

PyDRex: Predicting crystallographic preferred orientation in peridotites under steady-state and time-dependent strain

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Declaration

The contents of this thesis are the results of original research and have not been submitted for a higher degree to any other university or institution.

Most of the work in this thesis has been published in Geophysical Journal International (<https://doi.org/10.1093/gji/ggaf026>) and has undergone peer review. Any supplementary work included in this thesis has, to the best of my knowledge, not been previously published, except where appropriately credited.

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Abstract

Crystallographic preferred orientation (CPO) of peridotite minerals is frequently invoked to explain the widespread dependence of seismic wave speed on propagation direction in Earth’s mantle — a property known as seismic anisotropy. As established by rock mechanics experiments, CPO constitutes a direct signature of past and ongoing strain regimes experienced by rocks during mantle flow. Therefore, an improved understanding of CPO generation promises to yield valuable information on the rheology and corresponding deformation mechanisms activated through mantle dynamics. Simulating CPO in geodynamical models is computationally challenging and has often been restricted to steady-state mantle flows. However, within Earth’s vigorously convecting mantle the steady-state assumption is questionable, thus motivating the need to couple CPO simulations with time-evolving mantle flow models. Here, we present a new Python implementation of the D-Rex CPO model, called PyDRex, which predicts salient features of mineral grain size and orientation evolution whilst providing a well-documented, user-friendly interface that supports flexible coupling to geodynamical modelling frameworks. PyDRex also packages numerous post-processing routines for strain analysis and visualisation of grain orientation distributions. We provide a set of benchmark simulations based on previous D-Rex implementations that validate PyDRex and demonstrate sensitivities to model parameters for both steady-state and time-dependent flows. Analysis of benchmark results highlights the role of dynamic recrystallisation in controlling competing grain growth in both the softest and hardest crystallographic orientations. When employing a commonly used value for the grain boundary mobility parameter ($M^* = 125$), we also find that transient CPO textures are generally not well resolved if crystals are represented by fewer than 5000 “grains” (weighted orientation samples) — a configuration rarely employed in most previously published studies. Furthermore, kinematic corner-flow models suggest that CPO produced at mid-ocean ridges has a non-linear dependence on depth, which implies that even ostensibly simple mantle flows can result in complex distributions of seismic anisotropy. Our analyses motivate further experimental calibration of parameters controlling dynamic recrystallisation and potential improvements to the numerical treatment of subgrain nucleation.

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1 Introduction

Convection in Earth’s mantle operates over a range of spatial and temporal scales. Primary mantle flow features manifest as sinking lithospheric slabs and rising mantle plumes (e.g. H.-P. Bunge et al., 2002; Davies et al., 2012; Ballmer et al., 2017; Flament et al., 2017), whilst secondary components include dynamic instabilities arising from the base of the lithosphere and within the transition zone (e.g. Ballmer et al., 2011; Davies & Rawlinson, 2014; Rawlinson et al., 2017; Duvernay et al., 2021). These secondary flow components may be sustained by local buoyancy anomalies (e.g. Coltice et al., 2018) or time-varying pressure gradients (e.g. Semple & Lenardic, 2018; Stotz et al., 2018). Resolving such features is an ongoing challenge in both seismological (e.g. Eilon et al., 2022; Eakin et al., 2023) and geodynamical models (e.g. Hedjazian et al., 2017; Davies et al., 2023). Short-lived instabilities, for example, may not be visible to seismic imaging methods, which can only capture present-day, instantaneous snapshots of upper-mantle structure. Such methods are also generally unable to assess the strength of mechanical coupling between the lithosphere and the asthenosphere, which remains debated on global (e.g. Höink et al., 2011; Rychert et al., 2020; Arnould et al., 2023) and regional (e.g. Jadamec & Billen, 2010; van Benthem & Govers, 2010; Jadamec, 2016; Shi et al., 2022) scales. By contrast, extensive signatures of viscoplastic deformation in the upper mantle document an integrated history of flow patterns. One such signature is crystallographic preferred orientation (CPO), i.e. preferential alignment of crystallographic lattice orientations within a polymineralic volume in response to deformation. The ubiquitous physical effect of CPO is readily detected by seismic anisotropy studies, which measure the dependence of seismic wave speed on propagation or polarization direction (e.g. Long & Becker, 2010; Walpole et al., 2014; Debayle et al., 2016; Lin et al., 2016; Eakin et al., 2018; Becker & Lebedev, 2021).

However, unraveling the history of deformation from seismic observations alone is difficult. This history could be dominated by past deformation events within the lithosphere, (e.g. Shimamura, 1984; Tono et al., 2009), for example, resulting from intense stress in continental regions undergoing compression (e.g. Eken et al., 2013; Eakin et al., 2021) or in areas affected by vigorous, focused asthenospheric flow (e.g. Silver & Chan, 1991; Fontaine et al., 2007; Debayle & Ricard, 2013). Although the deformation history provides key information on the evolution of mantle rocks, it remains unclear how quickly anisotropic signatures respond to experienced strains. This relationship has critical implications for identifying the geological processes responsible for the observed anisotropy. Rheological studies suggest that the development and evolution of anisotropy usually depend on microphysical processes that produce CPO in upper-mantle peridotites (Kohlstedt & Hansen, 2015).

In this study, we present PyDRex, a new Python-based implementation of the D-Rex model (Kaminski & Ribe, 2001; Kaminski et al., 2004) that predicts deformation-induced CPO in peridotites. PyDRex computes CPO along flow-field pathlines, which are determined

either by backward propagation of material points in steady-state mantle flows or by forward advection of such points in time-dependent flows. Whilst many existing frameworks provide accurate numerical solutions to the relevant systems of equations governing geodynamical flows, few of them are currently able to additionally compute CPO predictions. This is partly due to the fact that simulations of viscoplastic deformation at large strains require the non-trivial ability to track the deformation history of modelled rocks. One potential numerical technique to approach this issue consists of advecting and tracking discrete material points in the simulated flow field. This is known as the “particle-in-cell” method: whilst the velocity is solved on an Eulerian grid, for example using the finite element method, deformation history is tracked by a separate set of Lagrangian material points, called particles (e.g. Moresi et al., 2003; Gassmüller et al., 2018). Some simple examples in the online PyDRex repository (see Section 8.1) demonstrate ways to interface PyDRex with computational geodynamics frameworks that support the particle-in-cell functionality. For reference, some of the results are presented in Section 7.6.

The reference implementation of the D-Rex model was designed for CPO simulations in steady-state flows within 2D domains (Kaminski & Ribe, 2001; Kaminski et al., 2004). Later adaptations by Lev and Hager (2008) and Faccenda and Capitanio (2013) extended the implementation to support time-dependent 3D flows. Furthermore, the feasibility of coupling the D-Rex model to geodynamical simulation frameworks was recently demonstrated in Fraters and Billen (2021), Kendall et al. (2022) and Faccenda and VanderBeek (2023). However, a systematic suite of benchmarks that explore the model behaviour and sensitivities in both steady-state and time-dependent flows has not yet been presented. In this thesis, we review the theoretical background for PyDRex, validate results obtained through the Python implementation against prior numerical and laboratory experiments, and provide examples for running CPO simulations in both steady-state and time-dependent strain regimes. The comprehensive suite of benchmarks presented herein can serve as a reference for future CPO modelling efforts, as the source code and parameters are publicly available at the online PyDRex repository (see Section 8.1), alongside a detailed package documentation. Furthermore, PyDRex development makes use of modern software engineering best practices, such as continuous integration (CI): the software is tested against core benchmarks each time changes to the code base are committed to ensure ongoing functionality and robustness of the implementation, facilitating future maintenance.

Corroborating CPO data used in the benchmarks has been digitised from previous numerical simulations (e.g. Kaminski & Ribe, 2002; Boneh et al., 2015; Signorelli & Tommasi, 2015), as well as studies of synthetic (Zhang & Karato, 1995; Bystricky et al., 2000; Jung & Karato, 2001; Katayama et al., 2004; Skemer et al., 2011) and natural (Warren et al., 2008; Skemer et al., 2009; Webber et al., 2010; Hansen & Warren, 2015) olivine samples. The compiled dataset can also be found in the PyDRex online repository. Methods for analysing characteristic properties of CPO and anisotropy, which have become available since the original D-Rex implementation, are incorporated in the PyDRex library. These include decomposition of the polycrystal elastic tensor into distinct symmetry class contributions (Browaeys & Chevrot, 2004), evaluation of CPO texture strength using the *M-index* (Skemer et al., 2005), and computation of various texture symmetry diagnostics via eigenvalue analysis of the spherical scatter matrix (e.g. Mainprice et al., 2014).

1 Introduction

In the next section, we present a summary of relevant theoretical and experimental results, as well as an overview of different approaches to peridotite texture modelling. A brief explanation of the PyDRex implementation is given in Chapter 3, followed by a demonstration of the benchmark results in Chapter 4. A discussion of numerical sensitivities and current limitations, as well as ongoing work, is presented in Chapter 5.

2 Background

2.1 Upper-mantle peridotite texture: theory and experiments

Mantle minerals naturally occur in polycrystalline form, which means that rocks are composed of grains of varying size (i.e. volume) and orientation. The orientation of a grain is defined by a rotation transform (matrix), which relates a unit cell of the grain's crystallographic lattice to a unit cell in arbitrarily chosen Cartesian reference coordinates. In this thesis, the term “texture” is used to refer to a combination of grain orientation and grain size distributions in a polycrystal. A texture characterised by a distribution of grain orientations near a particular plane (girdle symmetry) or clustering near a particular axis (point symmetry) describes a crystallographic preferred orientation (CPO, see Figure 2.1) – some authors use the equivalent term lattice preferred orientation (LPO). The development of CPO requires deformation mechanisms that cause permanent changes to the microstructure of crystals.

Viscoplastic deformation refers to a combination of viscous and plastic behaviour. It is characterised by both a proportionality between stress and strain rate, as well as the requirement for stress to exceed a critical threshold. These permanent changes in crystal microstructures result from two types of processes, which arise from the fact that crystalline solids contain defects and imperfections in their atomic lattice structure. The first kind, collectively known as plastic deformation mechanisms, are supported by dislocation or diffusion of crystallographic defects. At high stress, in coarse-grained rocks such as peridotites, they are most likely dominated by dislocation creep (Kohlstedt & Hansen, 2015), which involves the formation and “gliding” of atomic dislocations along lattice symmetry planes. By contrast, diffusion creep (stochastic movement of point defects within the crystallographic lattice) is unlikely to produce a strong, characteristic texture, because it does not involve any significant internal strain gradients within grains (Karato, 2010). Dislocation glide may be aided by dislocation climb, which allows dislocations to move orthogonally to slip planes in order to avoid obstacles (Karato, 2008; Hansen et al., 2021).

The second class of processes contributing to viscoplastic behaviour is called recrystallisation, referring to changes in the size or geometry of grains that can occur in both static and deforming crystals. Dynamic recrystallisation mechanisms, in particular subgrain rotation and grain boundary migration (GBM), are commonly observed in minerals experiencing high stresses (e.g. Zhang & Karato, 1995). These mechanisms are driven by heterogeneity in the distribution of dislocations (Karato, 2008). Subgrain boundaries are formed at sufficiently high gradients of dislocation energy (i.e. internal strain energy), and the new subgrain may rotate into a strain-free lattice orientation. GBM occurs when grains with sufficiently lower relative dislocation density gradually annex parts of neighbouring grains as a means to minimise

2 Background

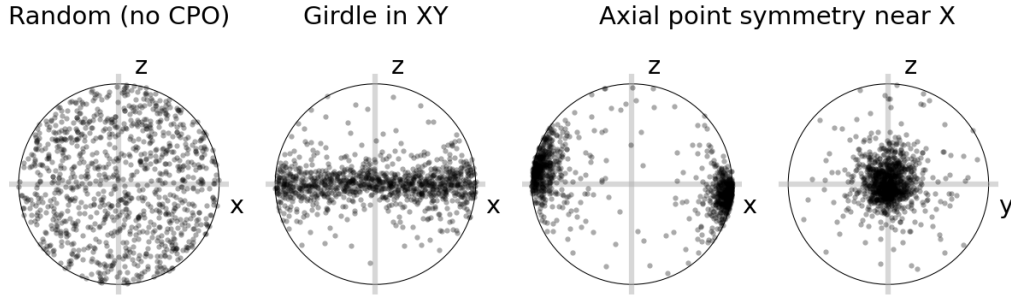


Figure 2.1: Example pole figures of end-member crystallographic textures. Pole figures display 3D spherical orientations as points on an equal-area lower-hemispherical projection. Polycrystals whose grains display a uniform (“random”) distribution of orientations do not produce any seismic anisotropy signature. However, polycrystals with preferentially girdled or axial orientations do. The strength of the seismic anisotropy is proportional to the degree of clustering, i.e. the “strength” of the crystallographic preferred orientation (CPO).

overall dislocation energy (Karato, 2008). In a deforming polycrystal, grains oriented favourably for dislocation glide will tend to incur a high density of dislocations. This increases their dislocation energy, causing them to gradually surrender atoms to neighbouring grains via GBM. At the same time, spatial heterogeneity of dislocations causes nucleation of new strain-free subgrains, which will also grow by GBM. Dynamic recrystallisation in mantle peridotites, therefore, manifests as a balance between GBM and subgrain nucleation (Kaminski & Ribe, 2001).

Early high-pressure and high-temperature deformation experiments on silicate minerals established that deformation under mantle conditions is restricted to unique crystallographic slip systems, defined by a combination of a slip plane and a slip direction (Heard et al., 1972). The experiments of Raleigh (1965, 1968) determined that the relative activity of these slip systems in olivine crystals is sensitive to temperature and strain rate. Carter and Ave’Lallemant (1970) subsequently identified the system (010)[100] as the dominant slip system at upper-mantle temperatures, where the values in parentheses and square brackets specify, in the Miller index notation, the normal to the slip plane and the direction of slip, respectively (see Figure 2.2). Olivine behaving in this way is now referred to as A-type olivine and is the most commonly observed olivine fabric type in mantle peridotite samples (Karato et al., 2008; Michibayashi et al., 2016; Demouchy et al., 2024). A-type fabric is also produced in high-temperature deformation experiments performed on synthetic peridotite aggregates (e.g. Bollinger et al., 2016; Bystricky et al., 2024). Further experiments by Jung and Karato (2001) and Katayama et al. (2004) found that slip system activities also depend on stress and water content, leading to the classification of four more olivine fabrics (B- through E-type), as described in Karato et al. (2008). In this document, the term “fabric” is used to classify variations of relative slip system activities within the same mineral phase, whereas “texture” strictly refers to static polycrystal microstructure.

Ave’Lallemant and Carter (1970) deduced that for olivine at mantle conditions, the primary microphysical deformation mechanisms should be dislocation glide, dislocation climb, and

2 Background

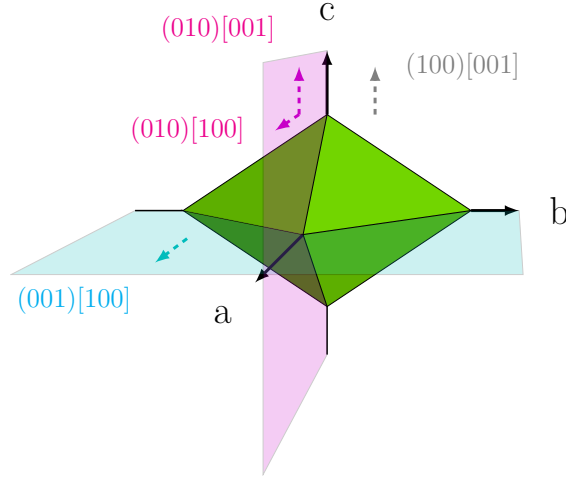


Figure 2.2: Diagram of an octahedron demonstrating orthorhombic dipyramidal symmetry. The axes $\{a, b, c\}$ correspond to crystallographic directions $\{[100], [010], [001]\}$. The shaded half-planes illustrate the (001) (aqua, horizontal) and (010) (pink, vertical) symmetry planes. The third symmetry plane, (100), spanned by $\{b, c\}$, is not illustrated. Olivine crystals, which are characterised by the same symmetry as the octahedron, have four known slip systems, each defined by a combination of a slip plane and a slip direction. They are shown here as arrows with Miller index annotations.

dynamic (“syntectonic”) recrystallisation. Later studies have supported this conclusion (e.g. Nicolas & Christensen, 1987; Bystricky et al., 2000; Bollinger et al., 2018), implying also that the strength of CPO in olivine is proportional to the accumulated strain.

