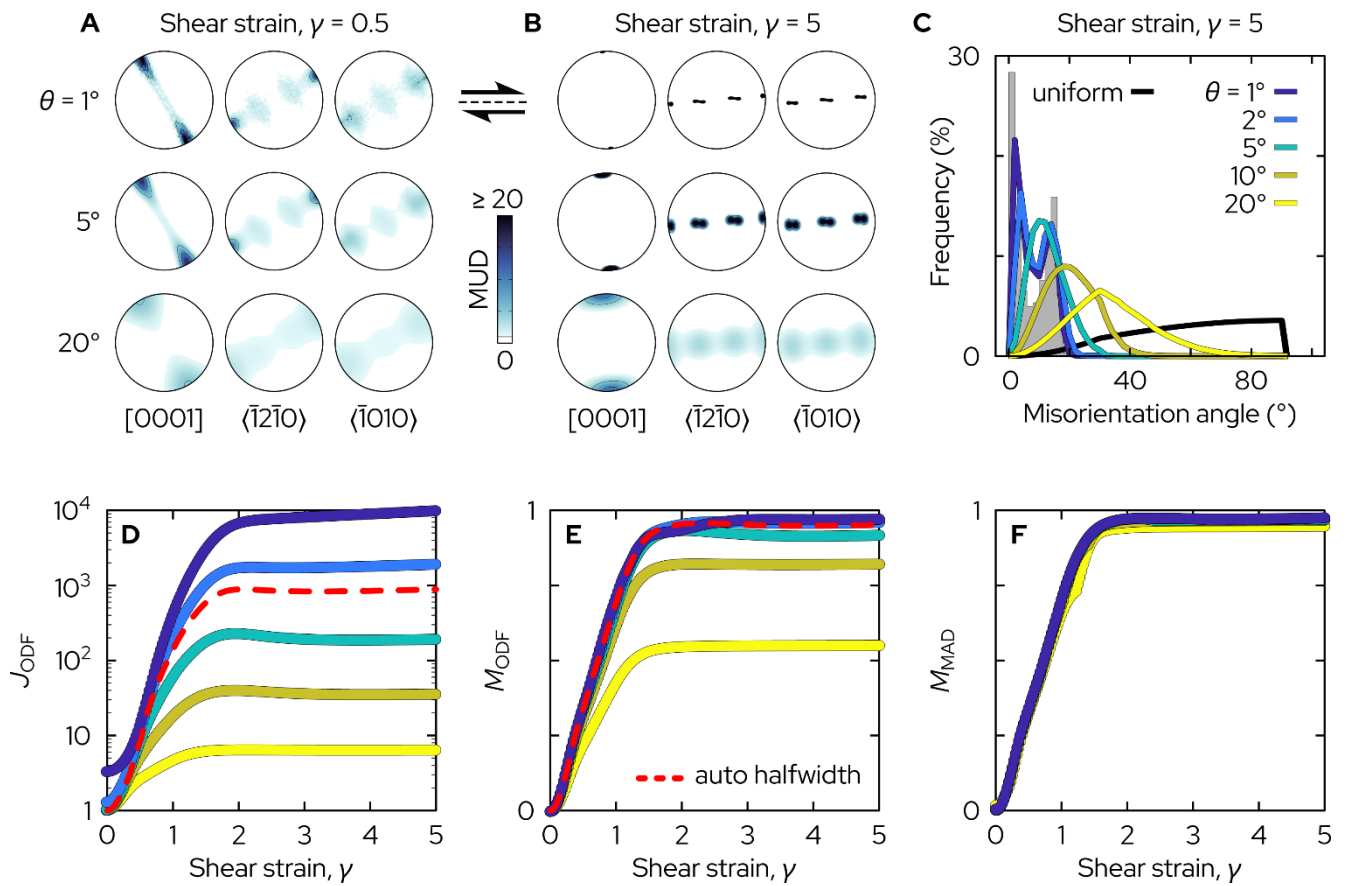
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Figure 3: CPO evolution in a numerical ice aggregate undergoing simple shear deformation (see main text for details). (A–B) Contoured pole figures of the [0001], $\langle 12\bar{1}0 \rangle$, and $\langle 1010 \rangle$ axes at shear strains of (A) $\gamma = 0.5$ and (B) $\gamma = 5.0$, produced using ODF kernel halfwidths of $\theta = 1^\circ$, 5° , and 20° . (C) The random-pair misorientation angle distribution (MAD) at $\gamma = 5.0$ (grey histogram; 2° bin width), alongside misorientation angle distribution functions (MDFs) constructed from ODFs with halfwidths of $\theta = 1$ – 20° (coloured lines) and the theoretical uniform MDF (black line). Note that the ODF-derived MDFs provide a poor description of the MAD at $\theta \geq 5^\circ$. (D–F) The J -, M_{ODF} -, and M_{MAD} -indices as a function of strain for (D–E) ODF halfwidths of 1 – 20° and (F) MAD bin widths of 1 – 20° . The red dashed line in (D) and (E) shows J and M_{ODF} when the ODF kernel (halfwidth, bandwidth) is chosen automatically using the default MTEX Kullback-Leibler cross-validation approach.

5.2.2. Parametric versus non-parametric ODF construction

The ODFs analysed in Figures 2 and 3 were all constructed using a parametric Fourier decomposition (i.e., harmonic series expansion) approach in which

$$f_{\text{Fourier}}(o) = \sum_{n=0}^W \sum_{k=-n}^n \sum_{l=-n}^n \hat{f}_n^{k,l} D_n^{k,l}(o)$$

(5)

where $o \in \text{SO}(3)$ denotes an orientation (rotation matrix) at which the ODF is evaluated in three-dimensional space, $\hat{f}_n^{k,l}$ are the Fourier coefficients, $D_n^{k,l}$ are the Wigner-D functions that serve as harmonic basis functions in $\text{SO}(3)$ space (analogous to sines and cosines in classical Fourier series expansion), and n is the harmonic degree, with W being the truncation order of the expansion; that is, the bandwidth (Hielscher & Schaeben, 2008).

However, ODFs may also be constructed using non-parametric kernel density estimation (KDE) whereby the distribution of orientations in $\text{SO}(3)$ is described through the superposition (i.e., summation) of radially symmetric unimodal model ODFs (kernels) centred around each orientation $o_1, o_2, \dots, o_M$:

$$f_{\text{KDE}}(o) = \frac{1}{M} \sum_{i=1}^M \psi(o o_i^{-1})$$

(6)

where $\psi : \text{SO}(3) \rightarrow \mathbb{R}$ is the radially symmetric kernel used to assign a real (scalar) value representing the probability density (e.g., multiples of uniform distribution, MUD) at each

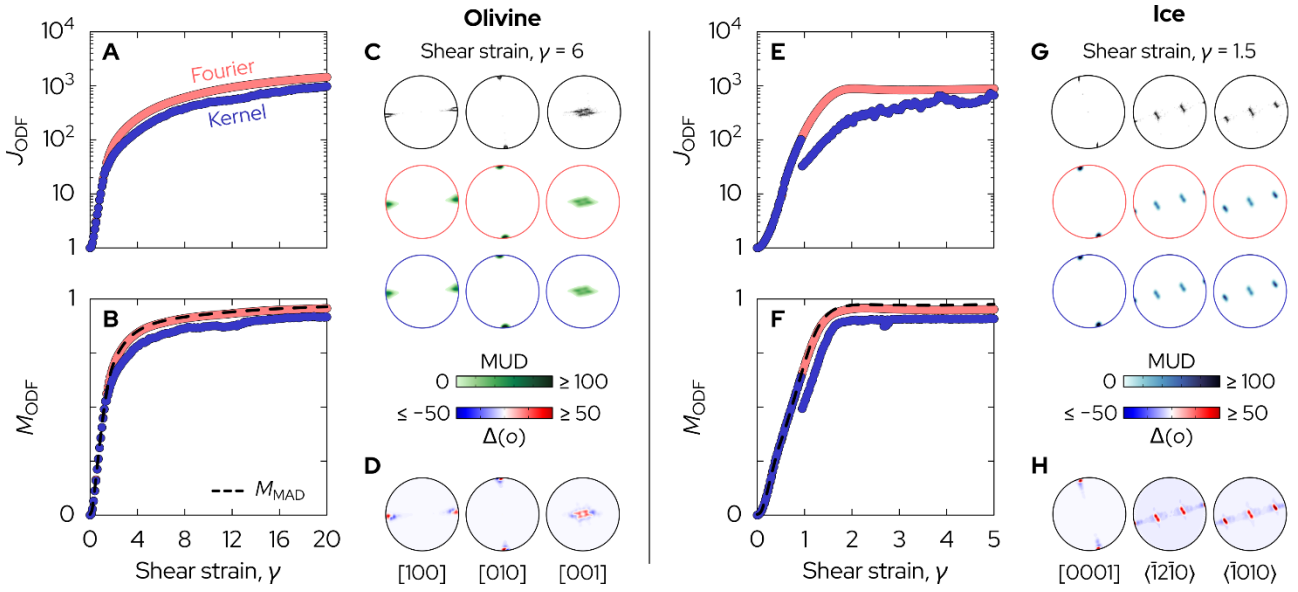
orientation in $SO(3)$ (Hielscher & Schaeben, 2008). In this approach, the main variables are the functional form of the kernel itself, ψ , and its halfwidth.

In MTEX, the choice between these approaches is made automatically according to internal heuristics such as dataset size, kernel bandwidth, and symmetry. Generally speaking, the KDE-based method is preferred when the ODF contains highly localised, high-intensity features (i.e., for smaller halfwidths), whereas Fourier-based representation is favoured when the ODF is smoother and can be efficiently represented using a truncated harmonic expansion (i.e., for larger halfwidths). However, either approach can be explicitly enforced by the user (as was done for Figures 2 and 3).

To assess the influence of the ODF construction method itself, Figure 4 compares CPO intensity derived using both the Fourier- and KDE-based implementations. In both cases, the MTEX-default de la Vallée Poussin kernel was used (Schaeben, 1997) with the kernel halfwidth selected automatically via Kullback-Leibler cross-validation.

Although both methods converge to similar J_{ODF} (Figures 4A, 4E) and M_{ODF} (Figures 4B, 4F) values at high strain, the KDE-derived values are relatively unstable—despite the VPSC simulations producing highly localised ODFs that are, in principle, best suited to kernel-based representation—evolving erratically, discontinuously, and non-monotonically as a function of strain for the ice simulations in particular (Figures 4E, 4F). In contrast, the Fourier-based ODFs evolve smoothly and strengthen monotonically, with values of M_{ODF} that are almost identical to M_{MAD} at any given strain (dashed line in Figures 4B, 4F). These marked differences are somewhat

surprising given the seemingly identical pole figures produced by each method (compare the pole figures outlined in red and blue in Figures 4C, 4G). However, significant local differences are found by subtracting the ODFs from one another: $\Delta(o) = f_{\text{Fourier}}(o) - f_{\text{KDE}}(o)$ (Figures 4D, 4H), with the Fourier-based method producing greater intensity around the primary ODF maximum (red colouring on Figures 4D, 4H) and the KDE-based method capturing the subsidiary features more precisely (blue colouring on Figures 4D, 4H).



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Figure 4: Comparison of parametric (Fourier-based) and non-parametric (KDE-based) ODF construction approaches for the (A–D) olivine and (E–H) ice VPSC simulations. (A, E) J-index and (B, F) M_{ODF} -index as a function of strain. The red data points represent ODFs obtained using Fourier series expansion, whereas the blue data points represent ODFs constructed via the superposition of radially symmetric kernel functions. The dashed black line in (B, F) represents M_{MAD} calculated via the original M-index method of Skemer et al. (2005). (C, G) Equal-area, lower-hemisphere pole figures showing the scattered point data (black outline), Fourier-based contouring (red outline), and kernel-based contouring (blue outline). The difference between the Fourier-based and kernel-based ODFs, $\Delta(o) = f_{\text{Fourier}}(o) - f_{\text{KDE}}(o)$, is shown in panels (D, H).

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6. Sensitivity to CPO type

Thus far, we have examined the limiting cases of random ($M = 0$; $J = 1$) and unimodal ($M \rightarrow 1$; $J \rightarrow \infty$) orientation distributions. However, as mentioned above, the J - and M -index are sensitive to both CPO intensity and CPO geometry. For example, a perfect [100]-fibre CPO in the orthorhombic crystal system (e.g., in olivine) will yield a value of M no greater than 0.436, far below the upper bound ($M = 1$) for a unimodal distribution. In some situations, it might therefore be desirable to use a scalar CPO metric that is insensitive to CPO geometry, enabling more meaningful, like-for-like comparison among specimens deformed under different conditions or mixed-mode kinematics.

