Melt network reorientation and crystallographic preferred orientation development in sheared partially molten rocks

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Abstract

As partially molten rocks deform, they develop melt preferred orientations, shape preferred orientations, and crystallographic preferred orientations (MPOs, SPOs and CPOs). We investigated the co-evolution of these preferred orientations in experimentally deformed partially molten rocks, then calculated the influence of MPO and CPO on seismic anisotropy. Olivine-basalt aggregates containing 2 to 4 wt% melt were deformed in general shear at a temperature of 1250°C under a confining pressure of 300 MPa at shear stresses of $\tau = 0$ to 175 MPa to shear strains of $\gamma = 0$ to 2.3. Grain-scale melt pockets developed a MPO parallel to the maximum principal stress, s1, at $\gamma < 0.4$. At higher strains, the grain-scale MPO remained parallel to s1, but incipient, sample-scale melt bands formed at ~20° to s1. An initial SPO and CPO were induced during sample preparation, with [100] and [001] axes girdled perpendicular to the long axis of the sample. At the highest explored strain, a strong SPO was established, and the [100] axes of the CPO clustered nearly parallel to the shear plane. Our results demonstrate that grain-scale and sample-scale alignments of melt pockets are distinct. Furthermore, the melt and the solid microstructures evolve on different timescales: in planetary bodies, changes in the stress field will first drive a relatively rapid reorientation of the melt network, followed by a relatively slow realignment of the crystallographic axes. Rapid changes to seismic anisotropy in a deforming partially molten aggregate are thus caused by MPO rather than CPO.

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Melt network reorientation and crystallographic preferred orientation development in sheared partially molten rocks
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Key Points
1. When a partially molten rock is stressed, its microstructural melt pockets reorient much
more quickly than its crystallographic axes.
2. Individual melt pockets orient parallel to the loading direction at the onset of
deformation.
3. Rapid changes to seismic anisotropy in a deforming partially molten rock can be
attributed to reorientation of melt pockets.

26 Abstract:

27 We investigated the co-evolution of melt, shape, and crystallographic preferred orientations (MPOs, SPOs and CPOs) in experimentally deformed partially molten rocks, from 28 which we calculated the influence of MPO and CPO on seismic anisotropy. Olivine-basalt 29 30 aggregates containing 2 to 4 wt% melt were deformed in general shear at a temperature of 1250°C under a confining pressure of 300 MPa at shear stresses of $\tau \le 175$ MPa to shear strains 31 of $\gamma \leq 2.3$. Grain-scale melt pockets developed a MPO parallel to the loading direction by $\gamma < 1$ 32 33 0.4. At higher strains, the grain-scale MPO remained parallel to the loading direction, while incipient, sample-scale melt bands formed at ~20° to the grain-scale MPO. An initial SPO and 34 CPO were induced during sample preparation, with [100] and [001] axes girdled perpendicular to 35 the long axis of the starting material. At the highest explored strain, a strong SPO was 36 37 established subperpendicular to the loading direction, and the [100] axes of the CPO clustered nearly parallel to the shear plane. Our results demonstrate that grain-scale and sample-scale 38 39 alignments of melt pockets are distinct. Furthermore, the melt and the solid microstructures evolve on different timescales: in planetary bodies, changes in the stress field will drive a 40 relatively rapid reorientation of the melt network and a relatively slow realignment of the 41 crystallographic axes. Rapid changes to seismic anisotropy in a deforming partially molten 42 aggregate are thus caused by MPO rather than CPO. 43 44

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47 Plain language summary:

We studied the influence of melt alignment and crystal alignment on the properties of partially melted regions in planetary bodies. Molten and crystalline elements within the rocks in these layers can deform and reorient in response to stress, but it is difficult to predict how the effect of realignment of each phase affects seismic properties of the rocks. Reorientation of melt networks during deformation of partially molten rocks is not well constrained, as experiments and computational models disagree on the most favorable alignment of melt pockets. Here, we measured the angles and shapes of melt and crystals in experimentally deformed partially molten rocks, then calculated seismic properties of the deformed rocks. We found that melt pockets change orientation and shape quickly, but crystallographic axes take longer to reorient. This observation indicates that immediate changes to seismic properties after a sudden change in stress field are caused by melt, rather than by crystals. Our results show that when stress fields abruptly change in Earth and other planetary bodies, melt pocket orientation controls seismic properties and is the best instantaneous indicator of stress changes.

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64 1. Introduction

Partial melting often occurs alongside sites of rapid deformation in Earth's lithosphere. In 65 response to deformation, the molten and crystalline components of partially molten rocks align, 66 67 leading to anisotropies in mechanical, transport, and seismic properties (Blackman & Kendall, 1997; Daines & Kohlstedt, 1997; Holtzman et al., 2003; Holtzman & Kendall, 2010; Long & 68 Becker, 2010; Savage, 1999; Taylor-West & Katz, 2015). The influence of microstructure on 69 seismic properties, in particular, is often considered only in terms of the crystalline components, 70 71 but this approach may not be sufficient for interpreting the effects of deformation in partially molten regions. Melt is known to change the physical properties of an aggregate even in small 72 concentrations, as the molten and solid rock components have distinct seismic properties. The 73 74 orientations of both phases therefore contribute to the seismic anisotropy observed in Earth's upper mantle and crust (Almqvist & Mainprice, 2017; Hansen et al., 2021; Lyakhovsky et al., 75 2021). Laboratory experiments provide an important tool for determining melt and 76 77 crystallographic preferred orientations in deformed partially molten mantle rocks. However, experimental results and modeling assumptions often disagree on the orientation of the melt 78 79 network. Previous experimental studies reported alignment of the long axes of melt pockets at 80 20° to the direction of the inferred maximum principal stress (Zimmerman et al., 1999, Soustelle et al., 2014, Danies and Kohlstedt, 1997) and, with increasing strain, the formation of melt-rich 81 "bands" at a similar orientation (Holtzman et al., 2003; King et al., 2010; see Kohlstedt & 82 83 Holtzman, 2009 and Daines & Pec, 2015 for comprehensive reviews of observed melt alignment 84 in experiments). In contrast, some viscoelastic models and theories assume grain-scale melt

alignment parallel to the direction of the maximum principal stress, σ_1 (Hier-Majumder, 2011;

86 Takei & Holtzman, 2009c; Taylor-West & Katz, 2015), an orientation of melt alignment which

has also been reported using ultrasonic measurements in experiments on analog materials (Takei,

88 2001). To resolve differences between modeling, nature, and experimental results, we

89 reexamined microstructures of deformed partially molten samples.