The amount of shear strain experienced by rocks is often quantified by the value $\Gamma = \tan(\alpha)$ (Reyne et al., 2021), where α is the angle of rotation of a material line that is normal to the shear plane in the reference (undeformed) configuration, as shown in Figure 2.3. In the cited literature, this quantity is most commonly denoted by the lowercase γ ; however, we use the uppercase Γ to avoid confusion with the “slip rate” introduced in Equation (3.5). Furthermore, to allow generalisation beyond simple shear, we will additionally use the strain measure $\varepsilon = \int D_0 dt$ for D_0 the largest eigenvalue of the rate-of-deformation tensor defined in Equation (3.3). Note that ε is equivalent to $\Gamma/2$ in steady-state simple shear (Hashiguchi & Yamakawa, 2012, p. 215). A graphical measure of strain, known as the finite strain ellipsoid (FSE; McKenzie, 1979), can also be obtained by considering changes to the shape of a material volume that was spherical before deformation; the long axis of the FSE corresponds to the axis of maximum finite extension in simple shear.

The first study of olivine texture in simple shear by Zhang and Karato (1995) demonstrated simultaneous strengthening and rotation of olivine CPO. Furthermore, at strains in excess of $\Gamma \sim 0.6$, the CPO direction was observed to rotate faster than the long axis of the FSE towards the shear plane. Their results suggested that the rate of rotation of olivine CPO is controlled by dynamic recrystallisation at large strains. Subsequent studies of olivine deformed in simple shear (e.g. Zhang et al., 2000; Lee et al., 2002) support the significance of dynamic recrystallisation, providing further evidence for the effects of subgrain nucleation and grain growth via GBM, as well as the possibility of grain-boundary sliding of small grains.

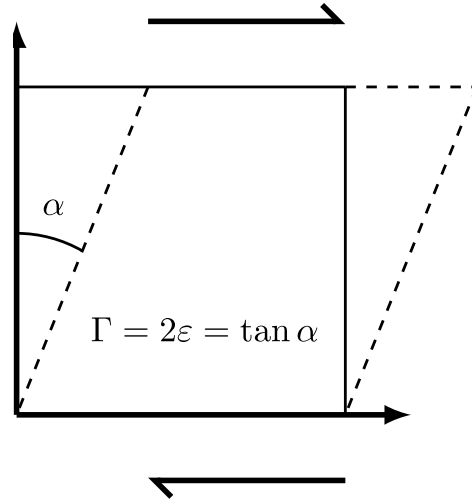


Figure 2.3: Diagram showing the angle defining the “engineering shear strain” measure commonly used in rock-deformation literature. Dashed lines represent the borders of the material after deformation. The shear strain value is $\Gamma = \tan(\alpha)$, which for simple shear is equivalent to $2\varepsilon = 2 \int D_0 dt$, with ε the accumulated “tensorial” strain and D_0 the largest eigenvalue of the rate of deformation tensor defined in Equation (3.3).

These early experiments used polycrystals with initially uncorrelated grain orientations, based on the simplifying assumption that CPO develops only once in a crystal that has not yet developed any significant textural symmetry. This assumption loses validity in many geological settings where multiple stages of deformation are expected, for example, below tectonic plates that have changed their direction of motion or near regions of impingement of buoyant upwellings. Torsional strain experiments on dunite samples (comprising over 90% olivine) published by Skemer et al. (2011) suggest that microstructures of peridotites exhibit CPO related to an integrated deformation history. Completely overprinting pre-existing CPO with a new texture seems to require larger strains than forming an initial CPO from an isotropic texture. Webber et al. (2010) offer a similar interpretation for CPO measured in naturally deformed samples from a lithospheric shear zone (Red Hills, New Zealand), which exhibit strains of up to $\Gamma \sim 11.4$. Evidence of dynamic recrystallisation is also observed in these naturally deformed samples, in agreement with experiments. Following these findings, Boneh and Skemer (2014) conducted deformation experiments on dunite samples with varying initial CPO, and they observed the development of transient textures, which are sensitive to the initial texture. Samples were subjected to strains progressing until $\Gamma \sim 1.2$, but the observed CPO did not reach a steady state, and the expected A-type fabric had not yet developed.

Samples from the Josephine Peridotite shear zone (Oregon, USA) also demonstrate protracted texture evolution in minerals with pre-existing CPO (Warren et al., 2008; Skemer et al., 2009; Hansen & Warren, 2015). Warren et al. (2008) reports texture evolution that is still fairly rapid, but texture strength remains low even in highly strained samples. Saturation of texture strength does not agree with early experimental results, which may suggest that pre-existing CPO or the presence of pyroxene additionally inhibits strong grain orientation clustering. Most recently, Hansen and Warren (2015) analysed more samples with A-type

fabric, confirming seismological assumptions that similar deformation mechanisms seem to operate in both dunite and harzburgite.

A comprehensive review of experimental and natural peridotite data is provided by Skemer and Hansen (2016). Based on these data, as well as more recent studies (e.g. Bollinger et al., 2016; Bystricky et al., 2024; Demouchy et al., 2024), it is clear that olivine texture is controlled by deformation geometry, with a non-unique sequence of deformation events contributing to the overall CPO. The combination of dislocation creep and dynamic recrystallisation produces CPO in peridotites by deforming olivine grains. However, these processes are not exhaustive controls on olivine texture. Grain orientations, in particular, may be influenced by complex interactions between neighbouring grains (e.g. Raterron et al., 2019), which remain difficult to unravel. Both dynamic recrystallisation and dislocation creep are also likely sensitive to environmental factors, such as pressure, temperature, and water fugacity (Karato, 2010). A formal description of these relationships at mantle conditions remains difficult to establish, in part due to the limitations of laboratory equipment and the difficulties in extrapolating laboratory results to the time-scales of geological processes (Karato, 2010). Kinematic models of CPO evolution, therefore, rely on empirical parameters that are often calibrated for specific combinations of simulation domains and initial configurations (Kaminski & Ribe, 2001; Boneh et al., 2015; Hansen, Conrad et al., 2016). We aim for the PyDRex implementation to provide sufficient flexibility so that users can easily change parameters and replace modular components as their situation requires.

2.2 Simulations of peridotite texture

CPO simulations provide a means of investigating plausible patterns of intrinsic anisotropy. An early approach to linking flow with CPO patterns assumed that the direction and length of maximum macroscopic extension could be used as proxies for the direction and strength of CPO. This approach avoids the need to develop models of any microscopic dynamics; it was explored by McKenzie (1979) to begin making sense of geophysical observations of anisotropy. Two key findings from that study are the dependence of CPO on strain rather than stress and the potential control exerted by the deformation gradient on upper-mantle anisotropy. A model of CPO as a function of finite strain was subsequently established by Ribe and Yu (1991) and Ribe (1992) for a pure olivine polycrystal. Such a model neglects dynamic recrystallisation processes (Lev & Hager, 2008), which have since been shown to control CPO evolution at large strains.

More recent polycrystal CPO models can be divided into three classes: full-field models, mean-field models, and kinematic models. Full-field, or “n-site”, models account for stress compatibility between grains and do not rely on empirical calibration. However, they require explicitly defined microstructures (usually a map of grain boundaries), which are generally unavailable in either experimental or natural environments. To capture the range of probable behaviours, the simulation must be repeated for a large number of different candidate microstructures. The fastest n-site model variants have an average computational complexity on the order of $N \times \log_2 N$ for N grains (e.g. Lebensohn, 2001), which makes this approach too expensive for use within geodynamic models.

2 Background

Mean-field models are more computationally tractable alternatives (with computational complexity that generally scales linearly with N) that introduce a statistical description of the microstructure in terms of lattice orientation (Castelnau et al., 2008). A single mean-field simulation can thus approximate an ensemble average of full-field simulations. The Visco-Plastic Self-Consistent (VPSC) model of Lebensohn and Tomé (1993) exemplifies this method. In these models, CPO evolution is investigated by considering interactions between each grain and an effective medium with averaged properties of the aggregate. The averaging procedure assumes a linear relationship between stress and strain. However, viscoplastic deformation is usually characterised by non-linear (i.e. non-Newtonian) rheology, which necessitates the use of a linearisation scheme (Hansen et al., 2021). Various linearisation schemes are discussed in Castelnau et al. (2008), and the “second-order” scheme proposed by Castañeda (2002) achieves the closest approximation of full-field mechanical models. A recent mean-field model extended the VPSC scheme to include limited recrystallisation effects (only subgrain rotation; Signorelli & Tommasi, 2015), which increased agreement with laboratory studies at the cost of computational efficiency. Mean-field models are still too slow for routine use in geodynamic simulation (Ribe et al., 2018) and generally omit simulation of dynamic recrystallisation.

Finally, kinematic models are the most approximate, but also the fastest. Starting from similar simplifications as the mean-field models, simulation of the local mechanical state is omitted, and intragranular strain heterogeneities are neglected. Instead, an empirically calibrated analytical expression for deformation-induced lattice rotations is employed. Solving this equation may yield either the lattice orientation for a discrete portion of the polycrystal (Ribe, 1992; Kaminski & Ribe, 2001; Moresi et al., 2003), or the average orientation for the whole aggregate (Goulding et al., 2015; Ribe et al., 2018). The D-Rex kinematic model introduced by Kaminski and Ribe (2001), which discretizes the polycrystal into a fixed number of volume fractions, was extended by Kaminski et al. (2004) to support polymineralic (olivine-enstatite) composition, thereby providing a more representative numerical analogue of mantle peridotite composition. It has been widely used to predict CPO in models of steady mantle flow (e.g. Kaminski & Ribe, 2002; Boneh et al., 2015; Hedjazian et al., 2017) and occasionally time-varying flow (Faccenda & Capitanio, 2013; Fraters & Billen, 2021). In the model, CPO evolves as a function of the mismatch between local and macroscopic deformation rates. Because this mismatch is only minimised, and not eliminated, by the best-fitting local deformation rate, the procedure implies strain incompatibility in the aggregate. This is addressed by ascribing the equilibration of any remaining strain mismatch to auxiliary mechanisms, such as grain boundary sliding or dislocation climb, which are assumed to have negligible effect on lattice orientations. The D-Rex model offers a reasonably accurate description of crystallographic texture at a relatively low computational cost (Hansen et al., 2021). Although it does not provide a way to extract local effects of CPO on viscosity, to our knowledge, it is the only model to both support polymineralic aggregates and offer parameters to control dynamic recrystallisation effects.

3 PyDRex

3.1 The kinematic texture simulation method

Laboratory studies of CPO, summarised in Chapter 2, provide ample evidence that CPO development depends not only on the mechanical properties of the deforming minerals but also on the history and geometry of deformation. To capture this behaviour, forward models of CPO evolution need to allow for interactions between microphysical mechanisms and time-varying macroscopic kinematics. Microscopic structure can either be tracked directly, which is not computationally tractable when combined with large-scale flow models, or via a more economical statistical description. In “kinematic” CPO models, additional simplifications are introduced to reduce the cost of computing grain-scale mechanical interactions. These simplifications generally derive from one of two homogenisation approaches: either stress or strain rate is assumed to be the same in every grain, following the Sachs or Taylor models, respectively (Mao, 2016). The Taylor approach has been more widely adopted because the mechanisms of dislocation creep are more readily expressed in terms of strain. However, dislocation creep mechanisms alone cannot accommodate arbitrary strains in minerals with fewer than five independent slip systems, such as olivine. Consider a mineral with slip systems indexed by $s \in \{1, 2, \dots\}$. The strain produced by dislocation glide on these systems can be expressed as

$$\epsilon_{ij} = \sum_s \frac{1}{2} \gamma^s (n_j^s l_i^s + n_i^s l_j^s), \quad (3.1)$$

where, for each independent slip system, γ^s is a stress-dependent slip activity, $\mathbf{n}^s$ is the vector normal to the slip plane, and $\mathbf{l}^s$ is a vector pointing in the direction of slip (Karato, 2008). Strain is symmetric, which means that the tensor ϵ has a maximum of six independent components. Furthermore, for incompressible flow, a reasonable assumption in Earth’s upper mantle (Jarvis & McKenzie, 1980), volume conservation implies that the strain cannot involve expansion or contraction, i.e. $\epsilon_{11} + \epsilon_{22} + \epsilon_{33} = 0$. This leaves five independent components which are necessary to describe an arbitrary strain ϵ . Only four slip systems are known for olivine, of which three may be active for any particular fabric type (see Section 8.2) meaning that deformation on these slip systems can only describe a strain with three independent components. This implies that dislocation creep cannot account for the total strain during viscoplastic mantle deformation.

The D-Rex kinematic CPO model developed by Kaminski and Ribe (2001) does not require dislocation creep to account for the complete deformation. Instead, active slip systems contribute to the macroscopic strain as much as possible, but may not fully accommodate it. Without consideration of any other mechanisms, incomplete strain accommodation would imply that unphysical incompatibilities have arisen in the microstructure, such as cavities

between grains or overlapping grain boundaries. However, the model is still applicable if the residual strain is assumed to be caused by auxiliary mechanisms, such as dislocation climb or grain boundary sliding (GBS). These auxiliary mechanisms are assumed to have no effect on grain orientations.

Deformation of the aggregate in a flow field is described by linear transformations from a reference state to the deformed state. These transformations are completely defined by nine coefficients, which constitute the *deformation gradient*. Along a flow pathline (i.e. a trajectory recorded by the motion of an aggregate), the deformation gradient F evolves according to

$$DF := \dot{F} + \mathbf{u} \cdot \nabla F = \mathbf{L}F, \quad (3.2)$$

where DF is the material derivative of F (McKenzie, 1979), related to the (Eulerian) temporal derivative $\dot{F}$ via convective transport by the local flow velocity $\mathbf{u}$. The quantity $\mathbf{L}$ is known as the *velocity gradient tensor* (Malvern, 1969) and can be decomposed as the sum of a symmetric rate of deformation (i.e. strain rate) tensor

$$\mathbf{D} = \frac{1}{2} (\mathbf{L} + \mathbf{L}^T), \quad (3.3)$$

and an antisymmetric rate of rotation (i.e. vorticity) tensor

$$\mathbf{W} = \frac{1}{2} (\mathbf{L} - \mathbf{L}^T). \quad (3.4)$$

It is convenient to extract the largest eigenvalue of $\mathbf{D}$ as a characteristic deformation scale, D_0 , and work with dimensionless variants of Equations (3.3) and (3.4) instead. Dimensionless quantities will be annotated with an asterisk, e.g. $\mathbf{L}^* = \mathbf{L}/D_0$.