Figure 5 shows an additional VPSC simulation in which randomly oriented olivine crystals were first deformed under uniaxial compression to a shortening strain of $\varepsilon = 60\%$, followed by simple shear deformation to a shear strain of $\gamma = 20$. During the initial uniaxial compression stage, a strong (010)-fibre CPO forms with (100) and (001) girdled in the plane normal to compression, and (010) aligning with the compression axis (Figure 5A). During the subsequent phase of simple shear, the (100) axes slowly rotate into alignment with the shear direction, forming a unimodal A-type CPO (Figures 5A, 5B). As expected, the M index increases during the compressive phase of deformation, approaching the theoretical maximum of $M = 0.436$ for a perfect (010)-fibre CPO (Figures 5B), before increasing further towards $M = 1$ as the unimodal A-type CPO develops under simple shear (Figure 5B, pale blue symbols).

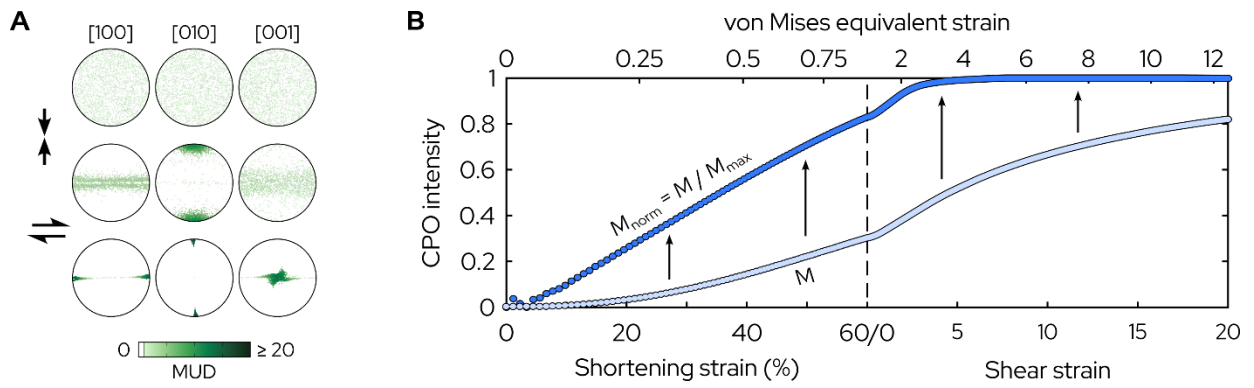


Figure 5: CPO evolution in a numerical olivine aggregate undergoing mixed-mode deformation.

Crystal orientations were subjected to 60% uniaxial flattening, followed by $\gamma = 20$ simple shear. (A) Lower-hemisphere, equal-area pole figures of the olivine [100], [010], and [001] axes at three points during the simulation: at the beginning, at the transition from compression to simple shear, and at the end. Each data point (orientation) is coloured according to multiples of uniform distribution, MUD. (B) CPO intensity a function of strain in the mixed-mode VPSC simulation. The vertical dashed line indicates the transition from uniaxial flattening to simple shear. The pale blue symbols show the raw (unnormalised) M -index values; the dark blue symbols show the M -index values after normalisation to account for differences in the upper limit of M for CPOs of different types.

In the simplest treatment, we could normalise M for the CPOs formed under axial compression by 0.436—the maximum attainable value for (010)-fibre CPOs in orthorhombic crystals—bringing them to the same $0 \leq M \leq 1$ scale as the unimodal CPOs. However, this procedure would produce a sudden, artificial jump in M at the transition from compression to simple shear. Moreover, such a procedure would only be applicable in instances featuring a known, stepwise change in deformation kinematics, which is rarely the case. A more suitable treatment would therefore account for the gradual change in the upper bound of M as the CPOs evolve from (010)-fibre to A-type unimodal. To this end, we can calculate the M -index of any given mixture of N end-member textures (Figure 6A). For simplicity, and for direct application to our mixed-mode simulations, we shall restrict this procedure to a ternary space defined by the

three end-member olivine CPOs found within our VPSC simulations: random ($M = 0$), (010)-fibre ($M \leq 0.436$), and A-type (010)[100] unimodal ($M \leq 1$). However, it should be possible to extend the same practice to N number of end-member textures (e.g., a binary for $N = 2$, a ternary for $N = 3$, a tetrahedron for $N = 4$, and so on) for CPOs containing components of various unique texture types.

Next, we need a method for placing our modelled CPOs within this ternary space. Conveniently, any point within the ternary can be described using a four-component eigenvalue spectrum. For our olivine VPSC simulations, we use the following end-members:

Random: $\lambda_{\text{random}} = [0.6175, 0.1275, 0.1275, 0.1275]$
(010)-fibre: $\lambda_{(010)\text{-fibre}} = [0.8183, 0.1817, 0.0000, 0.0000];$
A-type unimodal: $\lambda_{\text{unimodal}} = [1.0000, 0.0000, 0.0000, 0.0000];$

Note that unlike orientations in S^2 space (e.g., Cartesian vectors), which are described by a 3×3 orientation tensor with three eigenvalues, crystal orientations in MTEX are represented in the three-dimensional rotation group, $SO(3)$, using four-component unit quaternions (Supplementary Text S1). Consequently, the corresponding 4×4 quaternion orientation tensor is characterised by four eigenvalues (Kunze & Schaeben, 2004).

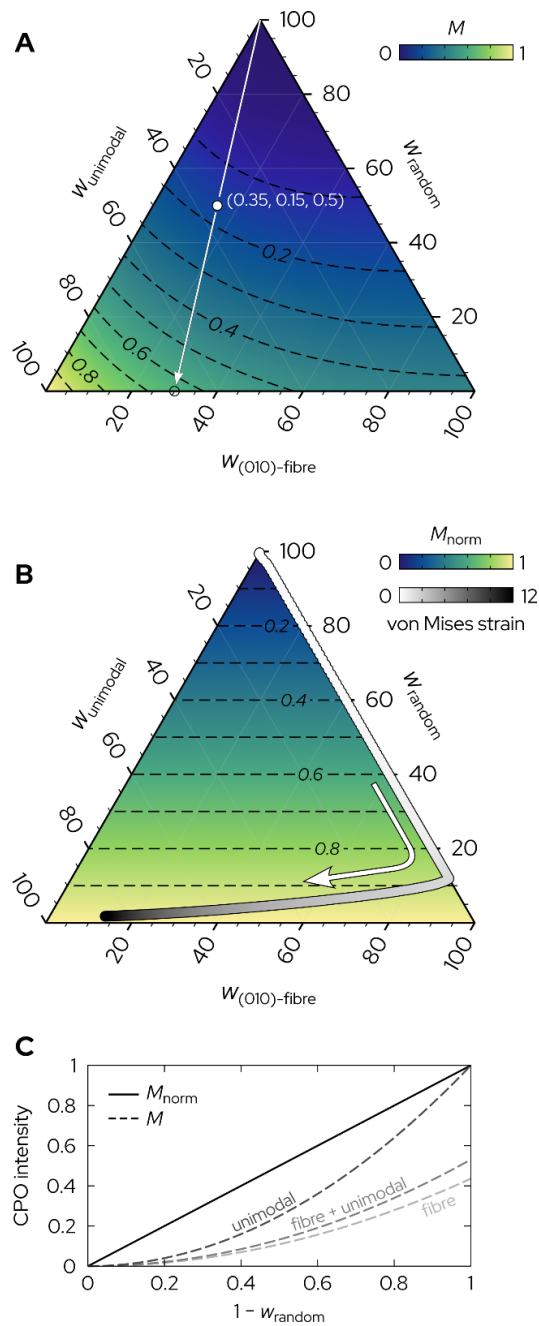


Figure 6: Normalisation of the M-index to account for CPO type. (A) The M-index calculated for synthetic mixtures of the three end-member CPOs observed in our VPSC simulations: unimodal, (010)-fibre, and random. Any CPO can be projected into this ternary space using its eigenvalue spectrum, providing barycentric coordinates representing the relative weights of the end-member CPO types. The M-index can be normalised using the M-index of a perfectly non-random CPO with the same proportion of the non-random components; that is, by projecting a ray to the bottom edge of the ternary. (B) The normalised M-index, M_{norm} , within the same ternary space. The symbols represent the CPOs from our mixed-mode VPSC simulations, projected into this ternary space using their eigenvalue spectra. (C) M_{norm} exhibits a linear relationship with the degree of CPO “non-randomness”, $1 - W_{\text{random}}$, whereas the original M-index varies nonlinearly.

514

515 By obtaining the eigenvalue spectrum of each modelled CPO, we can now project it into our
 516 ternary space to obtain barycentric coordinates representing the relative proportions of each
 517 endmember:

$$W = (W_{\text{unimodal}}, W_{(010)\text{-fibre}}, W_{\text{random}}) \quad (7)$$

520 with $w_i \geq 0$, and $\sum w_i = 1$. For example, the barycentric coordinates $w_{\text{unimodal}} = 0.15$, $w_{(010)\text{-fibre}} =$
 521 0.35 , $w_{\text{random}} = 0.5$ represent a CPO with a 15% unimodal component, 35% (010)-fibre
 522 component, 50% random component, and $M = 0.160$ (Figure 6A).

523

524 The M-index can now be normalised by the M-index value of a perfectly-ordered CPO (i.e.,
 525 $w_{\text{random}} = 0$) with the same relative proportion of the non-random components:

526

$$M_{\text{norm}} = \sqrt{\frac{M}{M_{\text{max}}(t)}} \quad (8)$$

529 where

$$t = \frac{w_{\text{unimodal}}}{w_{\text{unimodal}} + w_{(010)\text{-fibre}}} \quad (9)$$

532

533 As shown in Figure 6C, the square root in Eqn. 8 makes M_{norm} directly proportional to $1 -$
 534 w_{random} , with the latter representing the non-random component of the CPO in our ternary
 535 space. In contrast, the M-index increases non-linearly with increasing “non-randomness”.

For the example given above, the corresponding normalisation factor is the M-index of a CPO with the barycentric coordinates $w = (0.3, 0.7, 0)$, which, from our M-index ternary, is 0.612 (Figure 6A). Our example CPO therefore has a normalised M-index value of $M_{\text{norm}} = \sqrt{(0.160/0.612)} = 0.511$. For further details on the normalisation process and its derivation, see Supplementary Text S1.

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7. Sensitivity to population size

7.1 Numerical polycrystals

Our VPSC simulations also provide an opportunity to examine how CPO intensity varies with population size. As a general rule of thumb, it is often assumed that 200–500 measurements are required to obtain a representative estimate of microstructural “state” (e.g., grain size, CPO intensity; Humphreys, 2001; ASTM International, 2013; Cross et al., 2017b). However, recent work by Lopez-Sanchez (2020) shows that several thousand measurements may in fact be required to accurately represent grain size distributions, particularly when the distribution is broad.

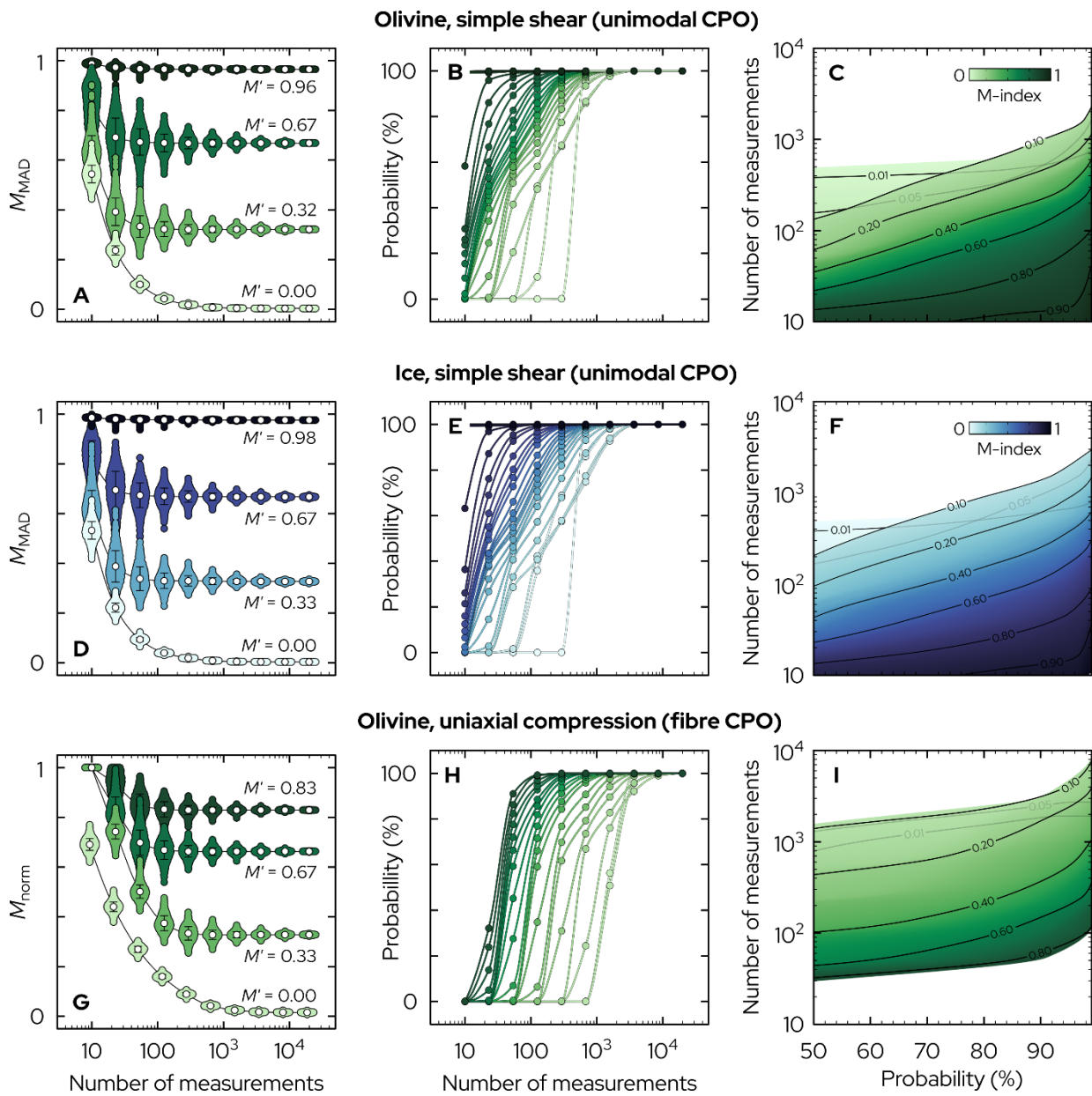
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To explore the effect of population size on measured CPO intensity, Figure 7 shows a Monte Carlo resampling analysis of the VPSC results. Although several scalar metrics have been examined thus far, the following analysis focuses primarily on M_{MAD} because it requires no kernel, such that its convergence with increasing population size reflects sampling alone. A comparable analysis for the ODF-derived metrics— J and M_{ODF} —would be complicated by the fact that the optimal kernel halfwidth itself varies with the number of measurements (Supplementary Figure S2), meaning that any change upon resampling would reflect the combined effects of sampling and kernel selection.