The present study investigates the microstructural behavior of several partially molten 90 olivine + basalt aggregates deformed in general shear experiments. The sample-scale behavior of 91 92 one set of samples was previously reported in Zimmerman et al. (1999). In addition, the behavior of two additional samples deformed at higher stress conditions was examined. We characterize 93 the co-evolution of melt preferred orientation (MPO) of the liquid network and crystallographic 94 and shape preferred orientations (CPOs and SPOs) of the solid phase, from which we infer the 95 influence of stress and strain on CPO, SPO and MPO development in the deformed samples. We 96 97 then use our experimental results to calculate predicted seismic anisotropy in these samples. Finally, we discuss the relative importance of the orientations of melt pockets and 98 crystallographic axes on seismic anisotropy in samples deformed to small strains. 99

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101 2. Methods

102 2.1 Experimental deformation and imaging details

Samples of olivine ± orthopyroxene and 2-4 wt% mid-ocean ridge basalt (MORB) were 103 created by hot pressing cold-pressed powders in a gas-medium deformation apparatus (Paterson, 104 1990) at 1250°C at 300 MPa for ~3 h. At these temperature and pressure conditions, MORB 105 inclusions melted, while solid olivine crystals did not, thus forming a dense, chemically 106 equilibrated partially molten aggregate (Cooper & Kohlstedt, 1984). Samples were then cored 107 and sliced from the hot-pressed cylinders and placed between thoriated-tungsten pistons pre-cut 108 at a 45° angle, as illustrated in Figure 1. These samples were subsequently deformed in general 109 shear at the University of Minnesota in the gas-medium deformation apparatus at 1250°C and 110 300 MPa confining pressure. Under strain rates of 10⁻⁶-10⁻⁴ s⁻¹, samples reached shear stresses of 111 $\tau = 50-175$ MPa and strains of $\gamma = 0.32-2.3$. A summary of the experimental conditions and 112 resultant MPO and SPOs presented in Table 1. 113

#	T (°C)	Υmeas	γ' (s ⁻¹)	σ _{effective} (MPa)	^τ final (MPa)	initial thickness (mm)	final thickness (mm)	ΜΡΟ α _p (°)	MPO b/a	SPΟ α _p (°)	SPO b/a	W _k
starting material	1250	-	-	-	-	-	-	160	0.97	20	0.88	-
PI-281	1250	0.32	1.7 x 10 ⁻⁶	110	55	0.65	0.61	135	0.8	13	0.94	-
PI-277	1250	0.4	6.5 x 10 ⁻⁵	132	66	0.82	0.8	134	0.72	11	0.89	0.99
PI-334	1250-1290	0.77	*	350	175	0.8	0.66	112	0.74	30	0.89	0.97
PI-314	1250	0.84	4 x 10 ⁻⁵	300	150	0.81	0.71	130	0.82	31	0.93	0.92
PI-274	1250	1.3	2.7 x 10 ⁻⁵	100	50	0.83	0.72	132	0.77	32	0.79	0.96
PI-273	1250	2.3	4.0 x 10 ⁻⁴	180	90	0.93	0.76	134	0.77	26	0.73	0.98

Table 1: Experimental parameters for starting material and six deformed samples. Here, γ 116 indicates strain, τ_{final} is the inferred shear stress, and W_k denotes the kinematic vorticity number, 117 expressing the ratio of simple shear to pure shear (see Section 4.2). The initial thickness of PI-118 281 was measured, but not its initial width, so its kinematic vorticity could not be calculated. 119 120 121 After deformation, samples were cut perpendicular to the shear plane and parallel to the 122 shear direction, as indicated in Figure 2. A Zeiss Merlin scanning electron microscope (SEM) in 123 the MIT Materials Research Laboratory was used to create backscattered electron (BSE) images 124 125 at 15 – 20 kV accelerating voltage of these 2-D flat sections. In addition, electron backscattered diffraction (EBSD) maps and energy dispersive spectra (EDS) maps were collected using a 126 Camscan X500FE CrystalProbe at the Université Montpellier 2 at an acceleration voltage of 20 127 kV and a step size of $0.2 - 0.6 \mu m$. 128



130 Figure 1: Schematic drawing of the sample setup for deformation experiments.



Figure 2: Sample preparation after deformation and orientation of cuts. (a) Experimental workflow for deformation and creation of 2-D sections. SEM images of orientation and appearance of the olivine-melt aggregates (b) prior to deformation, at initial thickness Th₀, and (c) after deformation, at final thickness Th_f, with melt highlighted in red. (d) Angle conventions used throughout this paper.

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139 2.2 Quantitative image analysis methods

We used the PARticle ORientation method (PAROR; Heilbronner and Barrett, 2014,
Chapter 14) to analyze the grain-scale MPOs and SPOs. This method yields the direction of the
longest and shortest projections of particle elements. In contrast to the more common ellipsefitting method of determining orientation of short and long axes, PAROR does not require the
shortest and longest projection directions to be perpendicular to each other and is therefore well

suited for analyzing shapes of irregular objects such as melt pockets. Any shape with long axis *a*and short axis *b* is characterized by a projection function at a range of angles α, such that

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$$P(\alpha) = 2\sqrt{a^2 \cos^2(\alpha_i + \alpha_r) + b^2 \sin^2(\alpha_i + \alpha_r)} \quad , \tag{1}$$

where α is constructed by starting at an initial orientation α_i and incremented by α_r over a range of angles. This projection is symmetric around 180°. $P(\alpha)$ will be largest at the same orientation as *a*, and smallest at the orientation of *b*. For aggregates of shapes, the distribution function at each value of α is characterized by the sum of the values of $P(\alpha)$, then scaled such that $\Sigma P(\alpha)_{max}$ = 1.