At the microscopic scale, the aggregate is modelled as a fixed number of surrogate “grains” of variable fractional volumes and associated lattice orientations. These elements do not directly correspond to physical grains, but rather provide a statistical discretisation of the polycrystal texture. Their shapes and locations are not tracked, and their number is fixed to a constant multiple of the number of relict (i.e. un-recrystallised) physical grains. In the literature, they are nevertheless simply referred to as “grains”. We will qualify these elements as “surrogate grains” to avoid confusion. For each of these surrogate grains, the microscopic velocity gradient tensor $\nabla \mathbf{v}$ ($\mathbf{L}$ describes the macroscopic state) is controlled by the rate of shear due to dislocation glide and the rate of rotation of the crystallographic reference axes (Ribe & Yu, 1991), which are represented as symmetric and antisymmetric tensors, respectively:

$$\nabla \mathbf{v}^* = \frac{\gamma \mathbf{G} + \mathbf{w}}{D_0}, \quad (3.5)$$

where γ is the rate of slip on the weakest (i.e. most active) slip system. $\mathbf{G}$ and $\mathbf{w}$ are defined as

$$G_{ij} = 2 \sum_s \beta^s l_i^s n_j^s \quad (3.6)$$

and

$$w_{ij} = \sum_k \eta_{ikj} \omega_k, \quad (3.7)$$

with β the scaling factor that determines relative activities on the different slip systems, ω_i the components of the crystallographic “spin” vector (rate of rotation of the crystallographic axes), and η_{ijk} the Levi-Civita symbol,

$$\eta_{ijk} = \begin{cases} +1 & \text{if } (i, j, k) \text{ is } (1, 2, 3), (2, 3, 1), \text{ or } (3, 1, 2), \\ -1 & \text{if } (i, j, k) \text{ is } (3, 2, 1), (1, 3, 2), \text{ or } (2, 1, 3), \\ 0 & \text{if } i = j, \text{ or } j = k, \text{ or } k = i. \end{cases} \quad (3.8)$$

The deformation of a given grain indexed by $n \in \{1, 2, \dots\}$ is obtained by minimising the mismatch between the macroscopic and the microscopic velocity gradients, which is expressed mathematically as the minimisation of

$$\langle R \rangle_n = f_n \|L^* - \nabla \mathbf{v}_n^*\|^2, \quad (3.9)$$

where the prefactor f_n is a weighting factor that encodes the fractional grain volume. Minimisation of $\langle R \rangle_n$ is achieved by substituting Equation (3.5) for $\nabla \mathbf{v}_n^*$, yielding linear equations for γ and ω_i , and solving the system of four equations

$$\begin{aligned} \partial_\gamma \langle R \rangle_n &= 0, \\ \partial_{\omega_i} \langle R \rangle_n &= 0, \quad i \in \{1, 2, 3\}, \end{aligned} \quad (3.10)$$

where ∂_γ and ∂_{ω_i} denote the partial derivatives with respect to γ and ω_i , respectively (Section 7.1). Finally, for an aggregate of N surrogate grains,

$$\langle R \rangle = \sum_{n=1}^N \langle R \rangle_n \quad (3.11)$$

gives the total (squared) deformation mismatch, such that $\langle R \rangle / \text{tr}(\mathbf{L}^* \mathbf{L}^{*\top})$ is the portion of deformation accommodated by auxiliary plastic mechanisms (suggested by Kaminski & Ribe, 2001, to be dislocation climb and grain boundary sliding). Thus, the solutions to Equation (3.10) control the rate of deformation of the grain and the rate of rotation of its lattice axes, respectively.

Dynamic recrystallisation mechanisms also influence the polycrystal texture by altering the fractional grain volumes. These mechanisms are controlled by the distribution of dislocations (Karato, 2008). In general, the density of dislocations in a particular grain will depend on its deformation history. To reduce computational complexity, in the D-Rex model, the density of dislocations is assumed to be a function of only the instantaneous local conditions. Empirical evidence suggests that this assumption is appropriate for olivine minerals, which exhibit a fast convergence towards steady-state dislocation density in deformation tests (e.g. Durham et al., 1977). Furthermore, the recrystallisation model of Wenk and Tomé (1999), which employs the same assumption and motivates the developments of the D-Rex model (Kaminski & Ribe, 2001), was used to obtain qualitatively good results in comparison with experiments.

The dislocation density, ρ_s , on slip system $s \in \{1, 2, \dots\}$, is proportional to a power of the critical resolved shear stress (CRSS) acting on the slip plane, τ_s ,

$$\rho_s \propto \tau_s^p. \quad (3.12)$$

The critical resolved shear stress τ_s is, in turn, proportional to the rate of deformation on the slip plane,

$$\tau_s \propto |D_s|^{1/n}. \quad (3.13)$$

The values of p and n are empirically determined parameters in the model. Olivine deformation experiments suggest that $p = 1.5$ and $n = 3.5$ are reasonable choices (Kaminski & Ribe, 2001).

Experimental data also constrain the shear stress required to initiate slip on different systems, which allowed Kaminski and Ribe (2002) and Kaminski et al. (2004) to propose simple distributions for normalised CRSS for the various olivine fabrics. For any particular olivine fabric, at least one slip system is always assumed to be active. The CRSS on the softest slip system, τ_0 , is used as a reference against which all τ_s are normalised, i.e. $\tau_s^* = \tau_s/\tau_0$. Values of τ^* for known olivine fabrics are given in Table 8.21. Combining Equation (3.12) and Equation (3.13) yields

$$\frac{\rho_s}{\rho_s^\alpha} = \left| \frac{D_s}{D_s^\alpha} \right|^{p/n}, \quad (3.14)$$

where ρ_s^α and D_s^α are arbitrary reference values of dislocation density and deformation rate, respectively, for the slip system s . The reference deformation rate for all slip systems is taken to be $D_s^\alpha = D_0$, where D_0 is the largest eigenvalue of the imposed deformation rate from Equation (3.3). The reference dislocation density is set as a model parameter, ρ_0 , that represents the dislocation density on the softest slip system. For the remaining slip systems, an additional relationship is introduced based on dislocation propagation theory (Kaminski & Ribe, 2001), which relates ρ_s^α to ρ_0 :

$$\frac{\rho_s^\alpha}{\rho_0} = \left(\frac{\tau_0}{\tau_s} \right)^{n-p} = \left(\frac{1}{\tau_s^*} \right)^{n-p}. \quad (3.15)$$

Thus, by combining Equation (3.14) and Equation (3.15), the dislocation density on an arbitrary slip system is given by

$$\rho_s^* := \frac{\rho_s}{\rho_0} = \left(\frac{\tau_0}{\tau_s} \right)^{n-p} \left| \frac{D_s}{D_0} \right|^{p/n} = \left(\frac{1}{\tau_s^*} \right)^{n-p} |D_s^*|^{p/n}. \quad (3.16)$$

Note that if slip system s is the softest system, then $D_s = \gamma$, with γ from Equation (3.5).

As noted in Section 2.1, the energy stored in dislocations drives both grain boundary migration and subgrain nucleation. A portion of the dislocation energy of an individual grain is consumed through mechanisms, such as subgrain rotation, that lead to the nucleation of new grains (Wenk & Tomé, 1999). Nucleation within solids remains an active area of study (e.g. Solas et al., 2001; Welsch et al., 2012; Signorelli & Tommasi, 2015; Bollinger et al., 2018). However, based on the theoretical analogue of solid nucleation in fluid solutions, Wenk et al. (1997) proposes that the fraction of a grain affected by subgrain nucleation is

proportional to an exponential function of the square of the dislocation density. This idea is adopted by the D-Rex model and gives the expression

$$E = \sum_s \rho_s^* \exp[-\lambda^* (\rho_s^*)^2] \quad (3.17)$$

for the amount of energy available in a single surrogate grain. The input parameter $\lambda^* = \lambda \rho_0$ encodes both the reference dislocation density ρ_0 and the efficiency of subgrain nucleation λ . Grain boundary migration acts to equilibrate dislocation energy between neighbouring grains. Because the D-Rex model does not track the relative location of grains, GBM is assumed to contribute to an overall minimisation of the difference between dislocation energy in individual surrogate grains and an averaged dislocation energy of the aggregate, $\bar{E}$. Therefore, the fractional grain volumes f_n , introduced in Equation (3.9), evolve according to

$$\partial_\varepsilon f = -M^* f(E - \bar{E}), \quad (3.18)$$

where $\varepsilon = \int D_0 dt$ is the accumulated strain, which is a (non-linear) function of time, and the input parameter M^* defines the grain boundary mobility, which determines the efficiency of grain growth.

In addition, Kaminski et al., 2004 introduced a third input parameter that defined a grain size threshold, f_{gbs} , below which surrogate grains were excluded from Equation (3.18). As surrogate grains smaller than the threshold value do not contribute to further texture changes, they represent portions of the aggregate in which grain boundary sliding is active. Evidence of grain boundary sliding was observed in experimental studies of deformed olivine (e.g. Lee et al., 2002; Bollinger et al., 2019).

Whilst the effects of recrystallisation mechanisms are much harder to constrain experimentally, the phenomenological approach taken in D-Rex to incorporate these effects contributes to the flexibility and versatility of the model. Although some theoretical rigour is sacrificed, such as in the neglect of activation energies for nucleation and GBM, or in the assumption that nucleated subgrains do not contribute to polycrystal texture, the benefit of a simple model controlled by three input parameters, λ^* , M^* and f_{gbs} , has proven uniquely attractive to the geodynamics community, as evidenced by its broad and growing use (e.g. Faccenda & Capitanio, 2013; Boneh et al., 2015; Hedjazian et al., 2017; Fraters & Billen, 2021).

3.2 Texture diagnostics

Crystallographic textures and, therefore, elastic properties of a polycrystalline medium may generally vary in all directions. Methods for representation, analysis, and classification of such textures (e.g. in order to quantify the degree of preferred orientation) have been developed and refined over recent decades (e.g. Browaeys & Chevrot, 2004; Morawiec, 2004; Skemer et al., 2005; Mainprice et al., 2014). In many cases, techniques were first developed for analysis of small experimental or natural samples and later adopted by modelling software. Whilst description of synthetic (numerical) textures is in many ways similar, the quantity of data is generally significantly larger. Experiments often describe samples in terms of hundreds of grains, whereas the D-Rex model requires thousands of “surrogate grains” to achieve

consistent outputs. To obtain useful synthetic models of seismic anisotropy, our goal is to employ many spatially distributed polycrystals, with texture snapshots taken at regular time intervals for each. Therefore, efficient descriptions of CPO are necessary.

Because seismic anisotropy is most commonly described by a single axis (the “fast direction” of seismic energy propagation) and a corresponding scalar value (the magnitude of anisotropy of either compressional or shear waves), we restrict ourselves here to those texture diagnostics that yield a CPO “axis” or some notion of CPO “strength”.

Impressions about the shape of a distribution of spherical data can be obtained by plotting 2D projections of the raw data. Crystallographic pole figures show Lambert equal-area projections onto a disc (see Figure 2.1). Such figures have been produced throughout the literature (e.g. Karato et al., 2008; Boneh et al., 2015; Hansen, Warren et al., 2016; Fraters & Billen, 2021), demonstrating a clear tendency for girdle or point symmetries in the grain orientations of deformed polycrystals. Fortunately, both of these symmetries lead to distinct characteristic eigenvalue properties of the spherical inertia or “scatter” matrix (Mardia & Jupp, 1999)

$$T_{ij} = \sum_{n=1}^N f^n x_i^n x_j^n, \quad (3.19)$$

where $n \in \{1, 2, \dots, N\}$ is the grain index, f is the grain volume fraction, and $\mathbf{x}$ is the grain orientation, represented as a 3-component vector. The components of $\mathbf{x}$ for a particular grain are direction cosines of a unit vector along its [100] axis. If $\mathbf{a}$ is a rotation matrix describing the grain orientation as per Equation (8.1), then $\mathbf{x}$ can be retrieved as the first row of this matrix. Due to the bipodal nature of peridotite textures, the vectors $\mathbf{x}$ and $-\mathbf{x}$ are equivalent (Mardia & Jupp, 1999).

In the case of a uniform distribution of grain orientations, all eigenvalues of T will be comparable. If only the two largest eigenvalues of T are similar, the distribution of orientations can be described by a girdle. Finally, if one eigenvalue is significantly larger than the others, this means that orientations are clustered near a particular axis. In the final case, the eigenvector of T corresponding to the largest eigenvalue is an estimate of the “mean” orientation axis of the data (Vollmer, 1990). This is often referred to as the *Bingham average* direction. Although straightforward to calculate, it does not provide a natural way to handle polymineralic compositions.

A second method for obtaining the CPO axis is based on the effective elastic tensor of a polymineralic aggregate obtained through *Voigt averaging* (Voigt, 1928; Man & Huang, 2010). Alternative averaging schemes for elastic tensors may also be used, such as Reuss or Voigt-Reuss-Hill schemes, the latter of which is described in detail in Man and Huang (2011). The Voigt method currently implemented in PyDRex computes the average as

$$\bar{\mathbf{C}} = \sum_v \mathcal{F}_v \left(\sum_{n=1}^N f_n \mathbf{C}'_n \right), \quad (3.20)$$

where $\mathcal{F}$ are the volume fractions of the constituent mineral phases indexed by v , N is the number of surrogate grains, which must be identical for each phase, and $\mathbf{C}'$ is the single-crystal elastic tensor rotated by the grain orientation. This rotation is achieved via the usual

fourth-order tensor rotation

$$C'_{ijkl} = a_{ip}a_{jq}a_{kr}a_{ls}C_{pqrs}, \quad (3.21)$$

where $\mathbf{a}$ is the direction cosine matrix of the grain orientation.

Once $\bar{C}$ is obtained, the CPO axis can be found by eigenvector analysis. Because anisotropy in Earth's mantle can be well approximated by a hexagonally symmetric medium (Becker et al., 2006), we first perform a further symmetry decomposition of $\bar{C}$ using the method introduced by Browaeys and Chevrot (2004) to obtain the component of this elastic tensor that is attributable to such a medium. The procedure also yields an estimate of the accuracy of the hexagonal approximation. A CPO axis obtained by this method will be called the “mean hexagonal axis” of the polycrystal; the seismological term “transverse isotropy axis” is equivalent.

The texture strength, which is related to the magnitude of observed P- or S-wave anisotropy, can be defined and calculated in various ways. Experimental studies first introduced the *J-index* to complement pole figure analysis (H.-J. Bunge, 1982). Whilst this value is still occasionally used (e.g. Warren et al., 2008; Hansen & Warren, 2015; Hansen, Conrad et al., 2016), it requires estimation of a continuous orientation distribution function (e.g., by fitting the observed orientations with spherical harmonic functions). The *J-index* also has no natural upper bound, making straightforward comparisons across simulations challenging, or being unsuitable for interpretation as a distance to an ideal point maximum, which is a common approximation of a-axis texture in deformed olivine.

Instead, we have implemented an alternative diagnostic introduced by Skemer et al. (2005). Comparison of the distribution of misalignment angles between every combination of surrogate grains observed in the results and the theoretical distribution for a polycrystal with randomly oriented grains yields the *M-index* value according to the sum

$$M = \frac{\theta_{\max}}{2n} \sum_{i=1}^n |R_i^T - R_i^O|, \quad (3.22)$$

where $\theta_{\max}$ is the maximum theoretical misorientation angle, R_i^T and R_i^O are the theoretical and observed counts for misorientation angles in the i -th bin, and n is the total number of bins. A value of $M = 0$ indicates a polycrystal with perfectly isotropic properties, according to the theoretical distributions proposed by Grimmer (1979), and increasing values of M , bounded at $M = 1$, correspond to increasing texture strength.

In practice, calculation of the *M-index* for synthetic data requires the following steps:

1. Define transform matrices that represent each unique symmetry operation from the chosen crystal lattice system.
2. For each pair of grain orientations $\{\mathbf{a}, \mathbf{b}\}$, apply symmetry operations to $\mathbf{b}$ until the smallest misorientation angle to $\mathbf{a}$ is found.
3. Generate theoretical distribution $\mathbf{R}^T$ and compute *M-index* using Equation (3.22).

Whilst this method offers the advantage of taking into account the lattice system symmetry, the computation time is proportional to $\binom{N}{2} \times S$, where N is the number of surrogate grains

and S is the number of symmetry operations. Based on our analyses, the maximum surrogate grain size could serve as a computationally cheaper proxy for texture strength in D-Rex models.

4 Validation and verification

The D-Rex theory has been used under different implementations, which have been accompanied by publications with disparate validation benchmarks and models (e.g. Lev & Hager, 2008; Faccenda & Capitanio, 2013; Hedjazian et al., 2017; Fraters & Billen, 2021; Kenyon & Wada, 2022). Furthermore, the computational resources and numerical frameworks required to run mantle convection simulations (e.g. Jadamec, 2016) have become significantly more accessible since the release of the original D-Rex model (Kaminski & Ribe, 2001; Kaminski et al., 2004), which motivates development and validation of an equally flexible, extensible, and reliable CPO simulation software. In this section, we present a systematic suite of benchmark cases for PyDRex, inspired by existing models and published results, which highlights consistencies and potential sources of discrepancy between PyDRex and previous implementations. The results presented serve not only to demonstrate the correctness of our implementation but also as a resource and basis to ground-truth future adaptations and improvements of PyDRex.