559

560 First, we find the model steps that correspond to 25 evenly spaced M values covering the range
 561 0 to 1 (i.e., in increments of ~ 0.04), which we define as the “true” (i.e., reference) M -index value,
 562 M' . For each of those steps, we recalculate M for 1000 random subsamples of orientations at
 563 each of 10 different population sizes, spaced evenly in logarithmic space between $N = 10$ and
 564 $N = 20,000$. Put simply, we recalculate the M -index 250,000 times as a function of CPO intensity
 565 and population size.

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Figure 7: M-index as a function of population size and true CPO intensity, M' , for the (A–C) olivine simple shear, (D–F) ice simple shear, and (G–I) olivine mixed-mode VPSC simulations

shown above. Note that only the CPOs formed under the uniaxial compression phase of the mixed-mode VPSC simulations are used in panels G–I. To allow like-for-like comparison of CPO intensity among the A-type (unimodal) and (010)-fibre CPOs, the M-index has been normalised to the range 0–1 following the procedure described in Section 6—note that no normalisation is necessary for the unimodal CPOs, as they already span the range $0 \leq M \leq 1$. (A, D, G) Monte Carlo calculations of M for orientation distributions of varying intensity and size. For each set of conditions, M is calculated using 1,000 random samples of N orientations. To better show the distribution of M , the data points are jittered in the x-direction according to a kernel density estimate along the y-direction. The mean of each distribution is shown by a white circle, with error bars corresponding to the 1-sigma standard deviation. (B, E, H) The probability of obtaining an estimate of M within 10% of the true CPO intensity, M' , as a function of CPO intensity and the number of orientation measurements. (C, F, I) Contour plots showing the number of orientation measurements required to reach a certain probability of obtaining M within $\pm 10\%$ of M' .

Figures 7A–C and 7D–F show the resampling analysis results for our olivine (Figure 2) and ice (Figure 3) simple shear VPSC simulations, respectively. In Figures 7G–I, we include a resampling analysis for the uniaxial compression phase of the mixed-mode simulations (Figure 5), allowing us to also examine the effects of CPO type on statistical convergence. Note that Figures 7G–I use the normalised M-index values, M_{norm} , to place the unimodal and fibre CPOs on a common 0–1 intensity scale.

For CPOs of any given intensity, M decreases with increasing population size, converging with the true M-index value, M' , at population sizes on the order of $N = 10$ to $N = 10,000$ (Figures

7A, D, G). However, there is much greater relative change in M for weaker CPOs—random orientation distributions ($M' \approx 0$) give M values that, on average, decrease by > 99% (i.e., from ≥ 0.6 to ~ 0) as N increases, whereas strong orientation distributions ($M' > 0.8$) give M values that decrease by only a few percent. Accordingly, weak CPOs require far more measurements ($N > 1,000$) to reach convergence with M' , while strong CPOs converge quickly ($N < 100$)—consider that only a single orientation measurement would be required to describe the CPO intensity of a monodisperse (i.e., single crystal) orientation distribution with 100% likelihood of obtaining the true value, M' . These findings are consistent with previous studies showing that fewer measurements are needed to accurately resolve a strong CPO than a weak one (Wagner et al., 1998).

To further quantify our observations, we calculate the probability, P , of obtaining the true value, M' , from the normal distribution of M-index values produced at each set of resampling conditions, within a given degree of acceptable uncertainty, ϵ (i.e., $\pm 10\%$ for the following analyses):

$$P(M' - \epsilon \leq M_{\text{MAD}} \leq M' + \epsilon) \quad (10)$$

where P is calculated using the cumulative distribution function (CDF) of a normal distribution, φ_M —with mean, μ_M , and standard deviation, σ_M , describing the distribution of the resampled M-index values (Figures 7A, 7D, 7G)—from z-scores corresponding to the desired bounds, $M' \pm \epsilon$:

$$P = \varphi_M(z_{\text{upper}}) - \varphi_M(z_{\text{lower}})$$

(11)

where

$$z_{\text{upper}} = \frac{M' + \epsilon - \mu_M}{\sigma_M}, \quad z_{\text{lower}} = \frac{M' - \epsilon - \mu_M}{\sigma_M}$$

(12)

For example, Figure 7A shows that resampling an A-type olivine CPO with $M' = 0.32$ produces a normal distribution of M_{MAD} values with mean, $\mu_M = 0.392$ and standard deviation, $\sigma_M = 0.0548$ when only 22 orientation measurements (i.e., 231 unique misorientation pairs) are selected at random each time. Thus, the probability of obtaining $M' = 0.32 \pm 0.032$ (i.e., $M' \pm 10\%$) is given by the z-scores, $z_{\text{upper}} = -0.7299$ and $z_{\text{lower}} = -1.898$, corresponding to $P = 0.204$. In other words, there is a ~20.4% chance of obtaining an accurate value of M_{MAD} (i.e., within $\pm 10\%$ of M') when describing that CPO using $N = 22$ arbitrary orientation measurements. It is not until $N > 293$ that M' can be obtained with >90% likelihood from a single sample of orientations.

Figures 7B, 7E, and 7H show the probability of obtaining an M-index estimate within $\pm 10\%$ of the true value, M' , when sampling orientation distributions of varying CPO intensities with varying numbers of measurements. To illustrate these data in a more intuitive manner, Figures 7C, 7F, and 7I present contoured heat maps showing the number of orientation measurements required to obtain a robust measure of the M-index at a particular probability level for various values of M' . The simple-shear VPSC simulations for olivine and ice behave very similarly (compare Figures 7C and 7F), as both develop unimodal CPOs. Interestingly, very weak but

640 non-random orientation distributions require the largest number of measurements to obtain a
641 robust measure of CPO intensity. For example, with an A-type olivine CPO, up to ~1,300
642 measurements are required to obtain an M-index estimate with 95% probability of falling
643 within $\pm 10\%$ of $M' = 0.10$ (Figure 7C), whereas only ~600 measurements are required to
644 measure $M' = 0.02$ at the same level of probability. For completely random orientation
645 distributions ($M \approx 0$), there is rapid convergence with M' beyond ~300 measurements (Figures
646 7B, 7E).

647

648 While the same general trends hold true for the olivine uniaxial compression simulations
649 (Figures 7G–I), the number of grains required to accurately describe the (010)-fibre CPOs is
650 generally greater for any given value of M_{norm} . For example, whereas a perfectly unimodal (i.e.,
651 $M = M_{\text{norm}} = 1$) orientation distribution could be accurately described using a single
652 measurement, many more measurements would be needed to describe a perfect olivine (010)-
653 fibre CPO ($M = 0.436$; $M_{\text{norm}} = 1$). However, when CPO intensity is expressed using the raw,
654 unnormalised M-index (see Supplementary Figure S3), fewer measurements are needed to
655 describe fibre CPOs compared to unimodal CPOs, as a fibre CPO of any given M value is
656 inherently stronger (i.e., closer to its maximum attainable M-index) than a unimodal CPO of the
657 same M-index. This result is convenient for two reasons. First, it implies that when CPO
658 intensity is expressed using the raw M-index, our unimodal resampling analyses may provide
659 an approximate upper bound on the number of measurements needed to describe CPOs of
660 the types examined thus far (i.e., random, unimodal, fibre). Second, it suggests that
661 population-size effects can be assessed from the raw M-index alone, without having to
662 normalise to account for CPO type.

663

664

665 7.2 Natural and experimental samples

666 To assess whether the population-size effects identified above are expressed in real specimens,
667 we can now perform the same resampling analysis on a diverse suite of natural and experimental
668 specimens spanning a wide range of crystal symmetries, CPO types, and deformation histories.
669 Six specimens containing minerals of various crystal symmetry classes have been selected for
670 analysis, as summarised in Table 2. All of the specimens had previously been mapped using
671 EBSD, and were selected for analysis on the basis that they 1) cover a wide range of CPO intensity
672 and symmetry, and 2) contain ≥ 5000 grains to ensure a robust reference measure of CPO.

673

674 In order of increasing CPO intensity (defined using M_{norm}), the specimens are as follows:

- 675 1) Sample LVT128 is a specimen of Carrara marble deformed in a torsional geometry using
676 a Large Volume Torsion (LVT) apparatus at 700°C, ~1.5 GPa confining pressure, and a
677 rotation rate corresponding to a shear strain rate of $4.8 \times 10^{-5} \text{ s}^{-1}$ at the outer radius of
678 the sample (Skemer et al., 2025). A maximum shear strain of $\gamma = 3.2$ was reached at the
679 outer radius of the sample, where calcite developed a multi-modal CPO featuring $r\{10\bar{1}4\}$
680 and $c(0001)$ planes sub-parallel to the shear plane, with $\langle\bar{2}021\rangle$, $\langle 20\bar{2}\bar{1}\rangle$, and $\langle\bar{1}2\bar{1}0\rangle$ axes
681 lying sub-parallel to the shear direction (Cross & Skemer, 2017);
- 682 2) STO-2-03 is a quartz-rich mylonite from the Alpine Fault zone, New Zealand, deformed
683 in a reverse dip-slip transpressional geometry under mid-crustal conditions (Cross et al.,
684 2015). Quartz exhibits an asymmetric type-I cross girdle CPO;

- 3) Sample PIL267 is a polycrystalline ice sample deformed in a general shear geometry in a cryogenic, triaxial gas-medium apparatus at -30°C and $1.67 \times 10^{-5} \text{ s}^{-1}$ shear strain rate to a finite shear strain of $\gamma = 1.1$ (Fan et al., 2021b). Under these conditions, ice develops a strong (0001)-axis maximum perpendicular to the shear plane, with a subsidiary (0001)-axis maximum rotated $\sim 45^{\circ}$ towards the shear direction;
- 4) DR538-R3 is an abyssal peridotite ultramylonite from the St. Paul's oceanic transform fault in the equatorial Atlantic Ocean. The sample was collected using a human-occupied vehicle during cruise AL170602 onboard the MV *Alucia*, and is composed primarily of olivine, pyroxene, amphibole, spinel, and low-temperature serpentinisation and carbonation products (Klein et al., 2024). The sample was mapped using a Zeiss Supra 40VP SEM equipped with an Oxford Instruments Symmetry S1 detector at the Marine Biological Laboratory (Woods Hole, MA, USA). Olivine exhibits a weak CPO comprising both (010)-fibre and A-type unimodal components. For the most part, DR538-R3 is fine-grained; however, the map also contains two large olivine porphyroclasts covering 10% of the total area;
- 5) Sample PT345 is an iron-rich olivine polycrystal deformed to a maximum shear strain of $\gamma = 3.7$ in a torsional geometry using a triaxial gas-medium Paterson apparatus at 1100°C , 300 MPa confining pressure, and a rotation rate corresponding to $2.3 \times 10^{-4} \text{ s}^{-1}$ shear strain rate at the outer radius of the sample, where a strong A-type CPO is found (Qi et al., 2021);
- 6) UM1787 is a quartz-rich mylonite from the Garhwal Himalayas, India, composed primarily of quartz, biotite, muscovite, garnet, and ilmenite (Saha, 2020). The sample was mapped perpendicular to foliation and parallel to lineation using a ThermoFisher Helios Hydra 5

scanning electron microscope (SEM) equipped with an Oxford Instruments Symmetry S3 EBSD detector at the Marine Biological Laboratory (Woods Hole, MA, USA). Because muscovite and biotite cannot be distinguished reliably using EBSD alone, all mica orientations were indexed using a muscovite match unit but are described here collectively as "mica". Furthermore, due to the relatively weak diffraction patterns produced by mica, the map was re-indexed using Oxford Instruments' MapSweeper pattern matching toolbox using the same procedures described by Hao et al. (2024), with a cross-correlation coefficient threshold of $R = 0.25$. Mica exhibits a strong (001)-fibre CPO, with [100] and [010] axes girdled within the foliation plane.