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The preferred orientation angle, α_p , is then calculated relative to the shortest projection direction α_{min} such that

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 $\alpha_{\rm p} = 90^{\circ} - \alpha_{\rm min} \,. \tag{2}$

As values of α_p are symmetric around 180°, for $\alpha_{min} > 90°$, negative values are converted to their positive conjugate (i.e., -30° is the same as 150°). Angles are measured counterclockwise from 0° (east) to 180° (west) throughout this manuscript, as illustrated in Figure 2d.

We described the orientations of grains and melt pockets using an orientation distribution function (ODF) visualized as rose diagrams, normalized such that the longest axis is 1 and the shortest axis is reported as a percentage relative to the longest axis, as illustrated in Figure 3.

164 The strength of the preferred orientation is quantified by its bulk aspect ratio, b/a, a 165 comparison of the longest, a, and the shortest, b, projections of all the analyzed melt pockets. The ratio is defined from 0 to 1, such that a b/a ratio close to 1 indicates that little difference 166 exists between the shortest and longest axes and that the shape is close to isotropic. In contrast, a 167 smaller value of b/a indicates a stronger preferred orientation. We also calculated the size of 168 169 segmented objects as an equivalent area circle with diameter d_{equ} . Because both melt pocket size and grain size distributions frequently follow a log-normal distribution, we report the mode of 170 the log-normal probability distribution as the most common size for melt pockets or grains in 171 172 each sample.

We analyzed the orientation of a sample-scale melt network with the autocorrelation
function (ACF; Heilbronner and Barrett, 2014, Chapter 20). The autocorrelation function
quantifies the orientation and spatial frequency of the patterns in an image without the

segmentation of individual features. For a given feature defined by the gray value function G(x,y) at coordinates (x, y), reoccurring at a displacement (x', y'), the ACF is defined as the

- 178 convolution of G(x,y) with itself such that
- 179

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$$G(x,y) * G(x,y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(x',y') \cdot G(x+x',y+y') dx'dy' .$$
(3)

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The output of the ACF shows the orientation of features, as well as the length scale over
which they repeat themselves. This approach is therefore well suited for analyzing large-scale,
fine-feature patterns.

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Figure 3: 2-D maps of two samples, one deformed to (a) low strain and the other to (b) high strain. The grains are outlined in black and melt pockets are highlighted in red. The melt and grain preferred orientations obtained from these images are represented as rose diagrams in red and blue, respectively.

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195 2.3 Melt network image analysis

Melt pockets, which are 2-D sections through a 3-D melt network, were analyzed at the
grain scale, where individual melt pockets are well resolved in the image (typically ~2000x
magnification), and at the sample scale, over which larger patterns become apparent (typically
~200x magnification). To measure grain-scale MPO, individual pockets were traced from SEMBSE, EDS, and band-contrast images such as those in Figure 3 and Figures 4a and 4b. These

traced images were then converted to binary, black and white images for segmentation. Only pockets above a minimum size of 10 pixels (at pixel resolutions of $0.02 - 0.4 \mu m$) were analyzed to avoid effects from poorly defined small melt pockets. We quantified the MPO and strength of alignment in a sample based on two factors, orientation (α_p) and bulk aspect ratio (*b/a*), as described above.

To identify larger-scale melt patterns, we used EDS composition maps of calcium, an element present at sufficient concentration within the basaltic melt but not in the olivine used for these experiments. We segmented these maps to create binary images of individual melt pockets, which we analyzed using the ACF method over the entire sample imaged.

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2.4 Grain-shape preferred orientation and crystallographic preferred orientation analyses

The shape preferred orientation was obtained from manual tracing of grains on SEM maps of the 2-D slices as well as from EBSD data. We characterize the shape preferred orientation of the grains in the same manner as the grain-scale MPO described above.

215 Representative data are displayed in Figure 3.

216 EBSD data were collected at two scales, analogous to the melt network analyses. A lowresolution map (0.6-µm step size) covered large parts of the whole sample, and a high-resolution 217 218 map (0.2-µm step size) focused on the intracrystalline deformation features, highlighted in Figures 4c-d. The EBSD data were analyzed using the MTEX toolbox () to characterize the 3-D 219 220 orientation of the crystallographic axes. The crystallographic preferred orientation is defined by an ODF describing the direction of the three mutually perpendicular crystallographic axes in the 221 222 olivine crystals in each sample. This ODF is represented graphically as a pole figure depicting multiples of uniform density (M.U.D.) in an equal-area, upper hemisphere projection, contoured 223 224 by areas of high and low concentrations of each of the three crystallographic axes of olivine, as 225 indicated in Figures 4e-f. We also collected the misorientations of the subgrains in the highresolution EBSD maps, defined by the difference in internal pixel orientations from the mean 226 orientation of an entire grain, which allowed us to examine internal deformation of grains. 227

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229 2.5 Calculation of seismic anisotropy

To constrain the microstructural contributions of MPO and CPO to the generation of
seismic anisotropy in olivine-melt aggregates, we followed the Gassman poroelastic differential

effective medium method as applied in a Matlab model, GassDEM (Kim et al., 2019). This
method uses the Voigt elastic tensor calculated from the CPO, then treats melt inclusions as an
oriented fluid-filled crack.

We modeled melt pockets as penny-shaped ellipsoids, per Faul et al. (1994). The axes of these ellipsoids were defined as 1:b/a:1, where b/a is the shortest projection length of the melt pocket normalized by the longest projection length (equivalent to the b/a reported for all MPOs), and using the orientations of our MPOs such that the azimuth of an inclusion is the angle at which *b* is oriented with $0^\circ = E$ and $90^\circ = N$. These orientations were rotated during input into the GassDEM interface, which takes $0^\circ = N$ and $90^\circ = W$. We took the high-frequency elastic constants of the resultant tensor calculated with 2.5 wt% melt.