PyDRex is structured as a Python package (library) with functionality split between various modules. The core module exposes a low-level interface to compute the derivatives of both grain orientations (Equation (7.25)) and grain volume fractions (Equation (3.18)), given the velocity gradient at the location of the polycrystal and some auxiliary model parameters. Typically this function will be called many times (once for each grain in each polycrystal at each timestep): it is therefore compiled using the Numba just-in-time compiler (Lam et al., 2015) to improve performance (some notes on performance and required memory resources are provided in Section 8.4, including an initial comparison with the original Fortran routines). Other modules include functions to compute diagnostics and track mineral phases of a deforming polycrystal.

4.1 Validation of the plastic deformation routine

The orientation of a grain with respect to the local (Eulerian) velocity gradient determines its propensity to undergo plastic deformation. Following standard crystallographic nomenclature, “soft” orientations are more favourable for plastic deformation, in contrast to “hard” orientations which are less favourable.

To validate our implementation of the D-Rex plastic deformation routine, we have derived analytical solutions for crystallographic rotation rates in various homogeneous simple shear flows (see Section 7.1). For simple shear with a deformation rate of D_0 along the Y axis in the model reference frame and a single crystal of A-type olivine undergoing dislocation glide on the (010)[100] slip system, the crystal orientation evolves according to

$$\frac{\partial \theta}{\partial t} = D_0 (1 + \cos 2\theta) \quad (4.1)$$

(Equation (7.23)), where $\pi/2 - \theta$ is the angle between the crystallographic [100] vector (a-axis) and the shear direction. The solution to this equation is

$$\theta(t) = \arctan(2D_0t + 1). \quad (4.2)$$

This can be compared to the rotation of a macroscopic finite strain measure. A popular strain measure in the finite (large) strain modelling literature is the finite strain ellipsoid (FSE; e.g. McKenzie, 1979; Ribe, 1992; Becker et al., 2003), which measures the deformation of a material volume that was spherical in the reference configuration. The orientation of this ellipsoid is defined by the normalised principal eigenvectors of the left-stretch (“Cauchy-Green”) tensor B , defined as

$$B = FF^\top \quad (4.3)$$

in terms of the deformation gradient tensor F , which is the solution to Equation (3.2). In general, solutions to Equation (3.2) are of the form

$$F = e^{tL}, \quad (4.4)$$

which in the simple shear case ($L^2 = 0$) simplifies to

$$F = I + tL, \quad (4.5)$$

with I the identity tensor (Huilgo & Phan-Thien, 1997). Solving for the eigenvectors of Equation (4.3) with substitution from Equation (4.5) and a simple shear velocity gradient L that has a single nonzero component, e.g. $L_{21} = 2D_0$, yields the vector describing the FSE long axis in simple shear:

$$\begin{bmatrix} 1 \\ \sqrt{D_0^2 t^2 + 1} + D_0 t \\ 0 \end{bmatrix}. \quad (4.6)$$

The angle between this vector and the X axis of the reference frame evolves as

$$\Phi(t) = \arctan\left(\sqrt{D_0^2 t^2 + 1} + D_0 t\right). \quad (4.7)$$

At low strains ($\varepsilon \approx 0.5$) the difference between θ and Φ reaches a maximum value of $\theta - \Phi \approx 5^\circ$ (Figure 4.1), but values converge for increasing strain, and both approach $\pi/2$ as $\varepsilon \rightarrow \infty$.

Numerical rotation rates of olivine [100] axes computed using the low-level PyDRex interface for the same simple shear case are shown in Figure 4.2; they are in excellent agreement with the theoretical prediction of Equation (4.1). Similar tests for other shear directions are provided in the PyDRex test suite, with results illustrated in the supplement.

4.2 Validation of recrystallisation for 2D textures

To aid discussion about simple shear geometry in this and following examples, we adopt the terms “shear plane” and “deformation plane”: in our definition, the shear plane refers to the

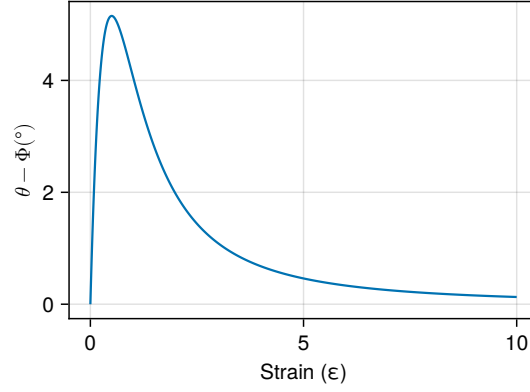


Figure 4.1: Theoretical misfit between single crystal olivine a-axis angle θ predicted by PyDRex and the long axis orientation Φ of a finite strain ellipsoid (FSE) in simple shear as a function of strain ($D_0 t \equiv \varepsilon$). For the olivine crystal, dislocation glide is active on the (010)[100] system. Values of θ and Φ are not identical, although they converge at large strain.

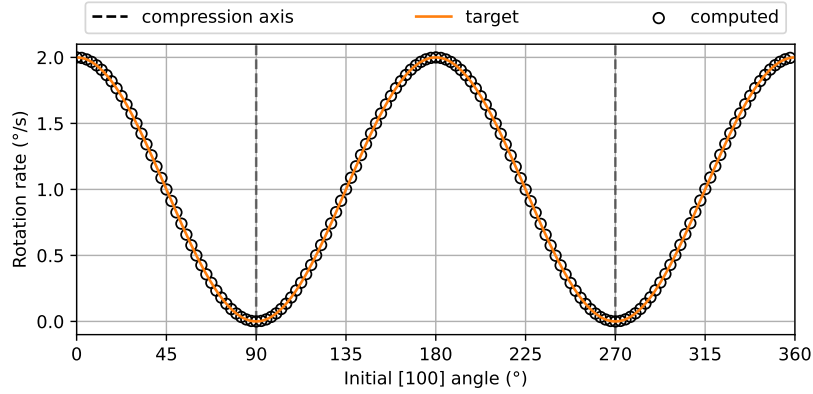


Figure 4.2: Numerical rotation rates (empty circles) for a single crystal of A-type olivine deforming via dislocation creep in simple shear with $L_{21} = 2D_0$. The initial [100] angle is measured from the X axis in the X-Y plane, so that at values of 90° and 270° (dashed lines), the [100] vector is aligned to the shear axis and the crystal does not experience rotation. Computed values follow the theoretical relationship (orange solid line) $\partial\theta/\partial\varepsilon = D_0 (1 + \cos 2\theta)$ derived in Chapter 7. The rotation rate, like the strain rate, is measured per unit time.

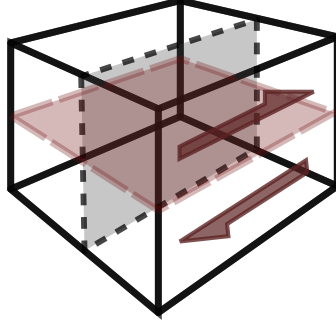


Figure 4.3: Deformation plane (gray, short-dashed border) and shear plane (red, long-dashed border) geometry for simple shear in a 3D domain as indicated by the harpoons. These planes are defined such that the line of their intersection contains the location of the tracked polycrystal aggregate.

zero-velocity plane that bisects regions of opposing velocity directions, while the orthogonal plane, containing the polycrystal of interest and spanned by the velocity and velocity gradient vectors, is called the deformation plane. This terminology is illustrated in Figure 4.3.

Analytical validation of the recrystallisation routines is possible if the initial orientations of $[100]$ vectors within an olivine polycrystal are isotropic in the deformation plane. For shear in the Y-direction, as in Section 4.1, the dislocation density on the single active slip system $(010)[100]$ is given by

$$\rho^* = |\cos 2\theta|^{p/n}, \quad (4.8)$$

according to Equation (3.16). The strain energy for each grain is, therefore,

$$E = \rho^* \exp[-\lambda^*(\rho^*)^2], \quad (4.9)$$

which allows calculation of the instantaneous change in grain sizes using Equation (3.18). Results illustrated in Figure 4.4 demonstrate that grain growth occurs for surrogate grains with both subparallel (i.e. soft) and suborthogonal (i.e. hard) $[100]$ orientations compared to the shear direction, as well as those with $[100]$ vectors at exactly 45° from the shear direction. Surrogate grains with suborthogonal orientations rotate fastest, as in the single crystal case, and those that are already aligned to the shear do not rotate.

A second recrystallisation test available in the PyDRex repository demonstrates that, for an initial ideal girdle texture in the shear plane, the evolution of the CPO is more complex due to the activation of a second slip system. Results are shown in Figure 7.2 in Chapter 7. Grain growth is restricted to surrogate grains in soft orientations, and rotation rates peak for those with $[100]$ vectors at 45° from the shear direction. Surrogate grains in hard orientations (i.e. suborthogonal to the shear direction) cannot rotate at all in this geometry and are instead passively consumed by recrystallisation. The maximum grain growth rate is higher than in Figure 4.4, which means that surrogate grains whose $[100]$ vectors lie in or near the shear plane will align quicker towards the shear direction compared to those whose $[100]$ vectors lie in or near the deformation plane.

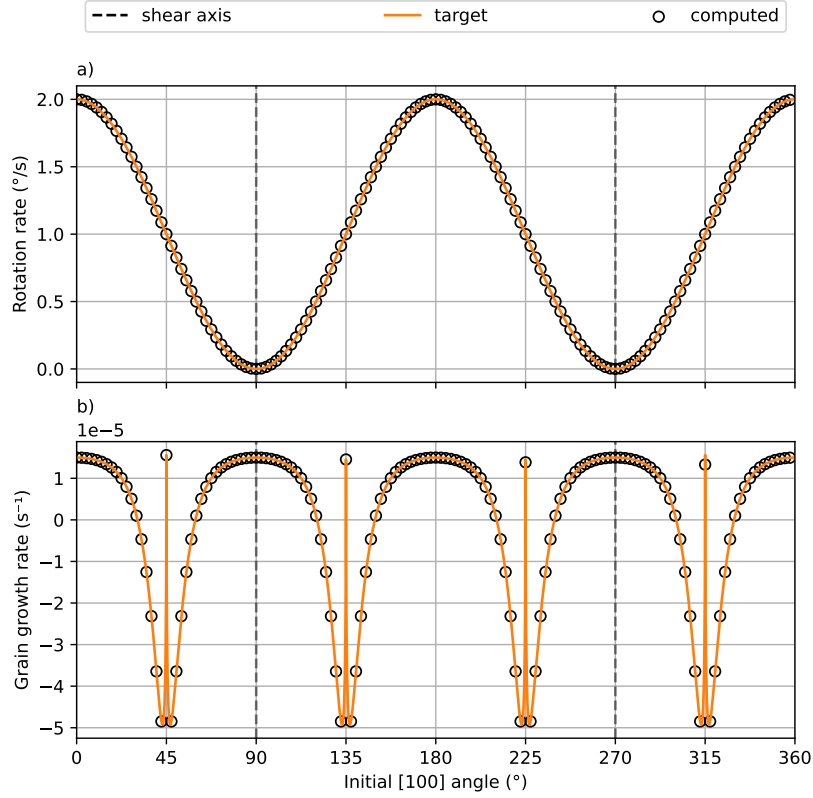


Figure 4.4: Numerical rotation rates (a) and grain growth rates (b) for an A-type olivine polycrystal, with an ideal girdle texture in the X-Y plane, deforming via dislocation creep in simple shear with $L_{21} = 2D_0$. The initial [100] angles for each grain are measured from the X axis in the X-Y plane, so that at values of 90° and 270° (dashed lines), the [100] vector is aligned to the shear axis and the grain does not experience rotation. Computed values (empty circles) follow the theoretical relationships (orange solid lines) derived using Equation (3.18) and Equation (4.9). The rotation rate is identical to the single crystal case in Figure 4.2. Rotation rate and grain growth are measured in units of inverse time.

4.3 Planar simple shear

Simple shear deformation is perhaps the simplest deformation mode applicable to Earth’s asthenosphere. Kaminski and Ribe (2001) used simple shear olivine deformation experiments to calibrate the original D-Rex model. They found that the rotation of the olivine a-axis follows the rotation of the FSE when $M^* = 0$ but occurs quicker as M^* increases. With the PyDRex package, we provide a subset of the D-Rex Fortran 90 subroutines (Édouard Kaminski – Pers. Comm.), which we slightly modified to set up stationary simple shear of olivine polycrystals without the need for meshes or pathlines. This code was used to validate PyDRex outputs, as shown in Figure 7.3 for the simple shear deformation just mentioned. Whilst the original papers only report individual D-Rex runs for any particular pathline (Kaminski & Ribe, 2001; Kaminski et al., 2004), we found that running the same model repeatedly led to different numerical outputs. The magnitude of these perturbations depended on various model parameters – a characteristic that we revisit in Chapter 5. We therefore obtained our reference data by averaging an ensemble of 500 Fortran model runs. For PyDRex, we similarly prefer to present ensemble averages in this study, as they capture a more complete and reproducible representation of the data. At strains smaller than $\varepsilon = 0.2$, our results deviate from the original D-Rex outputs due to stochastic variations in the initial random state (initial orientations of surrogate grains are randomised, i.e. drawn from an isotropic distribution). For all strains past $\varepsilon = 0.2$, average PyDRex and D-Rex outputs correspond within $\sim 4^\circ$ for $M^* = 0$, 1° for $M^* = 50$, and 1.5° for $M^* = 200$ (see Figure 4.5). Thus, the average D-Rex outputs match the PyDRex outputs to within one standard deviation.

Kaminski and Ribe (2001) suggested that CPO computed using $M^* = 0$ would follow the long axis of the FSE, however their simulation terminated at a strain of $\varepsilon = 1$. Our ensemble run with $M^* = 0$ reveals that the average $[100]$ angle computed based on D-Rex plastic deformation theory described in Chapter 3 deviates by up to $\sim 10^\circ$ from FSE theory at large strain ($\varepsilon \geq 1$). The theoretical relationship between plastic deformation and finite strain was investigated by Ribe (1992), however analytical solutions are only available under the assumption of a single active slip system. Whilst Ribe (1992) established that plastic deformation can be a unique function of finite strain under simplified conditions, our numerical analysis shows that the long axis of the FSE does not always correspond to the CPO direction (*Bingham average*) obtained from plastic deformation modelling, in particular at large strains for minerals that exhibit multiple slip systems. This is demonstrated by the mismatch between the $M^* = 0$ (blue) and FSE (dashed purple) results in Figure 4.5.