All of the EBSD maps were processed using the open-source MTEX toolbox for MATLAB (Bachmann et al., 2010). For each specimen, a reference M-index value, M' , was calculated using the original histogram-based approach of Skemer et al. (2005) and the mean orientation of 5,000 grains selected at random. To provide more like-for-like comparison of CPO intensity given the wide variety of CPO geometries, the M-index was also normalised using three ideal end-member CPOs for each sample: random, unimodal, and either a fibre (olivine, mica), cross-girdle (quartz) or bimodal (calcite, ice) CPO. Figure 8 shows each specimen within its corresponding ternary defined by these end-members, demonstrating that the chosen specimens represent both a broad range of CPO intensity and CPO geometry. This sample suite therefore provides a useful framework for evaluating whether the population-size trends observed in the VPSC simulations above are broadly applicable regardless of CPO geometry and crystal symmetry.

Table 2: Summary of EBSD data from natural and experimental specimens

Sample name	Sample type	Phase of interest	Symmetry class	# grains	CPO type	M'	M_{norm}
LVT128	Experimental	Calcite	Hexagonal	7155	Multimodal	0.046	0.217
STO-2-03	Natural	Quartz	Trigonal	11671	Cross girdle	0.043	0.403
PIL267	Experimental	Ice	Hexagonal	21924	Weak bimodal	0.217	0.469
DR538-R3	Natural	Olivine	Orthorhombic	29185	Weak fibre	0.131	0.545
PT345	Experimental	Olivine	Orthorhombic	5398	Unimodal	0.392	0.792
UM1787	Natural	Mica	Monoclinic	5590	Fibre	0.270	0.949

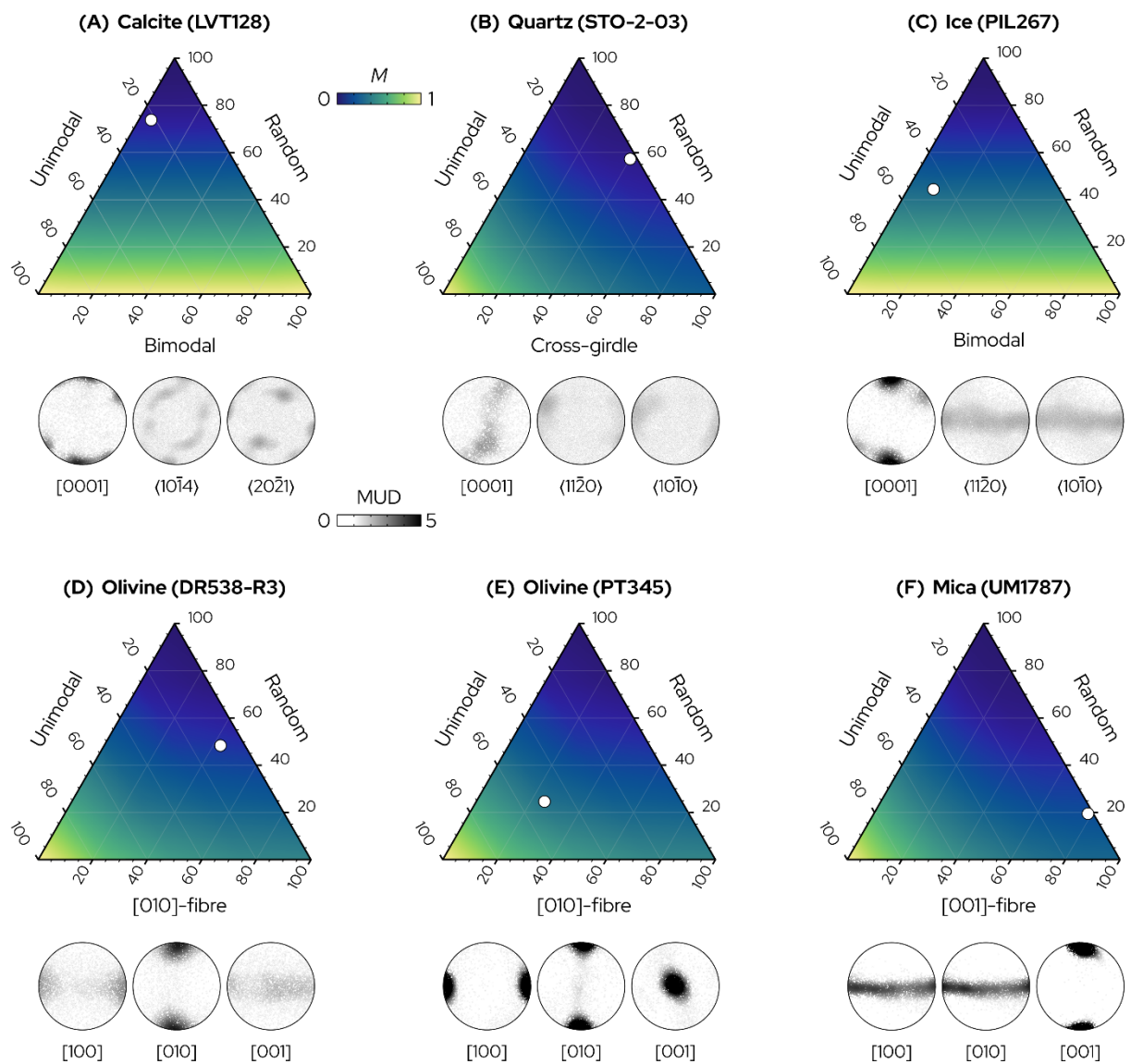


Figure 8: CPO intensity and geometry of the natural and experimental sample suite. The CPO of each sample has been placed into a ternary space (see main text) defined by three end-member CPOs: random, unimodal, and either a (A, C) bimodal, (B) cross-girdle, or (D–F) fibre CPO. Each ternary is coloured according to the M-index at each location in the ternary, constrained by mixing synthetic CPOs of the three end-members in varying proportions. The CPO of each sample is shown using scattered pole figures where each data point is coloured by multiples of uniform distribution (MUD). The pole figures are all lower-hemisphere, equal-area projections. Sample details are provided in the main text.

Figure 9 shows the resampling analysis results for the natural and experimental specimens. As expected, the probability of obtaining an M value within $\pm 10\%$ of the true, reference value, M' ,

748 increases as more orientation measurements are provided. Furthermore, as shown for the VPSC
749 simulations, the number of measurements required to obtain an accurate value of M increases
750 with decreasing CPO intensity. For example, for the sample with the lowest M-index value, STO-
751 2-03, roughly 1,000 measurements are required to obtain M within $\pm 10\%$ of M' with 95%
752 probability (Figure 9A, triangles), whereas only ~ 100 measurements are required to reach the
753 same probability in sample UM1787, which has a near-perfect (001)-fibre CPO (Figure 9A,
754 diamonds).

755

756 Again, these data are easier to interpret when plotted as the number of measurements required
757 to obtain M' ($\pm 10\%$) at a given probability. For reference, Figure 9B shows a contoured heat map
758 of this quantity, taken as the maximum across the olivine and ice simple-shear simulations
759 (Figures 7C and 7F). As noted above, these simulations—which produce unimodal CPOs—are
760 expected to provide an approximate upper bound on the number of grains required when CPO
761 intensity is expressed using the raw (unnormalised) M-index, at least for the idealised
762 simulations examined above.

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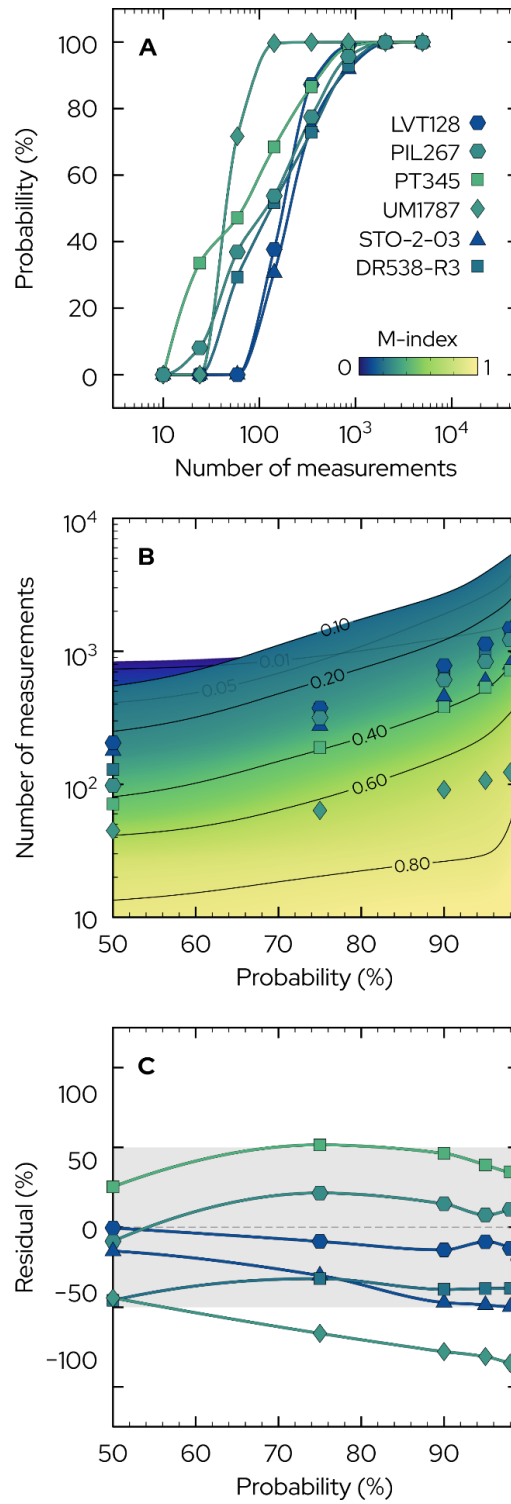
764 As shown in Figure 9B, there is generally close correspondence between the heat map derived
765 from the VPSC simulations and the real sample analyses (i.e., the symbols in Figure 9B). The
766 residual between the simulated and real data is typically within $\pm 50\%$ (Figure 9C), where positive
767 values indicate that more measurements are required for convergence with M' than suggested
768 by the VPSC simulations, and negative values indicate that fewer measurements are required for
769 convergence. The only noteworthy outlier is UM1787—the strong (001)-fibre CPO for mica—
770 which can be accurately described with up to ten times fewer measurements than suggested by

771 the VPSC analyses (−90% residual; diamonds in Figure 9C), consistent with our inference that

772 fibre CPOs require fewer measurements than unimodal CPOs at an equivalent raw, unnormalised

773 M-index.

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Figure 9: Resampling analysis for natural and experimental samples.

(A) The probability of obtaining an estimate of M within 10% of the true CPO intensity, M' , as a function of CPO intensity and the number of orientation measurements. (B) A contour plot showing the number of orientation measurements required to reach a certain probability of obtaining M within $\pm 10\%$ of M' . The heat map represents an upper bound derived from the simple-shear VPSC simulations. (C) The residual between the VPSC results, represented by the heat map in (B), and the resampling analyses of the real specimens, represented by the symbols in (B). Positive values indicate that more measurements are required to obtain a measure of the "true" CPO intensity than is suggested by the VPSC simulations; negative values indicate that fewer measurements are required for a representative measure of M than the VPSC simulations would suggest.

For convenience, Figure 10 replots the heat map presented in Figure 9B to show the number of measurements required to obtain a representative measure of M ($\pm 10\%$) at a range of probability levels. Table 3 provides the corresponding values in tabulated form for select M -index values and probability levels. Note that the values shown in Figure 10 and Table 3 have been doubled relative to Figure 9B to account for additional complexity not captured by the idealised VPSC simulations. With this adjustment the recommended sample sizes encompass all of the natural samples analysed here, including those requiring 50% more measurements than the VPSC simulations alone suggest (Figure 9C). Again, this calibration should be treated as a conservative upper bound as non-unimodal CPOs can be described using considerably fewer measurements at an equivalent raw M -index value.