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Figure 4: (a), (b) Band contrast images and (c), (d) orientation maps for sample PI-277.
Pole figures are equal-area projections scaled as multiples of uniform distribution (M.U.D.). (e)
Overview EBSD pole figures correspond to a larger number of crystals, while (f) high-resolution
EBSD pole figures include a smaller number of crystals in greater detail, resulting in more
pronounced point maxima.

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249 3. **Results**

250 3.1 MPO - Melt preferred orientation

251 *3.1.1 Grain-scale melt alignment*

Melt pockets reached a steady state-state orientation after a low degree of strain. The 252 orientations of all individual melt pockets ("grain-scale" MPO), which were collected for all 253 analyzed samples, are summarized in Figure 5. The melt preferred orientation in the starting 254 material is very weak, with the b/a aspect ratio of 0.97 from all aggregated individual melt 255 pockets indicating a nearly isotropic shape. The strength of the MPO increased at the onset of 256 deformation and was fully established by $\gamma \approx 0.5$, with melt pockets oriented close to the loading 257 258 direction at 135°. The values of α_p of these deformed samples were essentially independent of strain (per linear fitting to establish a first-order relationship, $R^2 = 0.02$, p =0.77) such that the 259 grain-scale MPO, once established, varied by only $\pm 5^{\circ}$ from parallel to the loading direction. 260 There was a moderate dependence of orientation on stress ($R^2 = 0.64$, p = 0.06) within the 261 studied range, with much of the variation due to the rotation of MPO in the highest stress test. 262 The strongest alignment, a b/a ratio of 0.72, formed by a strain of $\gamma = 0.4$ (Figure 5b). Once 263 established, b/a was insensitive to increasing strain (R² = 0.008, p = 0.95) and stress (R² = 0.003, 264 p = 0.90). 265

Melt pocket sizes also converged to a common value at a low strain and did not evolve further with increasing strain, as demonstrated in Figure 5c. Melt pocket size in the starting material was $d_{equ} \approx 2 \mu m$, while melt pocket size shrank to $d_{equ} \approx 0.9 \mu m$ by $\gamma = 0.4$ and converged to $d_{equ} \approx 0.5 \mu m$ by $\gamma > 0.4$ in a manner that did not significantly depend on strain (R² = 0.28, p = 0.22) or stress (R² = 0.42, p = 0.11)





Figure 5: Evolution of MPO as a function of strain. (a) Rose diagrams from orientation of longest axes of each individual melt pocket. (b) Projection functions based on equation (1) with minima (shortest projection axis) and the corresponding preferred orientation labeled. (c) Melt pocket size histograms with log-normal fit overlain. The mode of the distribution is labeled.

3.1.2 Sample-scale melt alignment

278 In addition to the grain-scale alignment, we observed larger patterns occuring over the spatial scale of the sample. The initial orientations and spatial distributions of all melt pockets at the 279 "sample scale" were isotropic, as revealed by the ACF analyses of the binary images in Figure 7. 280 At low strains, the spatial distribution of the melt remained isotropic, but the network of melt 281 282 pockets developed a preferred orientation parallel to the loading direction at the sample scale, in agreement with the orientation of melt observed at the grain scale. In the samples deformed to 283 the highest strain, melt began to segregate into relatively melt-rich and melt-poor regions, and a 284 secondary orientation at long correlation length scales (i.e., the spatial distance over which a 285 feature can be correlated with itself) began to form at $\sim 155^{\circ}$ ($\sim 20^{\circ}$ to the loading direction). 286 287 Short-correlation length scales (i.e., those close to the origin on the ACF plot) still retained an orientation sub-parallel to the loading direction. 288



Figure 6: Sample-scale melt network analyzed by the autocorrelation function (ACF). Conditions of our (a) hot-pressed starting material and (b)-(e) four deformed samples with each corresponding ACF (central column) and binary melt map contoured from low melt density, in white, to high melt density, in purple (rightmost column). The distance from the center of an ACF represents the length scale over which a feature can be correlated (i.e., closer to center of an ACF = shorter-scale feature correlation, while further away from the center of the ACF = longerscale feature correlation).

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299 *3.2 Grain shape and crystallographic preferred orientation (SPO & CPO)*

300 *3.2.1 SPO - Shape preferred orientation*

301 Grains in the deformed samples established an SPO with increasing strain, but did not 302 reach a steady state-state orientation over the range studied here. The SPO of all grains is reported in Figure 7. The long axes of grains were oriented at 10-20° from the shear plane of the sample at low strains and rotated to ~30° from the shear plane for $\gamma > 0.8$.

There was no clear dependence of the angle of preferred orientation, α_p , on either strain (per linear fitting to establish a first-order relationship, $R^2 = 0.26$, p = 0.30) or stress ($R^2 = 0.26$, p = 0.30). However, the bulk grain shape aspect ratio, b/a, did depend on strain ($R^2 = 0.72$, p = 0.016), but not stress ($R^2 = 0.02$, p = 0.76). The aspect ratios remained close to isotropic (with a minimum of 0.88 at $\gamma = 0$ and a maximum of 0.94 at $\gamma = 0.3$) for all but the sample deformed to the highest strain. A stronger SPO, indicated by a b/a of 0.79, formed by $\gamma = 1.3$, as long axes of the deforming grains began to align.

Grain size generally decreased with increasing stress ($R^2 = 0.66$, p = 0.026) and was less sensitive to strain ($R^2 = 0.32$, p = 0.16). The distribution of grain sizes in the starting material (Figure 7c) peaked between $d_{equ} \approx 5-10 \mu m$ after hot-pressing for 3 h. At $\gamma = 0.3$, grains exhibited a normal distribution curve with a peak at $d_{equ} \approx 9 \mu m$, while all samples deformed to higher strain had a log-normal distribution curve of grain sizes peaking at $d_{equ} \approx 2-4 \mu m$.