Higher values of M^* lead to faster rotation of the olivine CPO, and the relationship is generally non-linear, with variation of M^* beyond 100 having less effect than variation between 10 and 100. Kaminski et al. (2004) used a relatively high value of $M^* = 125$ to produce numerical results that provide a reasonable match to experimental results from Zhang and Karato (1995). However, using high values for M^* introduces an undesired side-effect: the olivine CPO quickly becomes unrealistically strong, displaying a high degree of clustering of a-axis orientations. This is observed in the Lambert equal-area projections of the orientation data (“pole figures”) shown in Figure 4.6. Such behaviour does not match the usual characteristics of pole figures from either self-consistent plastic models (e.g. Tommasi et al., 2000) or experimental results with dynamic recrystallisation (e.g. Zhang & Karato, 1995;

4 Validation and verification

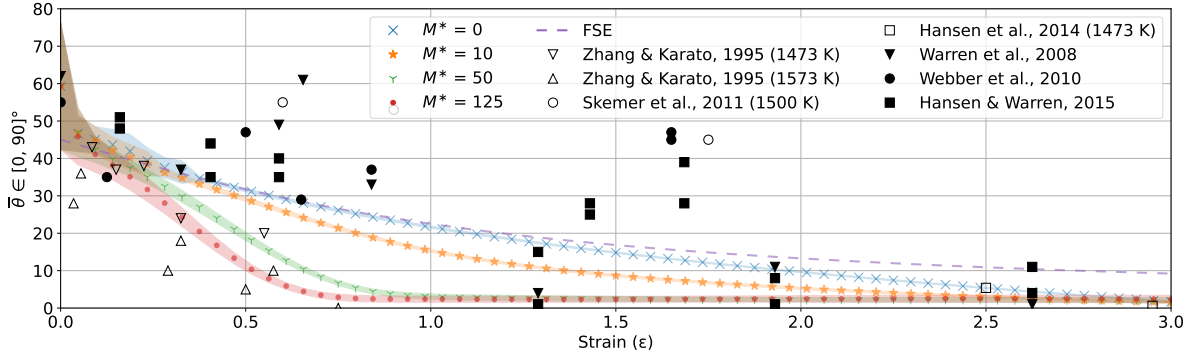


Figure 4.5: A-type olivine test demonstrating the effect of the grain boundary mobility (M^*) parameter. For our ensemble of 41 runs, a series of CPO vectors is computed using *Bingham averaging*. The mean angle between these vectors and the shear plane is plotted using the coloured markers, with shaded areas depicting one standard deviation. Results are compared to available data from experimentally (empty markers) and naturally (filled markers) deformed samples. Each simulation run in the ensemble uses a different state for the random initial grain orientations. Figure 7.3 shows that PyDRex reproduces the outputs of the original Fortran 90 code. Setting $M^* = 0$ prevents recrystallisation, and the CPO axis follows the long axis of the finite strain ellipsoid (FSE) for strains of $\epsilon \leq 1$, after which it aligns faster and reaches 0° by a strain of 3. For increasing values of M^* , the CPO direction is quicker to respond to imposed shear. Remaining model parameters are 1.5 for the stress exponent p , 3.5 for the deformation exponent n , 0 for the grain boundary sliding threshold, and 5 for the nucleation efficiency λ^* . The aggregate consists of 5000 surrogate grains.

Bystricky et al., 2000; Zhang et al., 2000; Lee et al., 2002). To address this issue, Kaminski et al. (2004) introduced the grain boundary sliding threshold, f_{gbs} , and a simple processing routine to exclude surrogate grains that have shrunk to a fraction f_{gbs} of their original size from the CPO routines, meaning they are simply advected in the flow and slide past other grains without deforming. This parameter restricts texture strength and alignment because a portion of the grains is no longer able to undergo changes in size either via dislocation creep or dynamic recrystallisation. The PyDRex model is much less sensitive to variations in f_{gbs} compared to variations in M^* , due to CPO being primarily controlled by few, large grains (see Section 5.2), and recommended values for this parameter are 0.2 – 0.3 (Kaminski et al., 2004).

For nonzero M^* , a secondary peak is also observed in the texture at moderate strains. Kaminski and Ribe (2001) attributed this feature to surrogate grains in hard orientations “that have not yet been consumed via GBM”. However, this explanation is at odds with the theoretical basis for GBM, as this mechanism should cause *growth* of those grains. We clarify this aspect of grain growth in Figure 4.4, from which it is clear that grains in both the softest and hardest orientations generally experience growth. The latter grow directly via GBM due to their low strain energy, while the former first birth nucleated subgrains which subsequently grow via the same mechanism. Therefore, the secondary peak is, in fact, generated as a direct consequence of GBM. Its rotation, caused by plastic deformation, is most visible in the lowermost row of Figure 4.6. The rapid disappearance of the secondary peak for large values of M^* can be attributed to the growth of nucleated grains outpacing the growth of grains in hard orientations. Note that in the D-Rex model, nucleated grains are not tracked

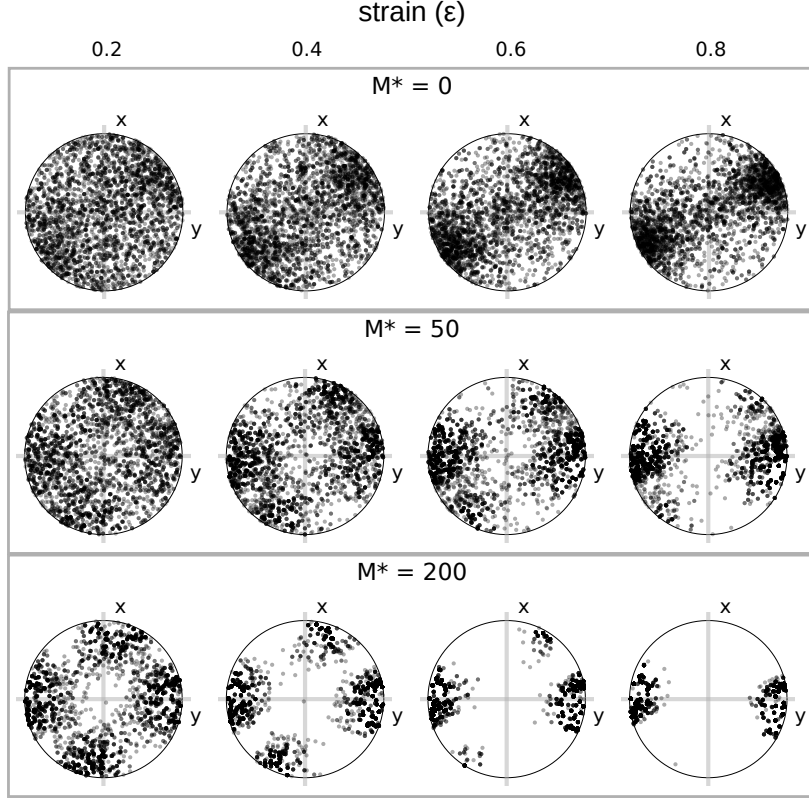


Figure 4.6: Y-X pole figures (lower-hemisphere projection) of PyDRex [100] (a-axis) orientations at strains of $\epsilon = 0.2, 0.4, 0.6$ and 0.8 (columns) for grain boundary mobilities $M^* = 0, 50$ and 200 (rows). Remaining parameters are identical to those used in Figure 4.5. The pure A-type olivine polycrystal is deformed in constant, uniform simple shear along the Y axis. As in Figure 4.5, increasing M^* causes the CPO to align faster. Pole figures of the remaining crystallographic axes, provided in Chapter 7, confirm that olivine a-axis orientations evolve towards a point maximum along the shear axis.

independently and instead contribute to growth of their “parent” surrogate grains.

An independent calibration of the D-Rex model was performed by Boneh et al. (2015), using experimental results from deformation of dunite samples with pre-existing CPO (Boneh & Skemer, 2014). They achieved a better match between D-Rex outputs and experimental results using a value of $M^* = 10$. Some subsequent modelling studies have adopted this value, which results in a slower CPO evolution and longer periods of transient CPO compared to $M^* = 125$ (e.g. Faccenda & VanderBeek, 2023). Data from torsion experiments (Skemer et al., 2011) and observations from natural samples (Warren et al., 2008; Webber et al., 2010; Hansen & Warren, 2015) seem to corroborate these expectations. We show results of available A-type olivine CPO observations in simple shear compared to PyDRex outputs for various values of M^* in Figure 4.5. Given the large variation in low-strain observations and the low number of high-strain data, it is difficult to provide a general recommendation for the value of the model parameter M^* . We suggest that a value of $M^* = 125$, as used in the original implementation, implies the assumption that CPO is generated in initially isotropic rocks. On the other hand, using $M^* = 10$ reflects a compromise between constraints from experimental

studies and observations of naturally deformed samples. Particular values depend on which approximation is more appropriate for the hypothesis being tested.

Whilst planar, uniform flow is trivial to simulate, mantle dynamics often exhibit complexity that cannot easily be reduced to such flows (e.g. Jadamec, 2016). In the next section we discuss a slightly more complex flow, which, while still planar and steady-state, generates spatial variations in strain rates.

4.4 Planar corner flow

At mid-ocean ridges, at the base of the newly forming oceanic lithosphere, the underlying asthenosphere is thought to experience high strains, leading to a characteristic CPO of peridotite minerals and measurable anisotropy of seismic wave velocities (Blackman et al., 2002). The simplest model of this flow field assumes a symmetric corner flow either side of the ridge. Corner flow models are popular in the texture-modelling literature due to their relatively simple dynamics. For example, the results discussed hereafter may be qualitatively compared to the “KR-ReX” pole figures presented in Castelnau et al. (2009), as well as the corner flow example for the original D-Rex implementation found in Kaminski and Ribe (2002). The shear experienced by aggregates following flow pathlines evolves from pure shear near the ridge axis to simple shear away from it.

The 2D flow field is defined by:

$$\mathbf{u} = \frac{dr}{dt} \cdot \hat{\mathbf{r}} + r \frac{d\theta}{dt} \cdot \hat{\boldsymbol{\theta}} = \frac{2U}{\pi}(\theta \sin \theta - \cos \theta) \cdot \hat{\mathbf{r}} + \frac{2U}{\pi} \theta \cos \theta \cdot \hat{\boldsymbol{\theta}}, \quad (4.10)$$

where U is the half-spreading velocity and θ measures the angle from the downwards direction beneath the ridge axis ($\theta = 0$) to the surface ($\theta = \frac{\pi}{2}$). Flow streamlines are parameterised by:

$$\psi = \frac{2Ur}{\pi} \theta \cos \theta, \quad (4.11)$$

which relates to the velocity through:

$$\mathbf{u} = -\frac{1}{r} \cdot \frac{d\psi}{d\theta} \cdot \hat{\mathbf{r}} + \frac{d\psi}{dr} \hat{\boldsymbol{\theta}}. \quad (4.12)$$

Conversion to the Cartesian (x, z) basis ($\hat{\mathbf{z}}$ pointing upwards) yields the following velocity field:

$$\mathbf{u} = \frac{2U}{\pi} \left[\arctan\left(\frac{x}{-z}\right) + \frac{xz}{x^2 + z^2} \right] \cdot \hat{\mathbf{x}} + \frac{2U}{\pi} \frac{z^2}{x^2 + z^2} \cdot \hat{\mathbf{z}}, \quad (4.13)$$

with the velocity gradient in the Cartesian (x, z) basis given by:

$$\mathbf{L} = \frac{4U}{\pi \cdot (x^2 + z^2)^2} \begin{bmatrix} -x^2 z & x^3 \\ -xz^2 & x^2 z \end{bmatrix}. \quad (4.14)$$

For small z and large x (i.e. close to the surface and away from the ridge axis), only the $L_{12} = x^3$ term is significant, which results in a simple-shear-type flow. Conversely, for $x \approx z$

(i.e. downwards from the ridge axis at a 45° angle), all four tensor components are comparable, but the L_{2i} entries are negative (because z is negative), leading to an antisymmetric tensor and, therefore, a pure shear. The bottom and right boundaries are permeable, while the velocity U (here 2 cm yr^{-1}) is imposed along the top. The left boundary is impermeable.

Results shown in Figure 4.7 were obtained for $M^* = 10$ and 125, $f_{gbs} = 0.3$, a nucleation efficiency of $\lambda = 5$, and 5000 surrogate grains per polycrystal. For higher M^* values, the texture of polycrystals that pass closer to the ridge axis ($x = 0$) is influenced by the upwelling flow. For $M^* = 125$, we observe sub-vertical CPO at a strain of $\varepsilon \approx 1$ for the pathline with $z_f = -20 \text{ km}$ (Figure 4.7b). Along this shallowest pathline, texture strength, measured using the *M-index*, briefly decreases at a strain of $\varepsilon \approx 1.3$ (Figure 4.7d), representing a transitional regime before horizontal deformation becomes the dominant control of the CPO. The development of an initial sub-vertical CPO during upwelling, which must subsequently be overprinted by the new sub-horizontal CPO, can explain the larger inclination of the CPO bars along this pathline in comparison to those on the shallowest pathline in Figure 4.7a.

For $M^* = 10$, texture strength begins to saturate for the pathline with $z_f = -60 \text{ km}$ at a strain of $\varepsilon \approx 2$, however on other pathlines the CPO remains in a transient regime. By contrast, for $M^* = 125$, a steady-state texture is reached on all but the deepest pathline ($z_f = -156 \text{ km}$). The deepest pathline is unique because the olivine polycrystal enters the domain far enough from the ridge such that it does not experience significant texture development during its limited vertical motion. Again, texture is established on the $z_f = -60 \text{ km}$ pathline at a strain of $\varepsilon \approx 2$, and the final CPO vectors on both $z_f = -60 \text{ km}$ pathlines are the most similar. On this pathline, only the texture strength (and therefore also the amplitude of seismic anisotropy) depends on the deformation parameters.

Transient CPO, however, is a function of deformation history, and therefore sensitive to the value of M^* . For $M^* = 10$, texture strength undergoes near-linear evolution on all pathlines (Figure 4.7c), whereas for $M^* = 125$, evolution is more complex due to the response of the CPO to the upwelling flow. The horizontal distance from the start of the pathline to the ridge axis influences the amount of perturbation of the CPO texture at strains between ≈ 0.5 – 1.5 (panel d), after which texture strength tends to plateau at a value of about 0.53. Saturation of texture strength is in part caused by the GBS parameter, which prevents development of unphysically strong texture in the model. Furthermore, at a strain of ≈ 1.5 , the angle (measured from the horizontal axis) of the CPO vector changes rapidly for both of the pathlines that start within $x < 200 \text{ km}$ of the left boundary (Figure 4.7b). For the pathlines starting beyond $x = 200 \text{ km}$, by contrast, the CPO angle follows a shallow, near-linear trend after $\varepsilon \approx 0.5$. This demonstrates the complex relationship between CPO predicted by PyDRex and deformation history of the simulated polycrystals. Of particular relevance for seismic anisotropy studies is the observation that the expected evolution of local, transient CPO should be sensitive to relatively small changes in past deformation experienced hundreds of kilometres away from the probing location.

We also provide an example of this model executed via the Fluidity geodynamical modelling framework (Davies et al., 2011; Kramer et al., 2012), in which Lagrangian particles are advected forwards along the same pathlines. This comparison, the results of which are presented in Figure 7.4 and match those obtained in pure Python, demonstrates that PyDRex can be successfully coupled to a larger geodynamics framework to predict the evolution of texture

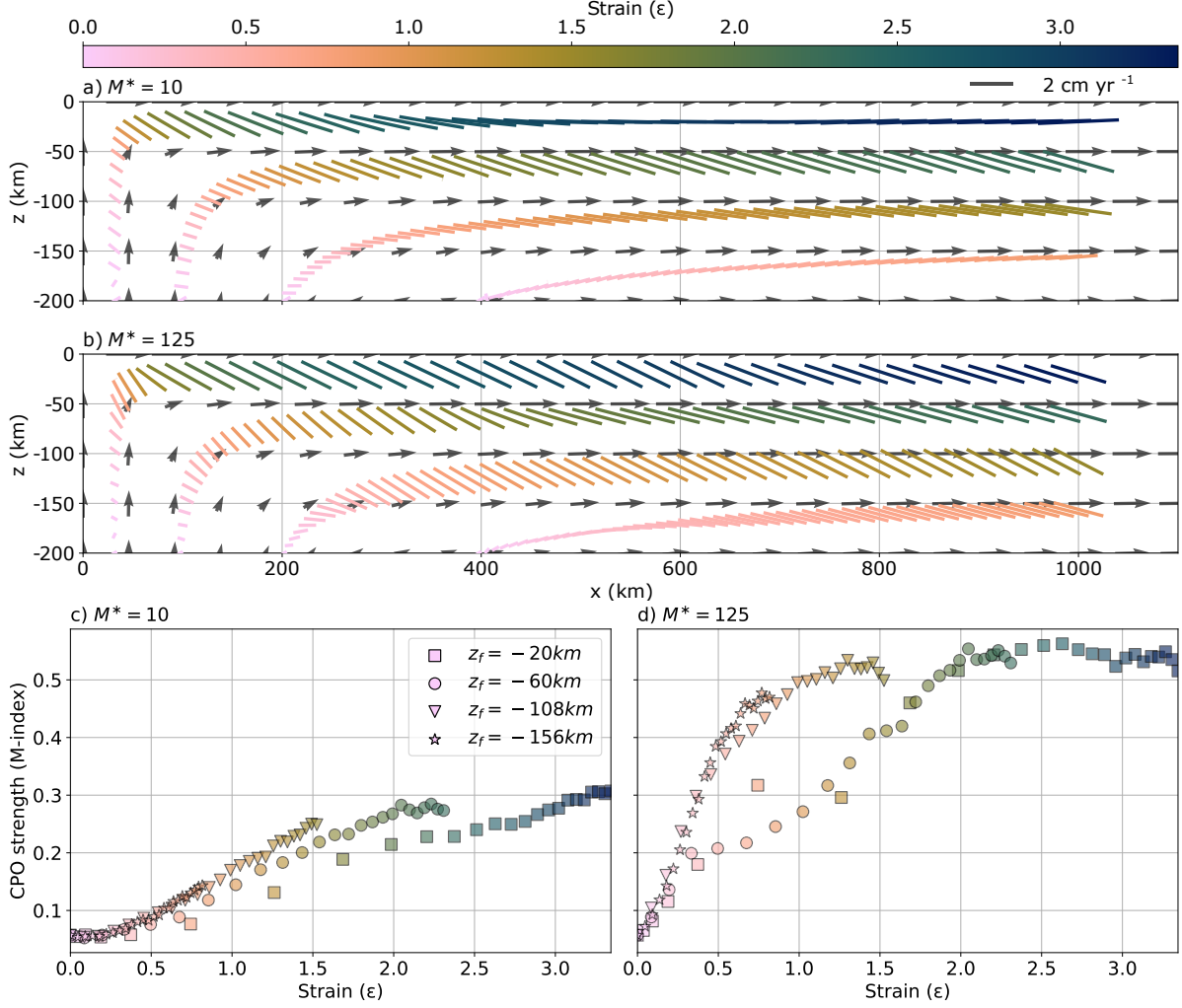


Figure 4.7: Texture evolution of A-type olivine in 2D corner flow from PyDRex. Panels (a) and (b) show the *Bingham average* of the orientations at each step (i.e. the olivine a-axis), for $M^* = 10$ and $M^* = 125$ respectively, plotted as bars at locations that follow pathlines. These CPO bars are scaled by the texture strength (*M-index*, Equation (3.22)); background arrows show the velocity field. Texture strength is plotted against accumulated strain in panels (c) and (d). The color of the markers corresponds to the position along the pathline, according to the color in panels (a) and (b). Unique marker symbols are used for each pathline; the value of z_f shown in the legend is the final vertical position on the pathline.

in more complex flows.