As Figure 10 demonstrates, counting-statistic requirements generally decrease with increasing CPO intensity; that is, fewer measurements are required for stronger CPOs. However, the number of measurements peaks for very weak but non-random CPOs, with up to 5,800 measurements

needed to describe CPOs with $M = 0.1$ at a 99% probability level (Table 3). Nevertheless, population sizes on the order of 1,000–2,000 independent measurements should provide sufficient confidence for most CPOs. These recommendations are broadly consistent with previous work showing that several thousand orientations are often needed to characterise weak ODFs (Jura et al., 1996; Bozzolo et al., 2007). Using synthetic orientation distributions, Billings and Skemer (2026) recently reported that 1,000–1,300 grains are required to constrain M for unimodal CPOs of intermediate strength in orthorhombic crystals. For comparison, their recommended population sizes are plotted on Figure 10 (grey symbols). Note that their recommendation is slightly stricter above $M \approx 0.2$, whereas ours is much stricter below $M \approx 0.2$. This difference arises because Billings & Skemer assessed CPO convergence using a fixed absolute tolerance (± 0.02), whereas we use a relative tolerance ($\pm 10\%$).

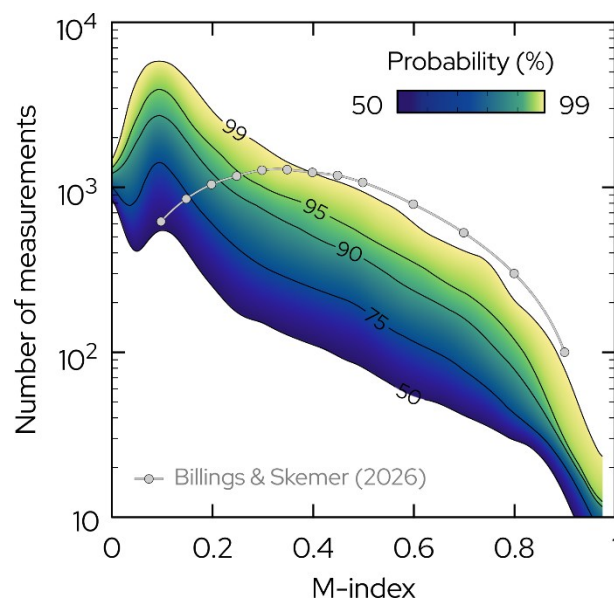


Figure 10: General guidance for the number of measurements required to accurately measure CPO intensity at various levels of probability. Heat map derived from resampling analyses of the VPSC simulations (i.e., Figures 7C and 7F). These values have been doubled relative to the resampling analyses shown in Figures 7C and 7F, and should therefore be considered a conservative bound, as the real (natural and experimental) samples analysed above show convergence at smaller population sizes.

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Table 3: The number of independent orientation measurements needed to obtain M within a tolerance, $\epsilon = \pm 10\%$, of the true value, M' , at a given probability level. Note that the relative ($\pm 10\%$) criterion collapses as $M' \rightarrow 0$, so we also impose an absolute floor of ± 0.001 . Note also that these values have been doubled relative to the resampling analyses shown in Figures 7C and 7F, to conservatively account for additional complexity not captured by the idealised VPSC simulations.

M-index	Probability (%)							
	50	70	75	80	90	95	98	99
0	839	941	997	1052	1215	1307	1404	1470
0.02	607	751	849	959	1349	1601	1922	2196
0.04	429	646	796	974	1680	2229	2994	3723
0.06	427	786	1009	1254	2178	3051	4188	5080
0.08	508	1047	1349	1646	2636	3750	5051	5717
0.1	549	1117	1427	1733	2720	3888	5256	5811
0.12	518	984	1246	1517	2457	3499	4819	5485
0.14	444	817	1026	1245	2076	2907	4034	4865
0.16	363	676	846	1019	1716	2373	3278	4134
0.18	298	566	711	855	1431	2004	2753	3447
0.2	250	482	609	739	1219	1752	2419	2892
0.25	174	337	433	536	901	1241	1837	2176
0.3	150	266	339	421	742	1006	1406	1761
0.35	127	228	287	350	611	862	1147	1413
0.4	111	199	249	302	507	745	1037	1219
0.45	94	176	220	267	435	621	910	1077
0.5	81	149	185	222	371	513	776	937
0.55	65	115	143	172	297	421	615	779
0.6	54	94	118	143	237	349	487	603
0.65	49	79	100	122	197	279	401	483
0.7	41	64	79	95	161	229	343	410
0.75	35	51	60	70	116	175	275	344
0.8	29	38	43	49	79	119	174	207
0.85	24	29	32	35	48	65	108	145
0.9	13	19	21	22	26	30	51	78
0.95	6	9	11	12	15	16	25	32

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8. One point per grain or all points?

830 When working with spatially resolved orientation data, a key consideration is whether to use all
831 of the available data ("all points") or just one representative measurement per grain ("one point

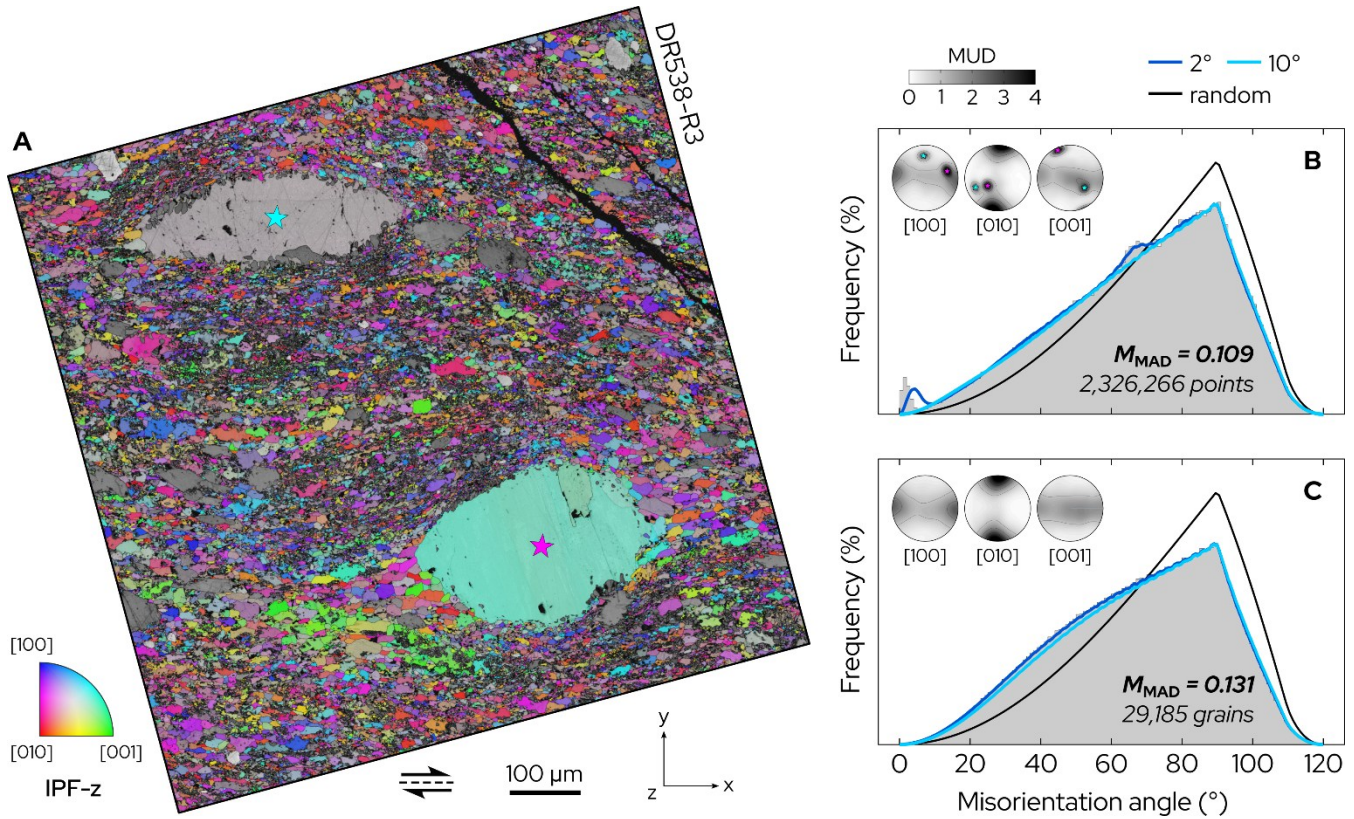
per grain"). In general, it is common practice to construct pole figures using only the one-point-per-grain data, particularly in specimens with bimodal grain sizes, to avoid obscuring the overall CPO with the orientations of just a handful of large grains (e.g., Figure 11). Of course, one strategy is to explicitly subset each population of interest—based on grain size, grain shape, or spatial region, for instance—and plot those subpopulations separately. Indeed, this approach is preferable when each subpopulation is expected to have distinct physical properties. However, there are also scenarios in which it is useful to visualise the all-points data together, particularly when the area- or volume-weighted data have direct physical meaning—for example, when examining the bulk elastic (seismic) anisotropy of a given specimen.

Likewise, CPO intensity can be calculated using either the all-points or one-point-per-grain data. To illustrate the impact of this decision, we examine specimen DR538-R3, which features a strongly bimodal grain size and modest A-type CPO. In Figure 11, we compare pole figures, misorientation angle distributions, and CPO intensities calculated for DR538-R3 using both the all-points (Figure 11B) and one-point-per-grain data (Figure 11C).

The all-points data for DR538-R3 produce distinct peaks at 2° and 65° misorientation angle (Figure 11B) due to the increased likelihood of sampling two orientations from within either of the two large olivine porphyroclasts. Consequently, the bulk A-type CPO becomes obscured and the all-points data produce an M value ($M = 0.109$) lower than that provided by the one-point-per-grain data ($M = 0.131$). However, it cannot be assumed that the all-points data will always produce lower CPO intensities than the one-point-per-grain data. Consider the case in which a coarse-grained, strongly textured aggregate contains a small fraction of fine, randomly oriented

855 grains. In this case, the coarse-grained, area-dominant grain population will introduce bias
 856 towards larger CPO intensity values; thus, the all-points (area-weighted) data will yield a greater
 857 value of CPO intensity than the one-point-per-grain data.

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861 **Figure 11: Comparison of all-points versus one-point-per-grain CPO data for a porphyroclastic**
 862 **abyssal peridotite mylonite, DR538-R3.** (A) An inverse pole figure (IPF) map showing crystal
 863 orientations relative to the z-direction. (B–C) Random-pair misorientation angle histograms and
 864 contoured pole figures for the (B) all-points and (C) one-point-per-grain data. The theoretical random
 865 angle distribution is shown in black. For comparison, angle distributions derived from the ODF (Mainprice
 866 et al., 2015) are shown for ODF kernel halfwidths of 2° (dark blue) and 10° (light blue).

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869 Whatever the approach, it is also important to ensure that each subpopulation contains a
 870 statistically robust number of measurements. This criterion is met for the fine-grained

871 population of DR538-R3, which is comprised of 29,183 grains—far exceeding the ~3,200
872 measurements needed to obtain a representative value of CPO intensity with 95% likelihood for
873 $M = 0.131$ (Table 3; Figure 10). However, the same criterion is clearly not met for the coarse-
874 grained population in DR538-R3, which features only the two large porphyroclasts. If we assume
875 for the sake of demonstration that the coarse-grained population exhibits a similar CPO intensity
876 of $M = 0.131$ (and that the porphyroclasts are homogeneously distributed in space), an area
877 ~500 times larger than that shown in Figure 11A would need to be analysed to achieve a similar
878 level of statistical robustness, equivalent to roughly one third of a standard 46 x 27 mm
879 petrographic thin section.