Grain sizes, aspect ratios, and shape fabrics wavered were roughly independent of strain at low strains ($\gamma < 1.3$); at the highest strains examined here, both aspect ratios and grain sizes showed a decrease. The strength of the SPO was dependent on strain, but the orientation was not systematically dependent on stress or strain. SPO thus required higher strains to develop a steady state state orientation and was less sensitive to the early stages of deformation than MPO.



Figure 7: Grain SPO evolution as a function of strain. (a) Rose diagrams from orientation of longest axes of individual grains. (b) Projection functions based on equation (1) with minima (shortest projection axis) and the corresponding preferred orientation labeled. (c) Grain size distribution with normal or log-normal fit overlain. The mode of the distribution is labeled.

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3.2.2 CPO – Crystallographic preferred orientation

The CPOs of deformed samples in Figure 8 evolved with increasing strain. The CPO was 329 well-developed in the starting material with [010] axes aligned perpendicular to the shear plane 330 of the sample and the [100] and [001] axes in weak girdles in the shear plane. As strain 331 increased, alignment of the [010] axes increased in strength, while the [100] and [001] axes 332 333 remained girdled. At low strains, the orientations rotated antithetically away from the shear plane, such that the [010] axes were 90-115° from the shear plane and the [100] and [001] axes 334 girdled within 5° of the shear plane. At the highest strain reached in our experiments, $\gamma = 2.3$, the 335 [100] axes began to cluster in the shear direction, while the [001] axes began to cluster in the 336 337 center of the pole figure. A secondary maximum orientation of the [100] axes developed roughly perpendicular to the loading direction. 338

The density and misorientation of subgrains increased as strain increased, and the effect 339 of increasing strain on intracrystalline structure is illustrated in Figure 9. As seen in Figure 9a, 340 341 the subgrain density was low and misorientation angles were small ($<10^{\circ}$) within subgrains in the starting material, while subgrains with relatively high misorientations (>10 $^{\circ}$) were present in 342 nearly every grain in the sample deformed to $\gamma = 2.3$. Inverse pole figures of the misorientations 343 in Figure 9 demonstrate that, with increasing strain, rotation around the [001] axis became 344 increasingly common. The development of a subordinate maximum also suggests rotation around 345 the [010] axis. 346

347 Similar to SPOs, CPOs did not change significantly in the early stages of deformation

348 (Figure 8). The orientations of the crystallographic axes shifted only slightly, as the [010] planes

349 first rotated antithetically to the shearing direction and then rotated into the shear plane. At

strains of $\gamma = 1.3 - 2.3$, the [010] planes were rotated slightly synthetic to the imposed shear

direction. The strength of the CPO generally increased as strain increased.



Figure 8: CPO evolution with increasing strain. Minima and maxima are reported as multiples of uniform distribution, M.U.D.; *n* is the number of grains surveyed in each map.



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Figure 9: Misorientation maps and inverse pole figures of misorientation axes in the crystallographic reference frame from (a) the starting material, (b) a sample sheared to low strain, and (c)-(d) two samples deformed to high strain. All images are at the same scale.

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3,3 Calculation of seismic anisotropy

We calculated seismic properties for each of our partially molten rocks, characterized in Figure 10 as the distribution of P wavespeed (Vp), the distribution of the normalized difference between the fast and slow S wavespeeds (Vs₁ and Vs₂), and the magnitude and polarization of Vs₁. We used three measures of seismic anisotropy, indicated as percentages within each tensor: 1) The normalized difference between the largest and the smallest values of P wavespeed (Vp), expressed in percent, calculated as $AV_p = 200 \frac{(V_{Pmax} - V_{Pmin})}{(V_{Pmax} + V_{Pmin})}$; 2) the % difference in fast (Vs₁) and slow (Vs₂) S waves, calculated as the greatest difference between Vs₁ and Vs₂ within the tensor, and AVs = $200 \frac{(V_{S1} - V_{S2})}{(V_{S1} + V_{S2})}$ for every point in

the tensor, with the maximum AVs reported;

374 3) the normalized difference between the largest and the smallest values of
$$Vs_1$$
,

375 calculated as AV_{S1} =
$$200 \frac{(v_{S1}max - v_{S1}min)}{(v_{S1}max + v_{S1}min)}$$
.

The seismic anisotropy calculated in our deformed samples evolved over the studied 376 strain intervals. Over a small increment of strain, the calculated values for the three indicators of 377 the seismic anisotropy decreased. However, for samples deformed to $\gamma \gtrsim 1$, the calculated values 378 of seismic anisotropy increased with increasing strain. This behavior parallels the development 379 380 of MPOs and CPOs with increasing strain. At low strains, the CPO was weak, and the MPO was oriented antithetic to the shearing direction and parallel to the loading direction. The melt 381 orientation was oblique to the orientation of the crystallographic axes, which were aligned in a 382 girdle parallel to the shear plane. The anisotropy determined for our lower strain tests reflects a 383 384 competition between MPO and CPO. As a result, inclusion of melt decreased the CPO-generated anisotropy with respect to a theoretical melt-free sample based on the same CPO. As strain 385 increased, the strength and direction of the preferred orientation of the melt network did not 386 change, but the CPO became stronger and the [100] axes became more aligned parallel to the 387 shear plane. At higher strains, the seismic anisotropy of Vp, Vs, and Vs1 all steadily increased. 388 As the MPO remained at a steady state strength and orientation at these strains, this increase is 389 due to the effect of CPO strengthening. 390









400 Figure 11. Summary of microstructural data. (a) Preferred orientation of melt 401 pockets (from $0^\circ = E$) as a function of strain. (b) Preferred orientation of melt pockets as a

function of stress. (c) Preferred orientation of grain shapes as a function of strain. (d) 402 Preferred orientation of grain shapes as a function of stress. In (a - d), Preferred 403 orientation is reported as $\alpha_{\rm p}$, and the strength of the preferred orientation is indicated by 404 405 the aspect ratio b/a of the fabric. (e)Orientation of the girdle formed by olivine [100] axes (θ_a) as a function of strain. (f) Orientation of the girdle formed by olivine [100] axes (θ_a) 406 407 as a function of stress. In (e-f), the strength of the preferred orientation is reported as peak multiples of uniform distribution, such that a higher M.U.D. represents a higher 408 409 concentration of axes aligned at this orientation. Note that CPO data are not available for 410 the two tests carried out at the highest stresses.