Whilst running these cornerflow models, we noticed that predictions of texture were affected by changes in the number of surrogate grains. For accurate CPO predictions, the texture evolution must be statistically resolved. In Chapter 5, we discuss a further benchmark that investigates the required number of surrogate grains for convergence of the numerical solutions to the D-Rex equations. We find that the CPO obtained from 5000 surrogate grains can consistently resolve some key transient features of polycrystal texture. Therefore, the result presented in Figure 4.7, as well as all further results presented in this section, are obtained from simulations using 5000 surrogate grains per polycrystal.

4.5 Changes in shear geometry and effects of enstatite CPO

The simulations presented so far all use steady-state flow regimes. However, the geometry of deformation may vary arbitrarily in the mantle, and it may, for example, evolve due to a sudden change in plate motion direction or the force balance dictating underlying mantle flow (e.g. Jones et al., 2017; Stotz et al., 2017; Torsvik et al., 2017; Iaffaldano et al., 2018). Fraters and Billen (2021) explored the effects of an instantaneous change in simple shear deformation geometry, and the next benchmark attempts to reproduce the behaviour demonstrated in Figure 5 of their study. We consider a polycrystal located in a 3D box at a point on the shear plane. The aggregate does not experience advective transport, but the velocity gradient drives rotation and deformation. Initially, the deformation plane is the X-Z plane, and the shear plane is the X-Y plane. At a later time, the shear geometry changes instantly so that the new deformation plane is the X-Y plane, and the new shear plane is the Y-Z plane. The simulation is run 500 times with 5000 surrogate grains, using $M^* = 125$ and $\lambda = 5$. Grain boundary sliding is enabled for surrogate grain sizes beneath the threshold of $f_{gs} = 0.3$.

Although anisotropy of peridotite aggregates will be dominated by the effects of olivine CPO, the presence of enstatite may also affect the overall CPO. Therefore, we use this benchmark to examine the evolution of both olivine and enstatite CPOs. As in Kaminski et al. (2004), we simulate enstatite rheology by ascribing enstatite grains a single slip system, (100)[001], on which dislocation creep is active. The CPOs of olivine and enstatite are tracked independently, and polycrystals for both mineral phases have the same number of surrogate grains. Figure 4.8a-c and j-l show results for control runs, where shear geometry does not change throughout the simulation. In the remaining panels, shear geometry changes once the indicated value of accumulated shear is reached. The rate of strain is constant in all simulations. For the results shown in Figure 4.8j, the imposed shear is always characterised by an X-Z deformation plane, and [100] vectors for both olivine and enstatite are swiftly rotated into this plane (before $\varepsilon \approx 0.25$). By contrast, results for the same shear in Figure 4.8k demonstrate that the identical [100] vectors take longer to rotate toward their steady-state orientations with respect to the X-Y shear plane. The corresponding symmetric result for shear characterised by an X-Y deformation plane is shown in Figure 4.8a and b.

As demonstrated in Figure 4.8, we observe that enstatite CPO evolves differently to olivine

CPO, in agreement with Fraters and Billen (2021). However, enstatite CPO in our simulations evolves more slowly, only beginning to reach a steady state by a strain of $\varepsilon \approx 2.2$. Considering that initial grain orientations are randomised for both olivine and enstatite, and that enstatite only has one active slip system in these implementations, it is plausible that fewer enstatite grains will be able to undergo plastic deformation, leading to slower texture evolution (and therefore lower texture strength). In Figure 4.8g and h, where the shear geometry is altered after half of the total strain accumulation, this slower texture evolution prevents reaching a steady-state enstatite CPO before the end of the simulation at $\varepsilon = 2.5$.

Texture strength, plotted in Figure 4.8c, f, i and l, was calculated after down-sampling the discrete orientation distribution from 5000 to 1000 surrogate grains. Computational requirements for the *M-index* calculations scale non-linearly with the number of surrogate grains, and down-sampling becomes unavoidable for high-resolution textures. Considering that the raw CPO outputs were captured for a population of 5000 surrogate grains, we do not expect this down-sampling procedure to result in significant loss of accuracy. Evolution of the texture strength in control runs, plotted in panels c and l, is nearly identical for olivine but not for enstatite. A truly isotropic enstatite aggregate should exhibit growth in texture strength that is independent of the imposed shear direction. We therefore suggest that 5000 surrogate grains may not even be sufficient for enstatite, which unlike olivine only has one particular slip system available, namely (100)[001]. The observed difference in *M-index* evolution for these two orientations of simple shear is not likely to be a function of the particular random state of the initial pseudo-isotropic orientation population, because we have used 500 distinct initialisation states in this case.

Inspection of Figure 4.8d-i reveals further characteristics of transient CPO texture in these simulations. After initial formation of CPO, demonstrated by the vanishing standard deviations (shaded regions) before $\varepsilon \approx 0.5$, the [100] vectors are already predominantly flattened into alignment with the initial deformation plane. When the shear geometry is changed, the mean axis of the CPO texture evolves towards the new steady state. The projected [100] angle measured from the original deformation plane, shown in Figure 4.8d and g, varies nearly linearly during this transient period, and standard deviations do not increase significantly, indicating that surrogate grains are rotating at similar rates. Angles of the [100] vectors from their projections in the new deformation plane, plotted in Figure 4.8e and h, show that the alignment perturbation in the X-Y plane lasts for $\varepsilon \approx 0.5$, under specified conditions. For olivine, maxima in the orientation perturbations displayed in panels e and h correspond to minima in texture strength (panels f and i), implying that the transient de-alignment caused by switching the shear plane would be difficult to detect for this geometry.

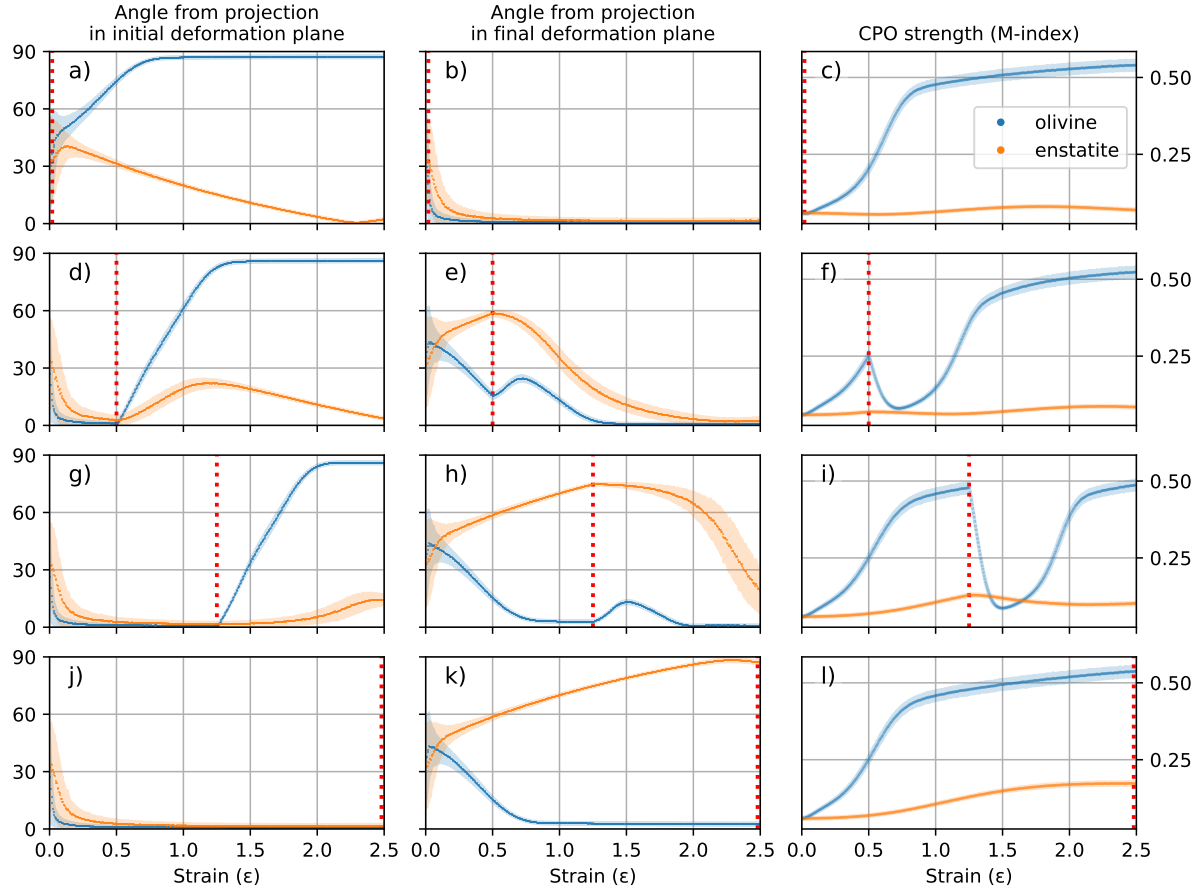


Figure 4.8: Angle in degrees (left and middle column) between a planar projection of the mean $[100]$ axis, calculated by *Bingham averaging*, and a reference vector, and texture strength quantified using the *M-index*. Blue (orange) traces show the angles for olivine (enstatite), which are averages of 500 model runs with distinct pseudo-isotropic initial states. Shaded areas are one standard deviation. In the left column, the angle is measured between the mean $[100]$ axis and its own projection onto the X-Z plane (initial deformation plane). In the middle column, the projection is instead performed onto the X-Y plane (final deformation plane). The change in shear direction occurs upon reaching the amount of strain indicated by the dotted red line. For the top row, the shear geometry is changed immediately, so the peridotites experience only the second shear. For the second and third rows, the geometry changes at a strain of 0.5 and 1.25, respectively. In the last row, the shear geometry is not changed and the peridotites experience only the first shear. General characteristics of these results agree with those shown in Figure 5 of Fraters and Billen (2021), although our enstatite texture evolves slower.

Similar results are presented in Figure 7.5, for a GBM parameter of $M^* = 10$ instead of $M^* = 125$ used here. In that case, neither olivine nor enstatite CPO reaches a new steady-state after the switch in shear orientation. The difference in texture strength for the control runs persists for enstatite and is additionally observed for olivine. Realignment of the mean angle in the initial deformation plane (X-Z) is no longer linear, instead displaying a diminishing rotation rate. Whilst the duration of transient texture strength is not significantly different in Figure 4.8f and i, the equivalent panels in Figure 7.5 demonstrate that this duration can depend on the amount of prior texture strength. However, the ability for existing texture to cause prolonged transient CPO seems to be restricted to weak textures ($M\text{-index} < 0.3$) and low GBM ($M^* = 10$).

5 Discussion

We provide a Python implementation of the D-Rex model, which can be used for rapid exploration of peridotite CPO using rectangular (2D) or orthopiped (3D) velocity meshes. Alternatively, the software allows for flexible simulation of peridotite texture evolution in any flow field by coupling to an existing geodynamical framework. Our review of the relevant theory and experiments highlights and clarifies the influence of dynamic recrystallisation mechanisms on kinematic texture evolution. In this section, we discuss the major implications of our investigation of the D-Rex model and outline the current limitations of the PyDRex software. Finally, we present plans for future PyDRex improvements, as well as potential applications, and discuss some avenues for advancement of kinematic CPO modelling in general.

5.1 Sensitivity to the number of surrogate grains

A possible source of confusion in the D-Rex literature is the use of the term “grains” to refer to orientation samples used to track texture evolution in the model. As we have highlighted, kinematic texture models do not track microstructures, instead using a simple discretisation of the medium into a fixed number of distinct elements which have some “size” (scalar statistical weight) and orientation. Each element interacts with the effective medium, which represents the averaged properties of all other elements. Importantly, the differences between these elements, which we have chosen to call “surrogate grains”, and more direct representations of physical grains prevent estimation of dimensional values for grain sizes from our results. The D-Rex model should be understood as providing an approximation of purely rheological behaviour, based on a surrogate discretisation of the crystallographic lattice.

For this reason, care must be taken when comparing the number of “grains” used in PyDRex simulations to the number of grains observed in experimental or natural peridotite aggregates, or indeed in “N-site” microphysics models, where grains have a defined spatial extent. Previous studies have often used 1000 surrogate grains or fewer for the kinematic texture discretisation (e.g. Lev & Hager, 2008; Faccenda & VanderBeek, 2023), which, according to our findings, is likely to result in significant stochastic variations in diagnostic outputs. These variations will be severe for simulations involving time-dependent strains. In all simulations presented thus far, we used 5000 surrogate grains: this was required for PyDRex to converge to a reproducible numerical solution for peridotite texture over time, especially if a large value is used for the grain boundary mobility parameter ($M^* \approx 125$), in line with the original calibration discussed in Kaminski and Ribe (2001).

This sensitivity is illustrated by the results presented in Figure 5.1, from a 2-D benchmark

case proposed by Lev and Hager (2008). For this case, velocity is defined by the equation

$$\mathbf{u} = \cos(\pi x/2) \sin(\pi z/2) \hat{\mathbf{x}} - \sin(\pi x/2) \cos(\pi z/2) \hat{\mathbf{z}}. \quad (5.1)$$

We compute CPO for a pure olivine polycrystal that follows the pathline shown in Figure 5.2. As in the corner flow case presented in Section 4.4, this velocity field incorporates dynamic pure shear contributions along the pathline. A sawtooth-like pattern is observed for the evolution of the smallest angle between the CPO axis (calculated using *Bingham averaging*) and the local velocity vector. However, a protracted period of misalignment occurs at strains of $\varepsilon \approx 5-6$ ($M^* = 125$), which is not captured for fewer than 5000 surrogate grains. Furthermore, as shown in Figure 5.1, the misalignment angle does not, on average, fall below 5° at strains around $\varepsilon \approx 3.8$ for 1000 surrogate grains, and the associated error based on 500 repeated runs remains significant.