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881 **9. Sensitivity to map quality and grain reconstruction**

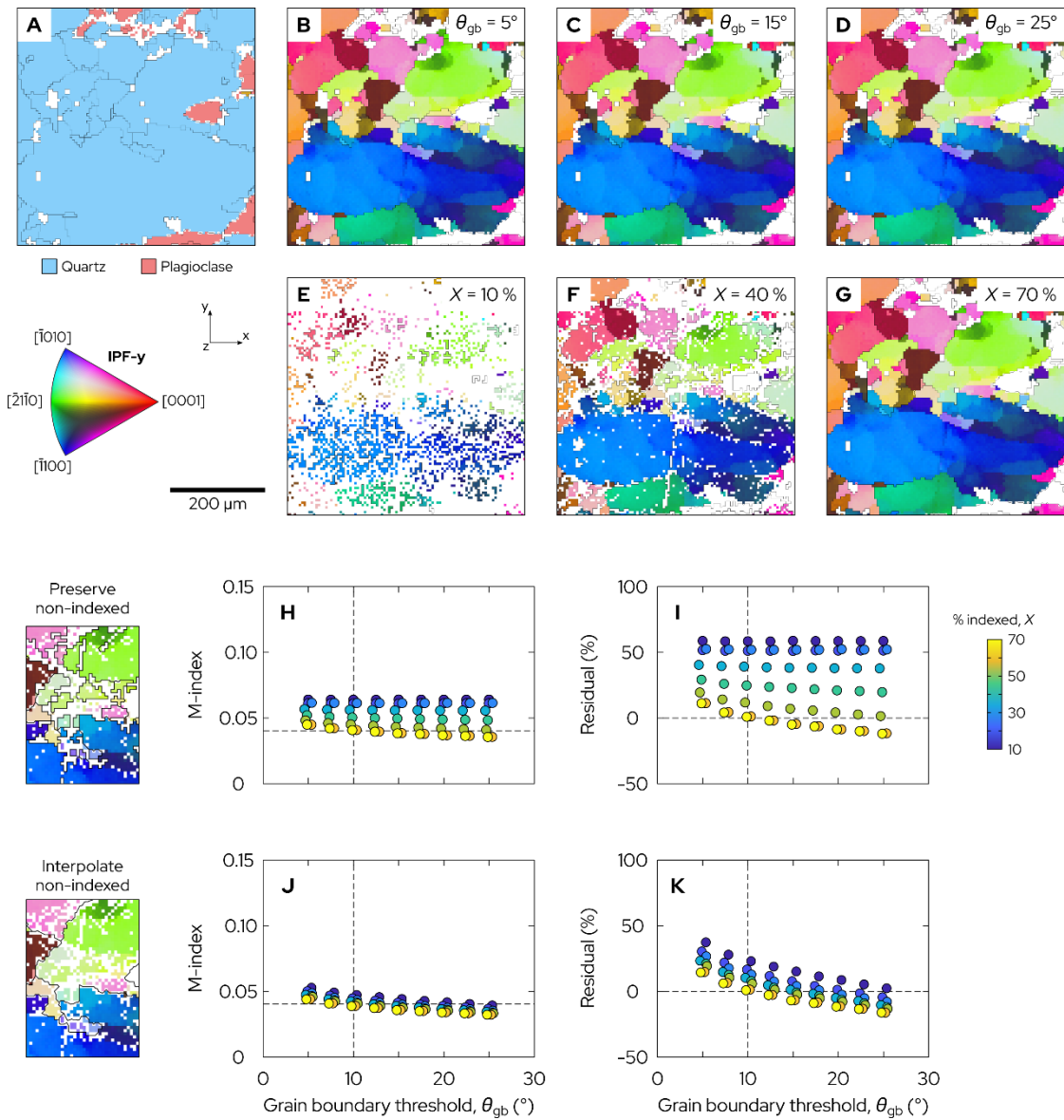
882 If CPO intensity is calculated from one-point-per-grain data, grain entities must first be
883 defined from spatially resolved (map) orientation data. Thus, the metric in question will
884 depend, to some degree, on map data quality (e.g., indexing rate, misindexing, clean-up
885 routines) and user-defined grain construction settings (e.g., the critical misorientation angle
886 used to define grain boundaries). While this dependence was raised as a specific criticism of
887 the M-index by Schaeben (2007), it applies equally to any CPO intensity metric calculated from
888 one-point-per-grain data (e.g., J-index, M-index, ball volume, fibre volume).

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890 Figure 12 illustrates how the M-index varies as a function of EBSD indexing rate and grain
891 boundary misorientation angle for specimen STO-2-03, the Alpine Fault mylonite described
892 above. Indexing rate was varied by nullifying pixels chosen at random but weighted according
893 to band contrast (i.e., EBSD pattern quality), such that regions of low pattern quality were more

likely to be nullified. Specimen STO-2-03 was chosen as it shows evidence for extensive subgrain rotation recrystallisation (Cross et al., 2015), and should therefore be maximally sensitive to the choice of grain boundary misorientation angle.

For a given grain boundary misorientation angle (varied between 5° and 25°), we randomly selected 100 subsamples of X % indexed pixels (with X ranging from 10 % to 80 %), and constructed grains using only those pixels (Figures 12A–G), generating 7,200 estimates of M . Generally speaking, the M -index is relatively insensitive to the choice of grain boundary misorientation angle, deviating by up to $\pm 15\%$ at any given indexing percentage. In contrast, the map quality—that is, the indexed fraction of the map area—exerts a significant influence over the M -index, with variations of up to $\pm 35\%$ when all non-indexed space is preserved (Figure 12I) such that poorly indexed grains may be counted several times as individual, unconnected grains. This effect can be mitigated to a large extent—with variation reduced to $\pm 15\%$ (Figure 12K)—by interpolating (“growing”) grains into all non-indexed space, ensuring that isolated grain fragments become joined together. Under extreme conditions where both the grain boundary misorientation angle and indexing rate are low, it is possible to obtain a value of M that deviates from the reference value by up to 60% when non-indexed space is preserved (Figure 12I), and up to 40% if grains are allowed to “grow” into non-indexed regions (Figure 12K). However, over a more reasonable range of conditions ($\geq 70\%$ indexing, 5–15 ° grain boundary angle), M deviates from the reference value by no more than $\sim 5\%$ (Figures 12I, 12K). Thus, measures of CPO intensity should be relatively insensitive to map quality or processing workflow over a typical range of conditions.



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Figure 12: Effect of EBSD map quality (indexing rate) and grain construction (misorientation threshold, interpolation) on apparent CPO intensity.

(A) EBSD phase map and (B–G) orientation maps for specimen STO-2-03, an Alpine Fault mylonite deformed under mid-crustal conditions (Cross et al., 2015). Only a small subregion of the full map is shown. (B–D) Grain boundaries, shown in black, were constructed using misorientation angle thresholds of 5–25°. (E–G) Maps with different indexing rates were generated by randomly nullifying pixels according to their EBSD band contrast values. (H, J) M-index versus grain boundary misorientation angle, θ_{gb} . Symbols are coloured according to the indexing rate, X , of their corresponding map. (I, K) The residual of each M-index value, expressed as a percentage relative to the reference value, $M = 0.043$ ($\theta_{gb} = 10^\circ$, $X = 70.4\%$). Panels (H–I) show the effects when all non-indexed space is preserved, whereas in panels (J–K), grains have been allowed to interpolate (“grow”) into non-indexed space.

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931 **10. Closing remarks and summary**

932 To improve reproducibility and reliability among studies involving CPO analysis, we establish the
933 following set of guiding principles, observations, and practical recommendations:

- 934 • Scalar representations of the orientation density function (ODF)—for example, the J-index
935 and M_{ODF} —are highly sensitive to the parameters used in their construction: namely, the
936 kernel halfwidth and the method used to construct the ODF (e.g., Fourier decomposition
937 or kernel superposition).
- 938 • ODF-derived metrics should not be compared without strict methodological consistency.
939 Comparisons are only meaningful when calculation parameters (e.g., halfwidth,
940 bandwidth, ODF construction method) are explicitly reported and when the same
941 procedure is applied to every dataset.
- 942 • Automatic kernel selection methods such as Kullback-Leibler cross-validation largely
943 overcome the sensitivity to halfwidth described above, and are recommended wherever
944 available. Unfortunately, such optimisation procedures may not be available in
945 proprietary software packages;
- 946 • When calculated following the original formulation of Skemer et al. (2005)—that is, using
947 the random-pair misorientation angle histogram—the M-index is computationally
948 efficient, has just one free parameter (the histogram bin width) to which it is largely
949 insensitive, and yields stable, reproducible estimates of CPO intensity across a wide range
950 of measurement conditions.
- 951 • The maximum attainable value of the M-index depends on the geometry of the
952 orientation distribution, such that a strongly developed fibre texture and a weakly

developed unimodal texture may return identical values. Normalisation offers a partial remedy, and here we provide one such method for normalizing the M-index using eigenvalue decomposition of the orientation tensor;

- Monte Carlo resampling shows that CPO intensity can be estimated (with 95% likelihood of obtaining a value within $\pm 10\%$ of the true value) using fewer than $\sim 1,000$ individual orientation measurements for moderate-to-strong CPOs ($M \geq 0.3$). However, for specimens with weak CPOs (i.e., $M \approx 0.1$), up to 3,900 measurements may be required for the same level of confidence. Given the speed with which quantitative microstructure data (e.g., EBSD data) can now be collected (e.g., Goulden et al., 2018), such population sizes are easily attainable and should not be considered an obstacle to robust microstructural analysis;
- When the volume-weighted data have direct physical meaning (e.g., seismic anisotropy), CPO intensity should be calculated using all available orientation data (i.e., all points per grain). Otherwise, one representative orientation per grain (e.g., the mean grain orientation) may be preferable, particularly for specimens with strongly bimodal grain sizes. In such cases, it may also be useful to analyse each distinct grain population separately (e.g., large porphyroclasts versus small recrystallised grains). Regardless of the approach, each distinct grain population must contain a statistically sufficient number of measurements.
- Grain reconstruction parameters (e.g., the critical misorientation angle) and EBSD map quality (e.g., indexing rate) introduce additional uncertainty—with the M-index deviating by up to 60% from its “true” value under extreme conditions in which indexing rate is very low ($< 25\%$). However, grain construction and map quality introduce no more than $\sim 5\%$

uncertainty for well-indexed maps—comparable to the $\pm 10\%$ tolerance adopted for the population-size recommendations above;

To close, the goal of this contribution is not to encourage the indiscriminate comparison of CPO intensity among specimens of different crystal symmetry, CPO type (unimodal, multimodal, fibre) or deformation history—such comparisons must always be approached with extreme caution. Rather, we aim to highlight the various sensitivities involved in CPO quantification, allowing the reader to make more deliberate, informed, and justified choices when reporting CPO data. By applying consistent methods, choosing calculation parameters appropriate to the data at hand—particularly the ODF halfwidth—and carefully reporting those procedures, the community can reduce ambiguity and make results more reproducible. Such practices will contribute towards a more robust understanding of the processes recorded by CPO formation.

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Author contributions

A. J. C. designed the study, performed the analyses, and wrote the manuscript.

Data availability

The EBSD maps for UM1787, DR538-R3, LVT128, and STO-2-03 are publicly available at <https://figshare.com/s/9e6687cfccf54478a4cc> (to be made public upon acceptance of the article), the EBSD map for PT345 at <https://doi.org/10.6084/m9.figshare.11838936.v1>, and the EBSD map for PIL267 at <https://doi.org/10.6084/m9.figshare.13456550.v2>. The repository entry for this article also contains the MATLAB function, `mIndexDiscrete.m`, that was used to calculate M_{MAD} for this study. This function provides the same results as the native MTEX function, `calcMIndex.m`, but runs up to ten times faster, and allows the user to specify the misorientation angle histogram bin width.

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**Quantifying the intensity of crystallographic preferred orientation (CPO):
some practical considerations and recommended practices**

A. J. Cross^{1*}

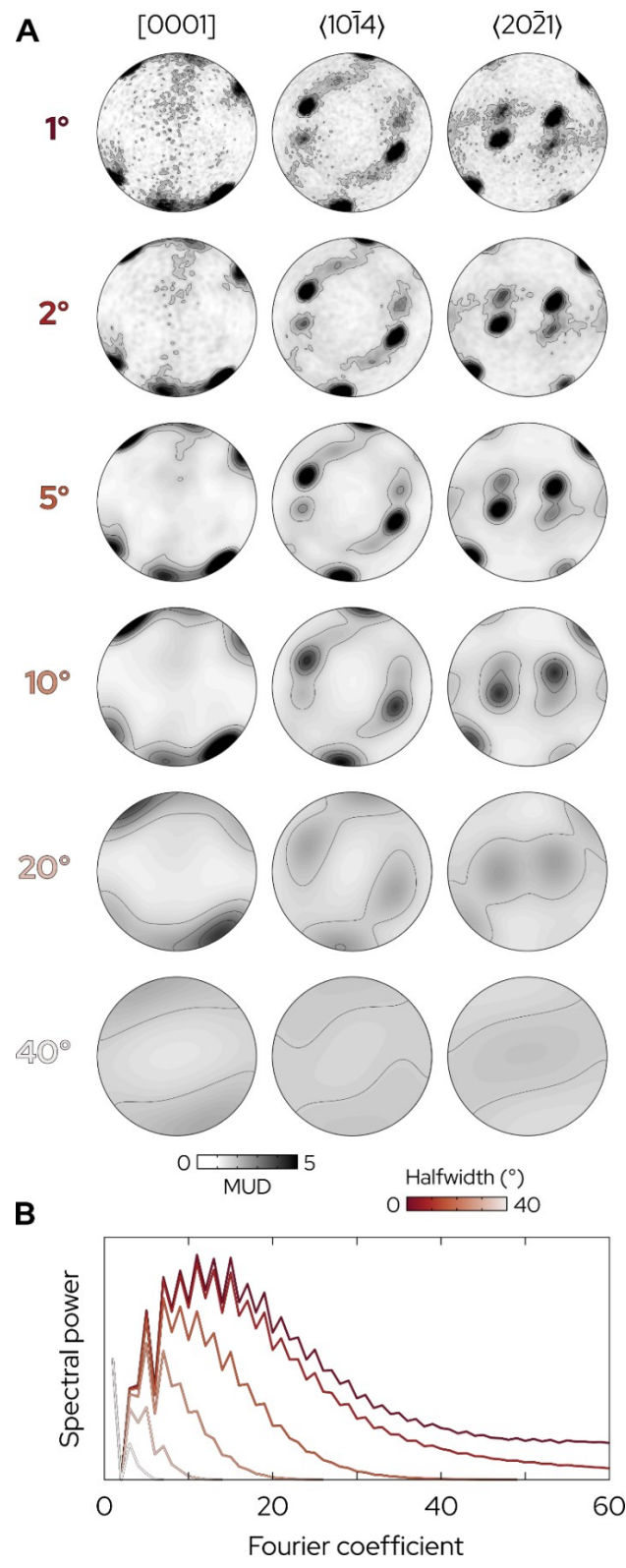
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Contents