411

412 4. Discussion

413 *4.1 MPO formation on the grain scale and on the sample scale*

414 Our results demonstrate that MPO evolves much more quickly in response to shear 415 deformation than either SPO or CPO of the solid grains, as summarized in Figure 11. A clear 416 grain-scale MPO is evident in our lowest-strain sample deformed to $\gamma = 0.32$; however, a change 417 in CPO and SPO is not apparent until $\gamma > 1$.

Previous examination of some of the samples used in this study with lower resolution optical images (tests PI-277, PI-281, PI-274, and PI-273, as reported in Zimmerman et al., 1999), led to the conclusion that the MPO is inclined at $\sim 160^{\circ}$ to the shear plane, antithetic to the shear direction (i.e., at $\sim 25^{\circ}$ to the loading direction). Likewise, analyses of low-resolution optical images of samples deformed in coaxial compression indicated that the MPO also formed at an angle of $\sim 20^{\circ}$ to the loading direction (Daines & Kohlstedt, 1997; Kohlstedt & Zimmerman, 1996; Zimmerman et al., 1999).

In contrast, our high-resolution SEM data demonstrate that the grain-scale melt pockets 425 426 in these samples are aligned parallel to the loading direction. The MPO alignment in our tests is in agreement with observations on an analog material (Takei, 2005) and is consistent with the 427 MPO needed to produce melt rich "bands" inclined $160 - 165^{\circ}$ to the shear plane on the sample 428 scale within the framework of two-phase flow theory with viscous anisotropy (Katz & Takei, 429 430 2013; Takei & Holtzman, 2009c, 2009b, 2009a; Takei & Katz, 2013; Taylor-West & Katz, 2015). Local variations in melt network orientation do exist, as seen in Figure 6; the orientation 431 of larger melt pockets, perhaps as an aggregation of several smaller pockets, can produce local 432

sub-maxima in orientation close to 155° in higher-strain samples in which incipient melt
segregation is observed.

The scale of observation and the method of analysis (projection-based and 435 autocorrelation-based methods vs. ellipse-fitting methods) may influence estimates of melt 436 orientation. We propose that individual melt pockets at the grain scale align subparallel to the 437 loading direction, while aggregated melt pockets on the sample scale form an en echelon pattern 438 aligned at a lower angle with respect to the loading direction (Figure 6). This observation 439 440 explains the discrepancy between experimentally obtained values of 155-165° for melt orientation and model assumptions of sub-parallel orientation with respect to applied maximum 441 principal stress: both are correct, just at different observation scales. 442

Only our highest-strain sample developed incipient bands, similar to those in other 443 experimentally sheared samples with a short compaction length that required strains of $\gamma \ge 1$ for 444 bands to form (King et al., 2010; Kohlstedt & Holtzman, 2009). The emergence of these bands 445 may then be the result of viscous anisotropy induced by grain-scale alignment of melt and 446 decreasing compaction length as grains recrystallize to a smaller grain size, documented in 447 Figure 7c. These observations again agree with predictions from the viscous anisotropy theory 448 framework and the experiments designed to test this theory (Katz & Takei, 2013; Qi et al., 2015; 449 Quintanilla-Terminel et al., 2019; Takei & Holtzman, 2009c) 450

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452 *4.2 Stress state in general shear experiments*

We observed that, in response to an applied stress, individual melt pockets relatively quickly established a preferred orientation, which remained essentially constant with increasing strain. The preferred orientation for the individual melt pockets formed parallel to the loading direction, which is often assumed to coincide with the maximum principal stress (σ_1).

However, as general shear experiments include an element of thinning, it is possible that the σ_1 direction may not be aligned with the loading direction. Since stress state is not directly observed during our high-pressure experiments, we used strain as a proxy for understanding the contribution of thinning within the imposed stress field. This thinning provides insight into the relationship between the orientation of the effective σ_1 and that of the loading direction. If all the deformation were simple shear, σ_1 would remain oriented at 135°, parallel to the applied load. As the contribution from pure shear increases, the maximum principal compressive stress would

rotate away from the loading direction. We quantified the imposed finite strain geometry by 464 measuring the sample thickness before and after deformation and calculating the kinematic 465 vorticity number (W_k), which quantifies the degree of pure (W_k \approx 0) vs. simple (W_k \approx 1) shear 466 during deformation (Fossen & Tikoff, 1993; Passchier, 1987). In our highest-stress test, W_k = 467 0.92; for all other experiments, W_k was >0.96 (see Table 1), indicating that the strain was close 468 to simple shear. Throughout this paper, we have presented examples mostly from low-strain 469 experiment PI-277 ($\gamma = 0.4$, $W_k = 0.99$) and high-strain experiment PI-273 ($\gamma = 2.3$, $W_k = 0.98$), 470 both of which deformed primarily by simple shear. Additionally, the calculation of the W_k 471 assumes that thinning is consistent throughout deformation. Based on examination of samples 472 annealed at high temperature and pressure but not deformed (e.g., starting material), most 473 thinning occurs during the annealing and pressurization stage of experimental setup, and does not 474 475 co-occur with shear deformation. The W_k values therefore represent the lowest possible degree of simple shear, and the deformation experienced by the samples is probably closer to 100% 476 simple shear (and thus, nearly no rotation of the σ_1 should occur). This result indicates that the σ_1 477 orientation is indeed close to the loading direction, at 135°, consistent with the MPO. 478