Further evidence is provided by analysing $\log_{10}(\bar{S})$, where $\bar{S}$ is the maximum normalised grain size, which varies as the CPO evolves. Grain sizes are normalised to the initial maximum grain size, which takes a value of 1. For this model, using $M^* = 125$, the minima in $\log_{10}(\bar{S})$ at strains of $\varepsilon \approx 3.7$ and $\varepsilon \approx 5.6$ are not well resolved for fewer than 5000 surrogate grains, as shown in Figure 5.1. Ensemble standard deviations overlap throughout for 5000 and 10000 surrogate grains (this is not true for cases with < 5000 surrogate grains), and do not decrease significantly from 5000 to 10000 surrogate grains. This implies that a minimum of 5000 surrogate grains are likely required to resolve CPO evolution when starting from an isotropic texture and using $M^* = 125$.

We have also investigated this benchmark using $M^* = 10$, in which case the sensitivity to the number of grains reduces. However, differences in the maximum normalised grain size remain clearly visible (on a logarithmic scale) in Figure 5.1 until 5000 surrogate grains. We note that convergence of the numerical solution is simultaneously affected by the number of timesteps along a pathline, which determines the temporal resolution of local changes in velocity gradients. Detailed analysis of this dependence is not presented here, as we have found stronger texture sensitivity to the number of surrogate grains and the GBM parameter M^* .

5.2 Dominance of a few large grains

In general, we find that CPO computed using PyDRex quickly becomes dominated by a few surrogate grains ($< 1\%$ of the total number) of very large size. Most remaining surrogate grains fall below the GBS threshold and therefore do not contribute to CPO evolution. This can be interpreted as a significant increase in homogeneity of the crystallographic lattice orientations of the real, physical grains in the polycrystal. Whilst such homogeneous lattice orientations are eventually required for shear-aligned CPO to form, the resolution (in strain increments) of current experimental results does not allow us to assess whether the speed of this process is physically sensible in PyDRex. Experiments generally demonstrate a decrease in the average grain size in strained rocks (e.g. Bystricky et al., 2000), partly because nucleated grains tend to be orders of magnitude smaller than their parents (e.g. Zhang et al., 2000). This behaviour is qualitatively similar in PyDRex, where the distribution of surrogate grain sizes,

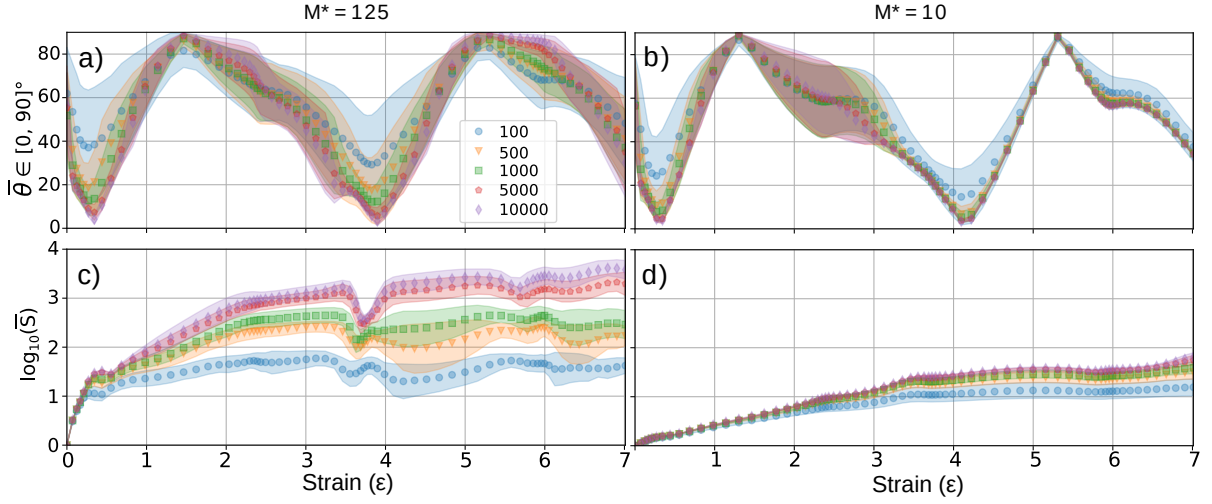


Figure 5.1: Ensemble results for the 2D cell geometry showing mean CPO angle relative to local velocity vector (a & b) and $\log_{10}(\bar{S})$, where $\bar{S}$ is the maximum normalised (non-dimensional) grain size (c & d). For example, a value of 3 indicates that the maximum grain size has increased by 3 orders of magnitude. Polycrystals follow the pathline shown in Figure 5.2, which also shows snapshots of the full grain size distribution. Markers are ensemble averages, colored according to the number of surrogate grains, and shaded areas depict one standard deviation, based on 500 runs with different randomised state of the initial grain orientations. Due to the lower value of M^* , the minima in CPO angle relative to local velocity vector in panel b is delayed (relative to that in panel a) until $\epsilon \approx 4.1$. Furthermore, the maximum surrogate grain size in panel d only grows to less than 100 times its original size, compared to the more than 1000 times increase in maximum surrogate grain size observed in panel c.

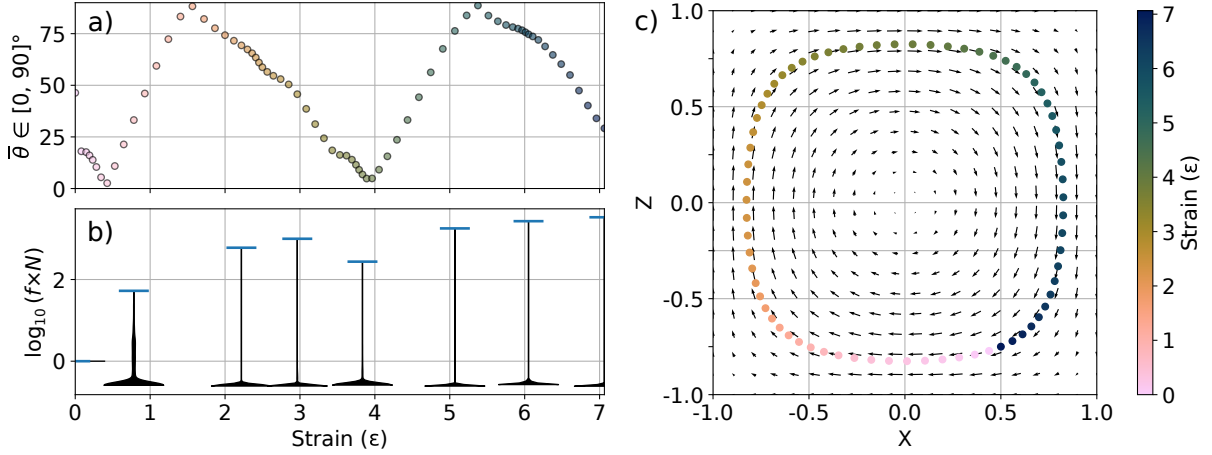


Figure 5.2: CPO angles compared to the local velocity vector (a), grain size distributions (b), and velocity field and pathline (c) for a 2D convecting cell simulation. The $\log_{10}$ normalisation method for grain sizes means that surrogate grains that are larger than their original size are represented as a positive value, whereas those that have shrunk are represented as a negative value. All original surrogate grains have a size of 1. The CPO misalignment follows a sawtooth-like pattern with some periods of protracted misalignment. Grain sizes become significantly heterogeneous before $\epsilon = 1$, so that the CPO is dominated by few surrogate grains which are more than 50 times their original size. Blue horizontal lines show the maximum grain size for the plotted snapshots, which is the value used in Figure 5.1c. Model parameters are identical to those used in Figure 4.7.

shown by the violin plots in Figure 5.2b, demonstrates rapid evolution towards a large number of small surrogate grains (bulge below 0) and a small number of large surrogate grains (thin, long neck).

The maximum grain size in PyDRex also provides a sense of texture strength; however our investigation indicates that it does not stabilise until extreme strains ($\epsilon > 10$). Nevertheless, it may be preferable in some situations, in particular sensitivity tests, because computation of the more robust *M-index* requires significant additional computational resources.

5.3 Non-linearity in depth dependence of CPO and importance of constraining M^*

Our 2D corner flow results (Figure 4.7) are characterised by non-linear changes in CPO with depth. Non-linear and complex patterns of CPO in such ostensibly simple flow regimes have been reported previously, for example using a similar corner flow model in a 2D rectangular box (Kaminski et al., 2004) or in a 2D quarter-annulus domain (Kendall et al., 2022). Such patterns result from the dependence of CPO on deformation history. In our 2D corner flow model, peridotite crystals experience different relative contributions of vertical and horizontal shear during their advection. Coupled with the fact that the three olivine slip systems allow different relative slip activities, this leads to the observed non-linearity. Further exploration of mantle flow regimes with time-varying strain geometry are required to fully characterise the

range of expected behaviours. Due to the significant differences in results obtained using $M^* = 10$ and $M^* = 125$, further calibration of this parameter using comprehensive comparisons against experimental and natural samples or seismic observations from, for example, shear-wave splitting analyses is important for the convergence of numerical modelling efforts.

5.4 Clarification of the effects of deformation history

The results shown in Figure 4.8 give some insight into the responses of olivine and enstatite phases to changes in shear direction. A strain of $\varepsilon \approx 0.75$ is required to generate a shear-aligned olivine texture (for $M^* = 125$ and assuming an isotropic initial texture). We note that under these conditions, this strain seems to be independent of whether grain orientations are initially random or already aligned to the previous shear direction (oriented 90° away from the new one). The duration of the transient olivine texture in panels a, d, and g of Figure 4.8 is similar, implying that rotation of an existing texture is quicker than forming a shear-aligned CPO from an isotropic initial configuration. By contrast, laboratory studies have suggested that pre-existing texture can induce protracted durations of transient CPO (e.g. Hansen et al., 2014; Boneh et al., 2015). In our numerical results, we observe that the duration of transient CPO, in particular CPO strength quantified by the *M-index*, can be prolonged by the presence of prior texture for low GBM activity (Figure 7.5), i.e. when using a value of $M^* = 10$, but not for $M^* = 125$. The characteristics of our results are most similar to those of natural samples analysed in Warren et al. (2008): CPO re-alignment is rapid, however changes in deformation geometry result in weak textures of transient strength.

The duration of transient CPO textures in olivine and, more generally, peridotite polycrystals requires further investigation and is significantly affected by the mobility of grain boundaries in these rocks (i.e. M^*). Furthermore, the instantaneous change employed in the simulation analysed in Figure 4.8 is an extreme end-member for how the flow regime likely evolves in the mantle. By coupling PyDRex to geodynamic frameworks that enable more sophisticated flow modelling, we anticipate that it will be possible to investigate CPO evolution under a wider range of relevant mantle flow settings, for example with both sudden and more gradual changes in plate motion directions and magnitudes (e.g. Iaffaldano & Bunge, 2015; Jones et al., 2017).

5.5 Limitations and anticipated advancements of kinematic CPO modelling

Currently, kinematic CPO models such as D-Rex and PyDRex, provide some of the most computationally efficient methods for simulating CPO generation and development in seismically relevant volumes of strained mantle peridotites. PyDRex is primarily controlled by a few parameters that allow for approximating the behaviour of dynamic recrystallisation and plastic deformation mechanisms based on empirical calibration. However, these parameters are difficult to constrain using currently available data from either experimental rock deformation or analysis of naturally deformed peridotite samples. Dynamic recrystallisation mechanisms,

in particular, are varied and complex, and there are no complete analytical models that capture their behaviour. Accordingly, when using PyDRex, or other D-Rex models, to predict CPO in the upper mantle, it is especially important to consider the implications of choosing a particular GBM parameter (M^*), which significantly influences results.

One limitation that is unique to current D-Rex-based models is the inability to separate relict and recrystallised grain populations in simulation outputs. Such separation could allow for more detailed comparisons with deformation experiments and further opportunity to refine key model parameters. We believe that this feature could be implemented using a similar technique as introduced by Signorelli and Tommasi (2015) for their modified VPSC models: instead of assuming that nucleated subgrains contribute to growth of the parent grain, it should be possible to track an additional population of recrystallised grains whose initial size is set to zero. Nucleation events, triggered by large residuals in dislocation density of individual grains compared to the polycrystal average, would involve prescribing a nonzero size to one of these extra grains. The parent grain would also need to decrease in size by the same amount. Overall, these changes would mostly be restricted to Equation (3.17).

The initial distribution of grain orientations is another important factor which influences CPO evolution (Boneh et al., 2015). At present, PyDRex uses a uniform distribution of grain orientations as the initial condition by default. This distribution is created by random sampling from normal distributions that cover the orientation space. However, it may be possible to reduce the number of surrogate grains required for numerical convergence by employing specialised distributions that can approximate an isotropic condition with fewer samples (e.g. Yershova et al., 2009). To further explore the effects of initial texture, the uniform axis random spin (“UARS”) spherical distributions introduced by Bingham et al. (2009) could prove useful, as these allow for compact description of non-uniform textures such as point maxima and girdles.

For simulations that use random initial orientations provided by normal distribution sampling, we recommend using 5000 surrogate grains for D-Rex-based simulations, which will ensure that outputs are reproducible and only minimally affected by stochastic properties of the initial simulation state. However, this makes computation of output diagnostics significantly more expensive (e.g. texture strength M -index), which necessitates prior down-sampling of the raw outputs.

PyDRex currently only considers dislocation creep and not other deformation mechanisms, such as diffusion creep. Upper-mantle deformation is likely accommodated by a composite dislocation and diffusion creep rheology (e.g. Karato, 2008; Garel et al., 2014; Garel et al., 2020). Future work could investigate the introduction of composite deformation mechanisms, as found in some previous D-Rex implementations (e.g. Faccenda & Capitanio, 2013; Hedjazian et al., 2017). This could potentially include alternative methods for influencing texture, as some studies suggest that even diffusive mechanisms can introduce predictable changes to CPO (e.g. Miyazaki et al., 2013).

The results presented in this thesis are limited to A-type olivine and enstatite. However, depending on the combination of CRSS values expected for the four slip systems of olivine, different plastic deformation behaviour and steady-state CPO is expected (e.g. Karato et al., 2008). These alternative “fabrics” become particularly important in upper mantle regions of high water content or stress (e.g. Jung & Karato, 2001; Katayama et al., 2004). Changing the

5 *Discussion*

CRSS values is trivially achieved in PyDRex, and these may be updated at any point during the simulation by modifying the relevant members of the tracked Python objects. Future work could perform further calibration of PyDRex using experimental results for other olivine fabrics.

6 Conclusions

We have presented a revised implementation of the D-Rex model written in Python, called PyDRex. Whilst reviewing the theory underpinning the model, we have clarified the effects of recrystallisation on polycrystal texture and demonstrated that the CPO direction obtained by *Bingham averaging* of kinematic CPO model outputs is distinct from the long axis of the FSE at large strain (regardless of the inclusion of dynamic recrystallisation effects). PyDRex CPO predictions have been validated against analytical, experimental and benchmark cases. Through a suite of systematic tests, which are included in the associated PyDRex software package, we demonstrate that PyDRex outputs (i) reproduce expected theoretical CPO results for A-type olivine in simple shear, (ii) are able to match general CPO characteristics of experimentally and naturally deformed A-type olivine samples, and (iii) are similar to the outputs of previous D-Rex model adaptations. Our numerical results suggest that the sensitivity of peridotite CPO to deformation history is a function of the grain boundary mobility, controlled by the M^* parameter. High values (e.g. $M^* = 125$) allow the simulated textures of peridotite aggregates to adapt quickly to changing shear geometry, whereas low values (e.g. $M^* = 10$) lead to a stronger dependence on deformation history. CPO strength in particular, quantified using the *M-index*, demonstrates protracted periods of transient evolution.