Figures S1–S6

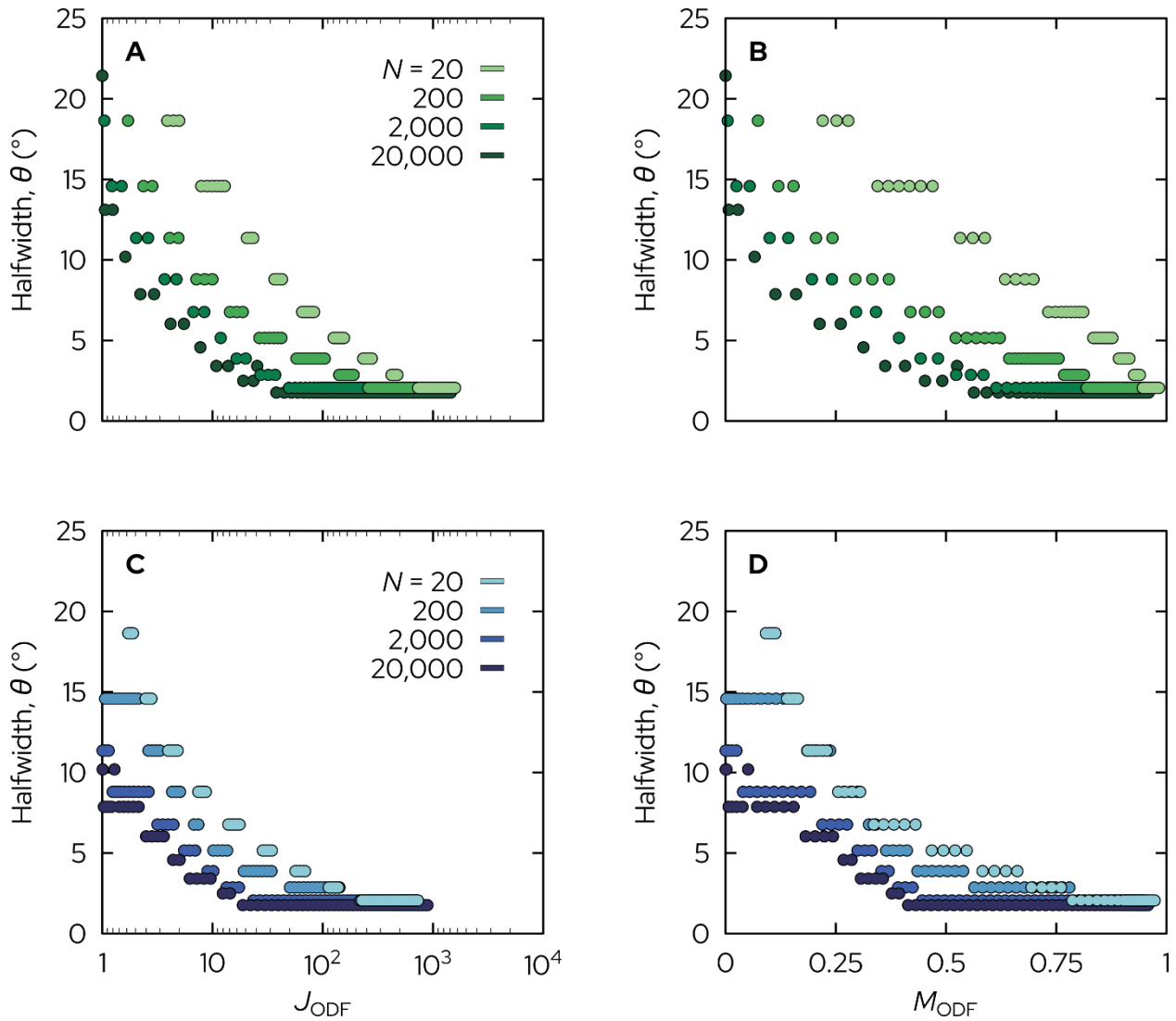
Text S1



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14

15 **Figure S1: The effect of kernel halfwidth on the orientation density function (ODF).** (A) Contoured pole figures
16 (lower hemisphere, equal angle) from a specimen of Carrara marble deformed in torsion, LVT128 (full description
17 in the main text). Contouring was performed using various halfwidths in the range 1–40°. Automatic halfwidth
18 selection using the default Kullback-Leibler cross-validation approach within MTEX (see main text) suggests an
19 optimal ODF halfwidth of 3° for this specimen. (B) ODF power spectra as a function of Fourier coefficient, coloured
20 according to ODF halfwidth. High-order information—corresponding to local, short wavelength features—is
21 progressively lost as the ODF halfwidth increases, producing smoothing of the contoured pole figures.



23

24

25 **Figure S2: Optimal ODF kernel halfwidth as a function of CPO intensity and population size (i.e., number of**
 26 **grains, N) for the (A–B) olivine and (C–D) ice VPSC simulations shown in Figures 2 and 3, respectively.** Kernel
 27 halfwidth was determined automatically using the Kullback-Leibler cross-validation approach (Bowman, 1984)
 28 implemented within MTEX.

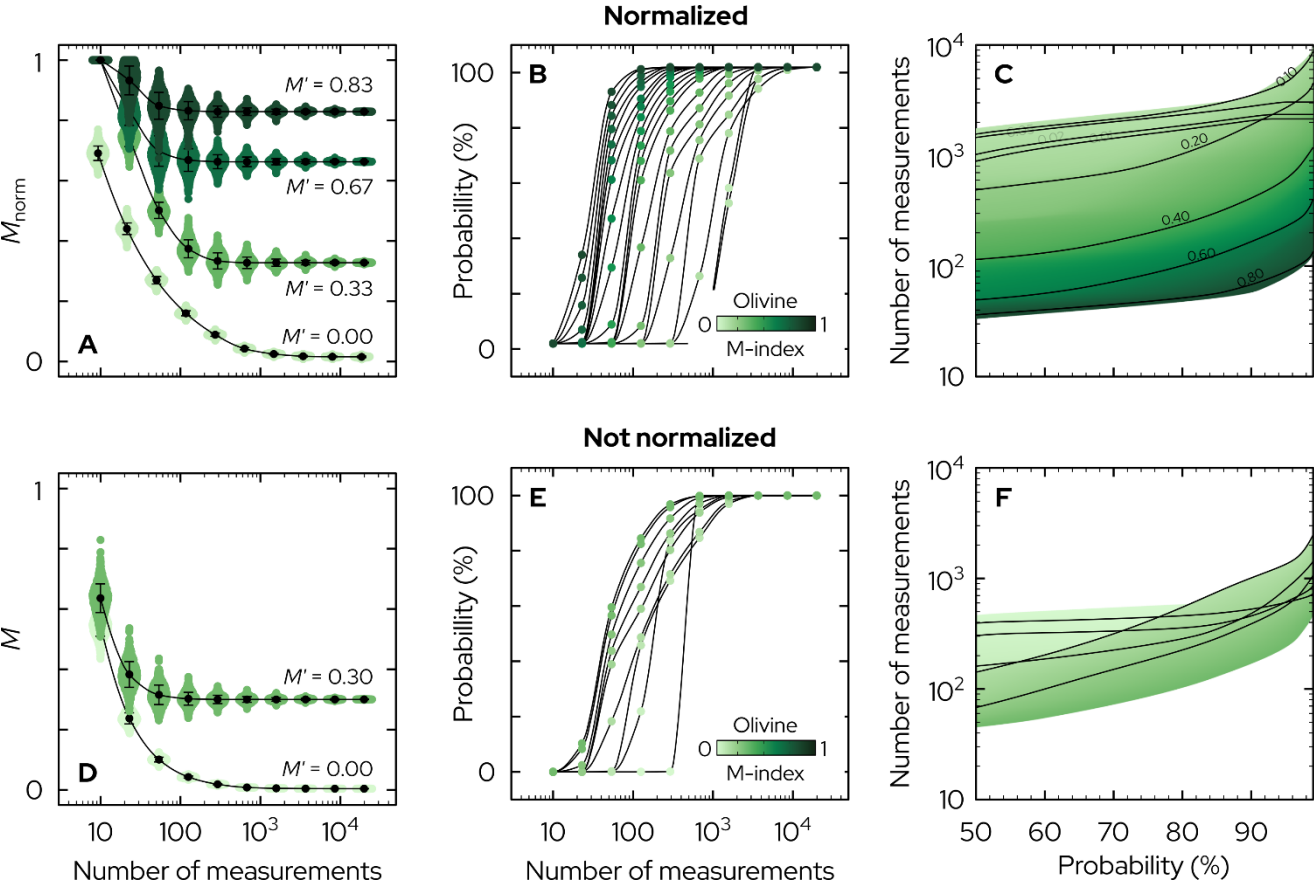


Figure S3: Comparison of the Monte Carlo resampling analyses for the (A–C) normalised and (D–F) unnormalised M-index for the mixed-mode olivine VPSC simulations. Note that only the CPOs formed under the uniaxial compression phase of the mixed-mode VPSC simulations are used. In (A–C), the M-index has been normalised to the range 0–1 following the procedure described in Section 6, using the following end-member texture components: unimodal, (010)-fibre, and random. (A, D) Monte Carlo calculations of M for orientation distributions of varying intensity and size. For each set of conditions, M is calculated using 1,000 random samples of N orientations. To better show the distribution of M, the data points are jittered in the x-direction according to a kernel density estimate along the y-direction. The mean of each distribution is shown by a white circle, with error bars corresponding to the 1-sigma standard deviation. (B, E) The probability of obtaining an estimate of M within 10% of the true CPO intensity, M' , as a function of CPO intensity and the number of orientation measurements. (C, F) Contour plots showing the number of orientation measurements required to reach a certain probability of obtaining M within $\pm 10\%$ of M' .

44 **Supplementary Text S1. Derivation of the normalised M-index**

45 The M-index of Skemer et al. (2005) measures the difference between the random-pair misorientation
46 angle distribution of a population of crystals, and the theoretical distribution of misorientation angles for
47 a randomly oriented aggregate of the same crystal symmetry (e.g., Figures 2C, 3C). For a random
48 orientation distribution, the overlap is maximised and $M = 0$. For a monodisperse (i.e., single crystal),
49 there is no overlap and $M = 1$. However, while the bounds $0 \leq M \leq 1$ hold for unimodal (i.e., single cluster)
50 CPOs, the maximum attainable M-index is < 1 for non-unimodal orientation distributions. For example,
51 a perfect (010)-fibre distribution of olivine crystals (orthorhombic symmetry class, mmm) cannot exceed
52 $M = 0.436$: a value that otherwise corresponds to a unimodal CPO of only moderate strength. To facilitate
53 comparison of CPO intensity among different texture types, it may therefore be desirable to normalise
54 the M-index to a common, texture-type-invariant 0–1 scale.

55
56 As described in the main text (Section 6), here we propose one method for normalising the M-index, in
57 which the M-index of a given CPO is normalised by the maximum attainable M-index value of an idealised
58 CPO with the same non-random texture components. In the example of our mixed-mode olivine VPSC
59 simulations (Figure 5), we can place each simulated CPO within a ternary defined by three end-member
60 textures, chosen to match the observed texture components: random, (010)-fibre, and A-type (unimodal).
61 This procedure is conceptually inspired by the point-girdle-random (PGR) index of Vollmer (1990), but
62 uses the eigenvalue spectrum of the entire orientation distribution in $SO(3)$ space, rather than the
63 eigenvalue spectrum of individual crystal axes projected into Euclidean S^2 space.