Small-scale variations in MPO do occur, which may be related to the degree of pure vs 479 simple shear in our experiments. The kinematic vorticity number, Wk was lowest in our highest-480 stress test, indicating that this sample experienced a higher degree of pure shear than all others. 481 In this high-stress test, the MPO rotated $\sim 20^{\circ}$ from the loading direction (synthetic to the sense 482 of shear). A similar misalignment between loading direction and σ_1 was observed in qtz + 483 feldspar samples deformed in general shear with a substantial thinning component; in these 484 experiments, the stress orientation could be inferred via the development of Dauphiné twins in 485 quartz (Pec & Al Nasser, 2021). Based on our observations, we propose that the grain-scale 486 orientation of melt pockets can be used as an effective proxy for the orientation of the maximum 487 principal stress. 488

489

490 *4.3 Grain SPO and CPO formation*

SPO and CPO evolve over higher strain intervals than MPO. Grains in the starting
material had a SPO and a CPO that developed during hot pressing of the starting material.
Individual olivine grains tend to be elongated along the [100] and [001] axes with the longest
straight grain boundaries lying in the [010] plane (Miyazaki et al., 2013; Qi et al., 2018). Axial

495 compression of these elongated crystals aligns the long axes of the SPO in a girdle perpendicular

- 496 to the loading direction. This process results in a SPO-induced CPO, characterized by girdles in
 - 497 [100] and [001] axes oriented perpendicular to the loading direction and clusters in poles of
 - 498 [010] planes parallel to the loading direction, as seen in Figure 8.
 - The strength of CPO alignment increased visibly with increasing strain for $\gamma > 1$, consistent with numerical models (Boneh et al., 2015) and other experimental results (Boneh & Skemer, 2014; Hansen et al., 2014; Qi et al., 2018). Although the alignment strength increased, the evolution of grain size and shape fabric still did not depend systematically on strain or stress at low strains. The pole figure geometry also did not change significantly until a strain of $\gamma > 2$.
 - The CPO of the deformed samples is commonly observed in sheared aggregates of meltbearing olivine. This CPO may develop if grains preferentially grow along the [001] direction and then align under the imposed kinematic boundary conditions; the relative fabric strength thus reflects competition between SPO-induced and dislocation-induced CPOs (Qi et al., 2018). Misorientation axes (Figure 9) also dominantly aligned with [001] with a subordinate maxima around [010], indicating that (010)[100] is the dominant slip system in our rocks, given that the subgrain walls have a tilt character (Prior et al., 2002).
 - The CPOs of our higher strain samples are similar to that of an A-type fabric, indicative of the easy slip system (010)[100] accommodating deformation in the shear plane (Karato et al., 2008; Zhang & Karato, 1995). The CPO-generating mechanisms (SPO-induced CPO and dislocation-induced CPO) are likely competing at low strains; at higher strains, the more prominent cluster in [100] axes alignment in the shear direction, together with large intragranular misorientations, indicate that dislocation glide is dominant in formation of the CPO.
 - 517 In the highest strain experiments, a secondary cluster in [100] axes orientations forms. 518 This secondary maximum, though relatively common in A-type fabrics, is not well understood. 519 Although Zhang et al. (2000) explained this secondary maximum as a signature of non-520 recrystallized grains in a matrix otherwise undergoing dynamic recrystallization, the grains with 521 this orientation in our sample do not have substantially different misorientations from the bulk 522 sample. They do, however, have a flatter and weaker SPO than all other grains in the sample. 523
 - 524 *4.4 Contributions to seismic anisotropy*

The CPO alignment strengthens, but remains relatively static in orientation angle in samples sheared to strains of $\gamma \leq 2.5$. In contrast, the grain-scale melt network develops a distinct preferred orientation over a very small strain interval, and the strength and angle of this orientation persists with increasing strain. The strength of the melt alignment saturates at low strains and does not increase with increasing strain or stress, as can be observed in Figure 5.

It follows that at early strain increments of deformation within the Earth, changes in the 530 531 orientation of the melt network will cause changes in seismic anisotropy. The CPO, which 532 evolves more slowly than MPO, will not contribute significantly to the seismic anisotropy until larger strains are reached. Previous studies of seismic anisotropy caused by an aligned melt 533 network in a rock with an isotropic CPO determined the strength of anisotropy caused purely by 534 melt orientation (Lee et al., 2017). In a series of calculations with the GassDEM model that 535 536 covered a range of hypothetical MPOs and crystalline fabrics, we found that the interplay of 537 MPO and CPO is crucial to modeling actual seismic anisotropy. As an example, we present 538 theoretical seismic properties for deformed sample PI-277 in Figure 12.



539

Figure 12: Seismic properties for deformed sample PI-277 using (a) the CPO alone, (b) the CPO and isotropic melt (idealized as circular melt inclusions), and (c) the CPO and aligned melt to create the elastic tensors. P wavespeeds (Vp), Vs anisotropy, and fast S-wave speeds (Vs₁) are shown in each case, along with the fast polarization direction for the Vs₁ wave traveling vertically through the sample.

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The addition of isotropic (equiaxial) melt pockets reduces seismic velocities and CPOinduced anisotropies but does not interact with the CPO-generated anisotropy (as in Figure 12b), and so its effect is less pronounced than that of oriented melt (Figure 12c). The presence of

aligned melt alone reduced seismic wavespeeds and influenced seismic anisotropies (Figure 549 12c), but the relative alignment of the MPO and CPO determined the extent and magnitude of 550 this change. The [100] axes of olivine and the angle of the MPO each indicate a likely fast 551 direction, so seismic anisotropy is highest if the [100] axes and the MPO are in a similar 552 orientation. Seismic velocities and anisotropies both decrease at the onset of deformation caused 553 554 by a change in stress; when the stress changes and a MPO forms or reforms, the new fast direction induced by the MPO competes with the steady state state [100] alignment. However, 555 calculated seismic anisotropy increases above $\gamma \approx 0.8$, as the CPO strengthens and the MPO 556 remains unchanged (Figures 10 and 11). The magnitude of this effect depends on melt fraction as 557 well, as the effect of co-aligned MPO and CPO increases with increasing melt fraction. 558 Anisotropy in P wavespeed (Vp), relative travel times of Vs, and Vs1 all followed the trend 559 described here, with Vs1 anisotropy being particularly sensitive to the effect of melt fraction. 560 The polarization of a vertically propagating S-wave (not necessarily a vertically polarized 561 S-wave; here, we use V_{S1} rather than V_{SH} or V_{SV}) is also particularly sensitive to the orientation 562 of melt: the addition of isotropic melt does not change this polarization direction, but the 563 564 orientation of the same degree of melt can rotate the fast direction by over 15°. Studies of CPO within the Earth, which invoke vertically propagating waves to explain seismic anisotropy thus 565

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4.5 Application to natural settings

may significantly mispredict the orientation of olivine axes.

Measurements of seismic anisotropy in the Earth's lithosphere are traditionally understood to result from CPOs, such that seismologists can use anisotropy measurements to infer the direction of flow in the mantle (Long & Becker, 2010). However, this approach does not sufficiently account for the presence and orientation of melt (Holtzman and Kendall, 2010; Mainprice, 1997).

Our results demonstrate that CPOs and MPOs evolve over distinct characteristic timescales,
complicating the interpretation of observed seismic anisotropy in terms of oriented mantle flow.
Natural strain rates are much slower than laboratory experiments, and the process of overprinting
extant CPOs during deformation likely involves a long transient interval (Boneh et al., 2015).
MPOs, however, require very small strain intervals to change, so the MPOs forming due to
changing stress will compete with established, steady state-state CPOs.

As such, abrupt changes to local stress field, such as those caused for example by an 580 earthquake or volcanic eruption, would only be visible in short-term perturbations to seismic 581 582 anisotropy as a result of readjustment of the orientation of the melt network. The almost instantaneous development of MPO in response to an applied differential stress also means that 583 MPO is a more reliable indicator of instantaneous changes in stress than the CPO. This behavior 584 of melt may be useful for observing results of stress changes within the Earth or for 585 understanding melt distribution in rapidly evolving planetary settings dominated by orbital tidal 586 587 stresses.

We can look to seismic studies of the Earth's crust for confirmation. Some crustal 588 seismic anisotropy is thought to result from the orientation of magmatic intrusions (Frothingham 589 et al., 2023; Hammond, 2014) and fluid-filled microcracks (Crampin, 1987; Crampin & 590 591 Zatsepin, 1997; Elkibbi et al., 2005) that form parallel to the local maximum compressive stress (Gerst & Savage, 2004; Johnson, 2015). Within geophysically observable timescales, microscale 592 593 crystallographic orientation is considered to be relatively static. Volcanically active crustal regions undergo short-term changes to magnitude and orientation of shear wave anisotropy 594 595 during episodes of melt infiltration (Araragi et al., 2015; Illsley-Kemp et al., 2018; Johnson et al., 2015), allowing researchers to track the local stress and deformation fields using anisotropy 596 597 measurements as a tracer for movement of melt.

Treating a small amount of melt as an oriented inclusion with distinct poroelastic 598 599 properties is a tested approach to interpreting seismic anisotropy in rapidly deforming regions. Our results indicate possible similarities in the seismic signatures of the melt-intruded crust and 600 601 partially molten mantle, suggesting that tomographic techniques used to infer near-surface stress and deformation could be applied to signals from deeper in the Earth. Studies of fast-deforming 602 603 zones in Eastern Africa have previously inferred that melt alignment contributes noticeably to 604 seismic anisotropy in the shallow upper mantle (Bastow et al., 2010; Chambers et al., 2021; Hammond, 2014; Kendall et al., 2005), and this framework may also be applicable to evolving 605 seismic anisotropy in subduction zones and mid-ocean ridges. 606

- 607
- 608

609 5. Conclusions

610

As a partially molten olivine-basalt aggregate deforms,

611	• Grain-scale melt alignment forms parallel to the loading direction at relatively
612	low strain ($0 < \gamma < 0.3$) and persists to the highest strains studied here. Strain does
613	not affect the orientation or strength of this grain-scale melt alignment above this
614	interval.
615	• A grain-scale melt preferred orientation forms parallel to the inferred local
616	maximum compressive principal stress (σ_1), which may rotate away from the
617	applied σ_1 with increasing shear stress or thinning.
618	• A distinct <i>sample-scale</i> melt preferred orientation forms at 155° (20° oblique to
619	the loading direction) at higher strain due to en echelon arrangement of grain-
620	scale melt pockets and incipient melt segregation.
621	• The CPO that developed during hot pressing does not change significantly in
622	orientation during subsequent deformation. However, the strength of the CPO
623	increases steadily with increasing strain.
624	• The relatively weak SPO produced during hot-pressing randomized at low to
625	intermediate strains $0.3 < \gamma < 1.3$, and grains develop a moderately strong SPO
626	oriented at ~30° to the shear plane at high strains ($\gamma > 1.3$).
627	• A MPO is established more quickly in response to changes in the stress field than
628	is a CPO or SPO.
629	• Once established grain-scale MPO does not change with increasing strain, but the
630	sample-scale melt network coalesces into bands with a distinct orientation. At
631	higher strains, the dislocation-induced CPO strengthens and contributes more to
632	seismic anisotropy than does the MPO.
633	• Immediately after a change in stress field, seismic anisotropy will be more
634	affected by changes to the MPO than by changes to the CPO. At small strains or
635	over short observable timescales, the MPO thus provides insight into the
636	orientation of the stress field in quickly deforming regions of the Earth's upper
637	mantle in ways that CPO-induced anisotropy cannot.
638	
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649	Data availability:
650	Melt maps, EBSD, and analyzed bulk MPO/SPO data are available at
651	10.5281/zenodo.7647271 (Seltzer, 2023).
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