64
65 In the open-source MTEX toolbox for MATLAB, crystal orientations are represented as rotations in $SO(3)$
66 space using unit quaternions, q , which describe the rotation required to map an orientation in the sample
67 coordinate system to an orientation in the crystal coordinate system (Kunze & Schaeben, 2004). Because
68 q and $-q$ describe the same rotation, it is useful to obtain a unique 4×4 symmetric matrix, Q , given by

$$Q = qq^T \quad (S1)$$

$$Q = \begin{pmatrix} q_1^2 & q_1q_2 & q_1q_3 & q_1q_4 \\ q_1q_2 & q_2^2 & q_2q_3 & q_2q_4 \\ q_1q_3 & q_2q_3 & q_3^2 & q_3q_4 \\ q_1q_4 & q_2q_4 & q_3q_4 & q_4^2 \end{pmatrix} \quad (S2)$$

75

76 The orientation tensor describing a population of N orientations can then be obtained as follows
 77 (Bachmann et al., 2010):

78

79

$$T = \frac{1}{N} \sum_{i=1}^N Q_i$$

80

(S3)

81

82 Importantly, the orientation tensor in SO(3) is a 4×4 symmetric matrix, such that spectral decomposition
 83 provides four principal eigenvectors, $a_1, \dots, a_4$, and four corresponding eigenvalues, $\lambda_1, \dots, \lambda_4$, which are
 84 ordered as such:

85

86

$$\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$$

87

(S4)

88 where

89

$$\sum_{i=1}^4 \lambda_i = 1$$

90

(S5)

91

92 Given that the eigenvalue spectrum sums to unity by definition, the eigenvalues can be used to plot any
 93 given CPO at a single, unique position within a three-dimensional space defined by the coordinates λ_1 ,
 94 λ_2 , and λ_3 . Furthermore, given that $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$, the accessible region of this eigenvalue space is
 95 limited to a tetrahedron defined by the vertices $(1,0,0,0)$, $(\frac{1}{2}, \frac{1}{2}, 0, 0)$, $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0)$, $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. As an
 96 example, Figure S4 shows the CPO for sample PT345 (Qi et al., 2021; see main text for details) placed
 97 within this eigenvalue space. Also shown on Figure S4 are the eigenvalue spectra corresponding to our
 98 three synthetic end-member textures, chosen according to the texture components observed in PT345.

99

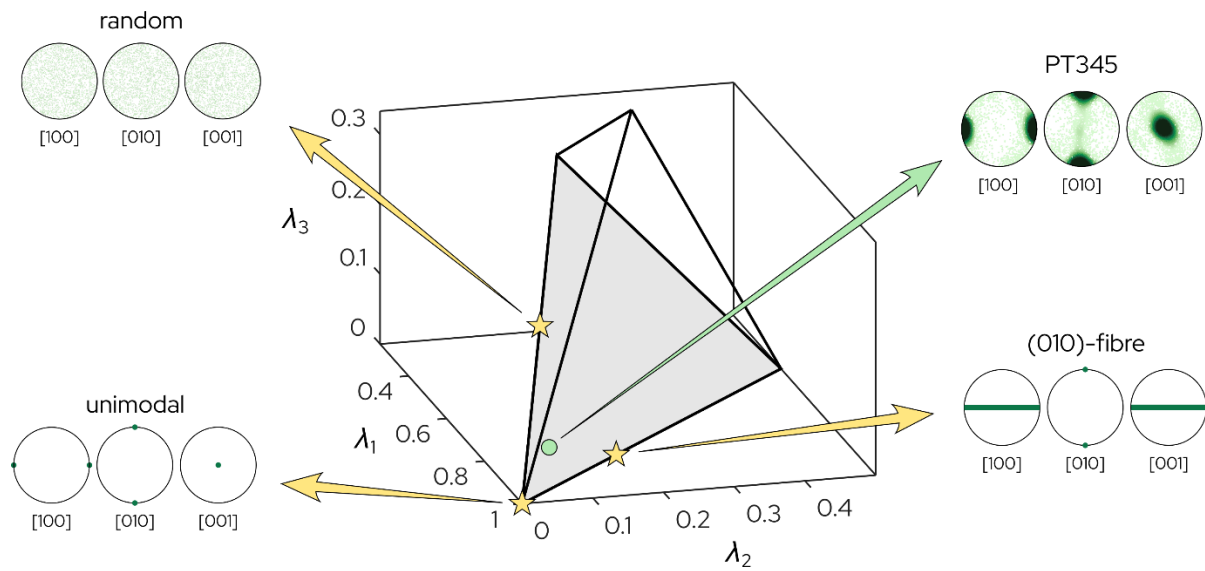


Figure S4. Projection of CPOs into eigenvalue space. Crystal orientations in MTEX are represented using unit quaternions, such that each CPO is characterised by a four-component eigenvalue spectrum. Because the eigenvalues sum to unity, any orientation distribution can be located uniquely within the three-dimensional space using the eigenvalues λ_1 , λ_2 , and λ_3 . Furthermore, given that $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$, all eigenvalue spectra must lie within the outlined tetrahedron. As an example, the green symbol marks the eigenvalue spectrum of specimen PT345 (see main text for details), along with corresponding pole figures in which each point is coloured according to local orientation density. Yellow stars mark the three end-member textures—random, A-type unimodal, and (010)-fibre—chosen to evaluate the texture components found within PT345.

To normalise the M-index, we need to calculate the proportions of the random and non-random (unimodal, fibre) textures expressed in PT345. This can be achieved by comparing the eigenvalue spectrum of our chosen sample against the eigenvalue spectra of synthetic CPOs generated by mixing our three end-member textures in varying proportions. Figure S5 shows the locations of these synthetic CPOs within eigenvalue space, calculated at modal proportion increments of 0.1 (i.e., 10%). When calculating these synthetic mixtures, we ensure that each component is defined by no fewer than 1,000 individual orientations, following the approximate population-size requirements established in the main text.

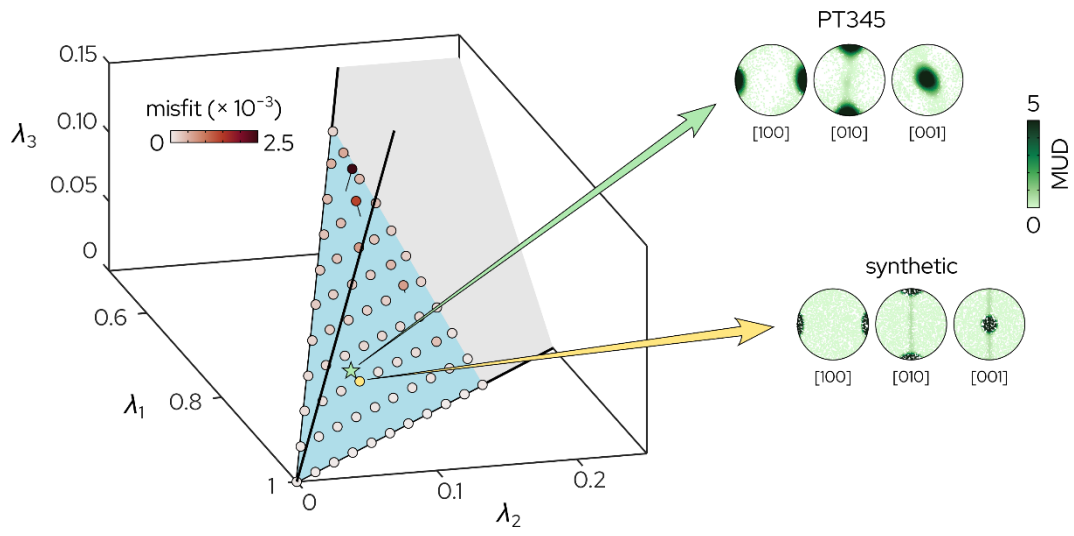


Figure S5: Eigenvalue distribution of synthetic end-member mixtures. Each circle represents a mixture of the three example olivine textures—unimodal, (010)-fibre, random—at increments of 10% modal proportion. The distribution of these synthetic CPOs can be well approximated by a plane (the blue surface) in eigenvalue space. Each symbol is coloured according to the misfit (i.e., Euclidean distance) between its calculated position and its ideal position on the fitted blue plane in eigenvalue space. Note that the misfit is $\leq 2.5 \times 10^{-3}$, indicating that a planar approximation is well justified in this specific case. The green star indicates the position (in eigenvalue space) of the CPO from olivine specimen PT345 (see main text for details). For comparison, pole figures are shown for specimen PT345 and for the closest synthetic CPO in eigenvalue space (yellow circle), which is composed of 50% A-type unimodal orientations, 20% (010)-fibre orientations, and 30% random orientations.

For PT345 and all of the other CPOs analysed in this study, the eigenvalue spectra conveniently lie close to a single plane (Figure S5), such that the spectrum of any given mixture is well approximated by a linear combination of the end-member spectra:

$$\lambda \approx w_{unimodal}\lambda_{unimodal} + w_{(010)-fibre}\lambda_{(010)-fibre} + w_{random}\lambda_{random} \quad (S6)$$

where w_i are barycentric coordinates representing the relative proportions, from 0 to 1, of each end-member texture.

Given that each eigenvalue spectrum contains three independent values, whereas the barycentric coordinates have only two degrees of freedom, Equation S6 is overdetermined and we can identify a unique position within our eigenvalue space that minimises

$$\left\| \lambda - \sum_k w_k \lambda_k \right\|^2$$

(S7)

where k corresponds to each of our three end-member textures. In other words, we use the least-squares misfit to find the position (and corresponding barycentric coordinates) that lies closest to the planar fit through our synthetic spectra in eigenvalue space (Figure S5).

The residual of the fit is given by

$$\varepsilon = \left\| \lambda - \sum_k w_k \lambda_k \right\|$$

(S8)

which measures how completely a CPO is described by the three end-members. Note that CPOs of a type not represented within the ternary—a small-circle distribution of [100], for instance—would return large residuals, indicating that their normalised M-index values should be treated with caution. Accordingly, it is important to emphasise that the chosen reference frame represents a reduced form of the full SO(3) orientation space and that, inevitably, information about the full orientation distribution is discarded. Nevertheless, this reduced-SO(3) reference frame retains more information than a scalar measure of CPO intensity alone (e.g., the M-index, the J-index).

Having placed a CPO within our chosen ternary framework, we can now determine how to normalise its M-index. The normalisation factor is the M-index of a CPO with the same relative proportions of the non-random components, and $w_{\text{random}} = 0$. In simpler terms, we construct a line between our CPO and the random vertex of the ternary, and then project that line onto the binary between the two ordered end-members: unimodal and (010)-fibre, in this case (Figure S6). The normalisation factor is the M-index of a CPO at this position along the binary.

In practice, the relative proportion of the two ordered components, is obtained from the barycentric coordinates as

$$t = \frac{w_{\text{unimodal}}}{w_{\text{unimodal}} + w_{(010)\text{-fibre}}}$$

(S9)

180 The normalised M-index is then given by

181

182

$$M_{\text{norm}} = \sqrt{\frac{M}{M_{\text{max}}(t)}}$$

183

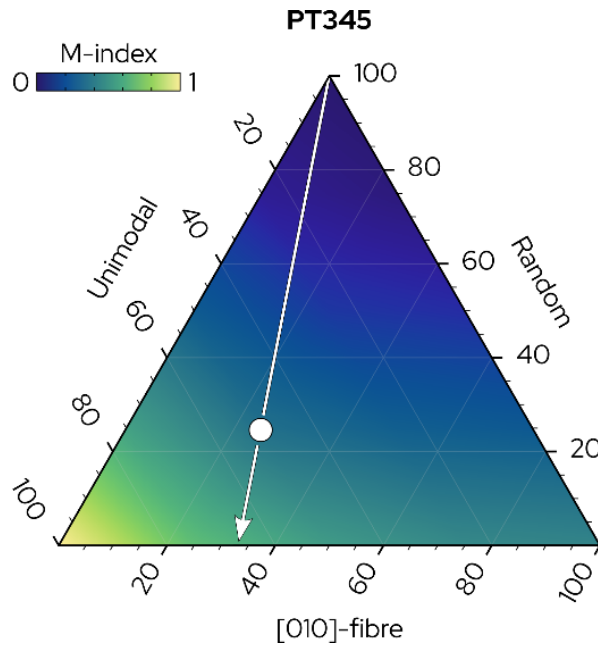
(S10)

184

185 with the square root introduced to provide linearity between M_{norm} and $1 - w_{\text{random}}$, the latter
186 representing the “non-randomness” of a given CPO.

187

188



189

190

191 **Figure S6: Normalising the M-index within a ternary reference frame.** The chosen ternary space for specimen
192 PT345, bounded by unimodal, (010)-fibre, and random end-members. The CPO for PT345 (white circle) has been
193 projected into this space using its eigenvalue spectrum. To normalise the M-index to the range 0–1, we take the
194 M-index of a CPO with the same modal proportion of non-random (unimodal, 010-fibre) components, but with no
195 random component (i.e., a perfectly ordered CPO of the same type). In effect, this value is obtained by projecting a
196 ray (white arrow) through PT345 onto the bottom edge of the ternary, which represents the binary between the
197 two non-random end-members.