It is difficult to constrain M^* using currently available experimental data, and values used in the literature (1–200) vary by two orders of magnitude (e.g. Kaminski & Ribe, 2001; Lev & Hager, 2008; Faccenda & Capitanio, 2013; Boneh et al., 2015; Fraters & Billen, 2021; Faccenda & VanderBeek, 2023). Due to the substantial influence of this parameter on CPO predictions, we suggest testing a range of values and exercising caution during model comparisons. Furthermore, our results suggest that resolving transient CPO textures requires a larger number of grains (5000), especially for high- M^* simulations, than has been used in most previous publications. On the other hand, for low- M^* simulations, large portions of the simulation domain may be characterised by transient CPO for long durations, leading to complex CPO patterns, and therefore non-trivial seismic anisotropy characteristics.

Results of kinematic CPO simulations from PyDRex can be used to corroborate both seismological and microphysical observations. By understanding plausible distributions of peridotite CPO for idealised mantle flow models, seismological studies of upper mantle anisotropy will be able to curb non-uniqueness in inferences about mantle dynamics and structure. Furthermore, in-situ observation of slip activity and dynamic recrystallisation intensity in microphysical deformation experiments is often challenging, and may similarly benefit from numerical comparisons.

7 Supplementary Material

7.1 Analytical single crystal D-Rex rotation rates for A-type olivine

Analytical expressions for single crystal DRex rotation rates were derived for the case of A-type olivine. Derivation for other olivine fabric types (e.g. Karato et al., 2008; Long & Becker, 2010) follows the same approach and will not be included here. These analytical expressions were used to validate the plastic deformation routines of our PyDRex implementation.

In the following derivations, some common definitions will be referenced. DRex allows four slip systems of olivine, which by convention are ordered as follows:

$$(010)[100] \quad (7.1)$$

$$(001)[100] \quad (7.2)$$

$$(010)[001] \quad (7.3)$$

$$(100)[001] \quad (7.4)$$

Each slip system is associated with a particular normalised critical resolved shear stress (CRSS) value. The mapping of CRSS values to slip systems is characteristic of the olivine fabric. For A-type fabric, the CRSS values τ^* are

$$1 \quad (7.5)$$

$$2 \quad (7.6)$$

$$3 \quad (7.7)$$

$$\infty \quad (7.8)$$

The permutation symbol ε , with dimensions indexed by i, j and k , is also employed:

$$\varepsilon_{ijk} = \begin{cases} +1 & \text{if } (i, j, k) \text{ is } (1, 2, 3), (2, 3, 1), \text{ or } (3, 1, 2), \\ -1 & \text{if } (i, j, k) \text{ is } (3, 2, 1), (1, 3, 2), \text{ or } (2, 1, 3), \\ 0 & \text{if } i = j, \text{ or } j = k, \text{ or } k = i \end{cases} \quad (7.9)$$

7.1.1 Simple shear $\partial v / \partial x$ with slip on (010)[100]

Consider a simple shear defined by the velocity gradient

$$L = \begin{bmatrix} 0 & 0 & 0 \\ 2D_0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (7.10)$$

7 Supplementary Material

with the only non-zero component as $\partial v / \partial x$ for v the velocity in the positive Y direction. The deformation rate is D_0 and the initial crystal lattice rotation around the Z-axis is

$$\mathbf{a} = \begin{bmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (7.11)$$

The first step in deriving the rotation rate due to dislocation glide is to extract the slip system vectors for all four allowed olivine slip systems from the orientation matrix $\mathbf{a}$, where the angle θ is measured counter-clockwise from the positive X-axis. This is done by taking the products $\mathbf{a}\tilde{\mathbf{n}}^s$ and $\mathbf{a}\tilde{\mathbf{l}}^s$, where $\tilde{\mathbf{n}}^s$ and $\tilde{\mathbf{l}}^s$ are the slip plane normal and slip direction vector for the s -th slip system in the reference frame, respectively. The slip normals and directions are given as values enclosed in parentheses and square brackets in equations (7.1) to (7.4), respectively. This yields the slip system normals and directions in the rotated (grain-local) frame:

$$\mathbf{n}^1 = \begin{bmatrix} -\sin \theta \\ \cos \theta \\ 0 \end{bmatrix} \quad \mathbf{l}^1 = \begin{bmatrix} \cos \theta \\ \sin \theta \\ 0 \end{bmatrix} \quad (7.12)$$

$$\mathbf{n}^2 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \quad \mathbf{l}^2 = \mathbf{l}^1 \quad (7.13)$$

$$\mathbf{n}^3 = \mathbf{n}^1 \quad \mathbf{l}^3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \quad (7.14)$$

$$\mathbf{n}^4 = \begin{bmatrix} \cos \theta \\ \sin \theta \\ 0 \end{bmatrix} \quad \mathbf{l}^4 = \mathbf{l}^3 \quad (7.15)$$

where the superscript s is not an exponent, but rather denotes the slip system.

The strain rate invariants (“slip invariants”) for each slip system can now be computed according to

$$I^s = l_i^s n_j^s D_{ij} = l_i^s n_j^s \cdot \frac{1}{2} (L_{ij} + L_{ji}) \quad (7.16)$$

In this case,

$$I^1 = D_0 (\cos^2 \theta - \sin^2 \theta), \quad I^2 = I^3 = I^4 = 0 \quad (7.17)$$

The slip system activities are proportional to the ratio of slip invariants to CRSS values. For A-type olivine, CRSS values are given in equations (7.5) to (7.8). In this case, only a single system will be active, which is unsurprising as the crystal is only experiencing a simple shear in one direction. The general formula for slip activities is

$$\beta_s = \frac{\tau_R^* I_s}{\tau_s^* I_R} \left| \frac{\tau_R^* I_s}{\tau_s^* I_R} \right|^{n-1} \quad (7.18)$$

where once again s is the slip system index, n is a model parameter that defines the power law relationship between shear stress and slip activity, τ_s^* and I_s are the CRSS value and slip

invariant value, respectively, for the s -th slip system, and the reference system $s = R$ is chosen so that $\left| \frac{L_R}{\tau_R^*} \right| \geq \left| \frac{L_s}{\tau_s^*} \right|$. Here, since only one system is active, we simply have $\beta = 1$ for that system.

Having determined the slip activities, it is now possible to construct the “slip tensor”, G , which encodes the geometry of plastic deformation of the grain. The equation is

$$G_{ij} = 2 \sum_s \beta^s l_i^s n_j^s \quad (7.19)$$

where the superscript s is once again an index not an exponent. Continuing our example, we determine that

$$G = 2 \cdot \begin{bmatrix} -\cos \theta \sin \theta & \cos^2 \theta & 0 \\ -\sin^2 \theta & \sin \theta \cos \theta & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (7.20)$$

Next, the slip rate factor γ [not to be confused with the finite strain measure $\gamma = \tan^{-1}(\alpha)$] is computed, according to

$$\gamma = \sum_k \sum_n \frac{2G_{ij}L_{ij} - (L_{k,k+1} - L_{k+1,k})(G_{k,k+1} - G_{k+1,k})}{2G_{lm}G_{lm} - (G_{n,n+1} - G_{n+1,n})^2} \quad (7.21)$$

which for this example yields

$$\gamma = \frac{-8 \sin^2 \theta D_0 + 4D_0}{8 - 4} = (-2 \sin^2 \theta + 1) D_0 = D_0 \cos 2\theta \quad (7.22)$$

The rate of rotation of the crystallographic axes is given by a vector with components

$$\omega_i = \frac{(L_{i+2,i+1} - L_{i+1,i+2}) - \gamma(G_{i+2,i+1} - G_{i+1,i+2})}{2} \quad (7.23)$$

which in this case only has one nonzero component

$$\omega_3 = \frac{2D_0 - 0 - D_0 \cos 2\theta \cdot 2(-\sin^2 \theta - \cos^2 \theta)}{2} = (1 + \cos 2\theta) D_0 \quad (7.24)$$

Finally, the updated orientation matrix is obtained from

$$\partial_{t^*} a_{ij} = \varepsilon_{jkl} a_{il} \omega_k \quad (7.25)$$

where ε_{ijk} are the components of the permutation symbol given in equation (7.9). This operation can optionally be split into computation of $\varepsilon_{ikj} \omega_k$ followed by $\omega^\top \mathbf{a}$. The result is

$$D_0(1 + \cos 2\theta) \cdot \begin{bmatrix} \sin \theta & \cos \theta & 0 \\ -\cos \theta & \sin \theta & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (7.26)$$

7.1.2 Other slip systems

The rotation rate and updated orientations for other shear and slip system configurations can be similarly derived. These examples cover the remaining slip systems of olivine that are allowed to be active in the original code.

Simple shear $\partial u/\partial z$, for velocity u in the positive X direction, with slip on (001)[100], produced by the setup

$$L = \begin{bmatrix} 0 & 0 & 2D_0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{a} = \begin{bmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{bmatrix} \quad (7.27)$$

leads to the rotation rate

$$\omega_2 = (1 - \cos 2\theta) D_0 \quad (7.28)$$

and new orientations given by

$$D_0 (1 - \cos 2\theta) \begin{bmatrix} \sin \theta & 0 & -\cos \theta \\ 0 & 0 & 0 \\ \cos \theta & 0 & \sin \theta \end{bmatrix} \quad (7.29)$$

Simple shear $\partial v/\partial z$ with slip on (010)[001], produced by the setup

$$L = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 2D_0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{a} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{bmatrix} \quad (7.30)$$

leads to the rotation rate

$$\omega_1 = (-1 - \cos 2\theta) D_0 \quad (7.31)$$

and new orientations given by

$$D_0(1 + \cos 2\theta) \cdot \begin{bmatrix} 0 & 0 & 0 \\ 0 & -\sin \theta & -\cos \theta \\ 0 & \cos \theta & -\sin \theta \end{bmatrix} \quad (7.32)$$

Note that the fourth slip system can never activate for simple shear due to the CRSS value of ∞ . These default CRSS values assume that the fourth system merely facilitates dislocation climb or other auxiliary mechanisms and does not contribute to dislocation glide in the olivine crystals.

7.2 Analytical single crystal D-Rex rotation rates for enstatite

Although more recent studies, such as Bernard et al. (2021), have demonstrated that orthopyroxenes may exhibit a range of rheological fabrics like olivine, the original DRex model

(and current PyDRex implementation) only considers a single type of enstatite fabric, which would be classified by those authors as the enstatite-AB type. This enstatite fabric responds to stress by plastic deformation on the (100)[001] slip system.

With a macroscopic initial condition given by Equation (7.27), the $\mathbf{n}$ and $\mathbf{l}$ vectors for the (100)[001] system are

$$\mathbf{n} = \begin{bmatrix} \cos \theta \\ 0 \\ -\sin \theta \end{bmatrix}, \quad \mathbf{l} = \begin{bmatrix} \sin \theta \\ 0 \\ \cos \theta \end{bmatrix} \quad (7.33)$$

and using Equation (7.16), $I = D_0 (\cos^2 \theta - \sin^2 \theta)$. Since only one slip system is active, the normalised activity is $\beta = 1$. The slip tensor is found using Equation (7.19),

$$\mathbf{G} = 2 \cdot \begin{bmatrix} \cos \theta \sin \theta & 0 & -\sin^2 \theta \\ 0 & 0 & 0 \\ \cos^2 \theta & 0 & -\sin \theta \cos \theta \end{bmatrix} \quad (7.34)$$

The slip rate is calculated according to Equation (7.21), which yields

$$\gamma = \frac{-8 \sin^2 \theta D_0 + 4D_0}{8 - 4} = (-2 \sin^2 \theta + 1) D_0 = D_0 \cos 2\theta \quad (7.35)$$

Next, the rate of rotation of the crystallographic axes is found from Equation (7.23) to be

$$\omega_2 = (1 - \cos 2\theta) D_0 \quad (7.36)$$

Leading to new orientations which are identical to Equation (7.29).

For enstatite crystals oriented orthogonal to the plane of deformation in any simple shear, this system cannot activate and therefore AB-type enstatite does not undergo plastic deformation, and only rotates passively with the flow.

7.3 Derivation of the FSE long axis in simple shear

The finite strain ellipsoid is a macroscopic measure of deformation. It is defined by three axes, which evolve as a function of the shear.

Consider a simple shear imposed by the velocity gradient from equation (7.10). The deformation gradient tensor $\mathbf{F}$ is

$$\mathbf{F} = \mathbf{I} + t\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 \\ 2D_0 t & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (7.37)$$

Therefore the left stretch (“Cauchy-Green”) tensor $\mathbf{B}$ is

$$\mathbf{B} = \mathbf{F}\mathbf{F}^T = \begin{bmatrix} 1 & 2D_0 t & 0 \\ 2D_0 t & 4D_0^2 t^2 + 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (7.38)$$

and the eigenvalues are found by evaluating the determinant and solving

$$\begin{vmatrix} 1 - \lambda & 2D_0t & 0 \\ 2D_0t & 4D_0^2t^2 - \lambda & 0 \\ 0 & 0 & 1 - \lambda \end{vmatrix} = 0 \quad (7.39)$$

which yields

$$(1 - \lambda) [(1 - \lambda)(4D_0^2t^2 - \lambda) - 4D_0^2t^2] = 0 \quad (7.40)$$

$$\equiv -\lambda^3 + \lambda^2(4D_0^2t^2 + 2) - \lambda(4D_0^2t^2 + 1) = 0 \quad (7.41)$$

This cubic equation has three distinct roots which are

$$\lambda_1 = 1 \quad (7.42)$$

$$\lambda_2 = -2D_0t\sqrt{D_0t + 1} + 2D_0t + 1 \quad (7.43)$$

$$\lambda_3 = 2D_0t\sqrt{D_0t + 1} + 2D_0t + 1 \quad (7.44)$$

The corresponding eigenvectors are found to be

$$\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ D_0t - \sqrt{D_0^2t^2 + 1} \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 1 \\ D_0t + \sqrt{D_0^2t^2 + 1} \\ 0 \end{bmatrix} \quad (7.45)$$

of which the last describes the long axis of the finite strain ellipsoid.

Note that some authors define the finite strain ellipsoid (FSE) in terms of the *right* stretch (“Cauchy-Green”) tensor $C = F^\top F$, e.g. in Appendix B of Kaminski et al. (2004). This formulation results in an FSE that visualises the forthcoming deformation, instead of the last experienced deformation. If F is the deformation gradient defined, as we have done here, using the Eulerian velocity gradients L readily obtained from fluid dynamics solvers, then B measures strain with respect to the global Eulerian frame, which facilitates simple comparisons with the direction of shear defined in the same frame. In any case, both B and C are symmetric and positive-definite and measure only strain, which means they offer no information about the rigid body rotation of the particle.

7.4 Numerical rotation and growth rates for A-type olivine

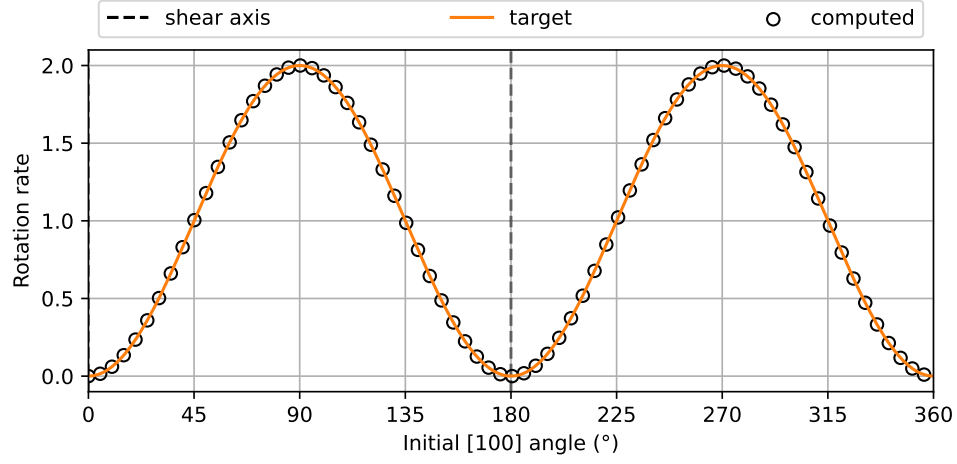
This section contains some auxiliary test results for A-type olivine in simple shear. Outputs are produced by PyDRex and can be reproduced using the PyDRex test suite.

7.4.1 Single crystal rotation rates

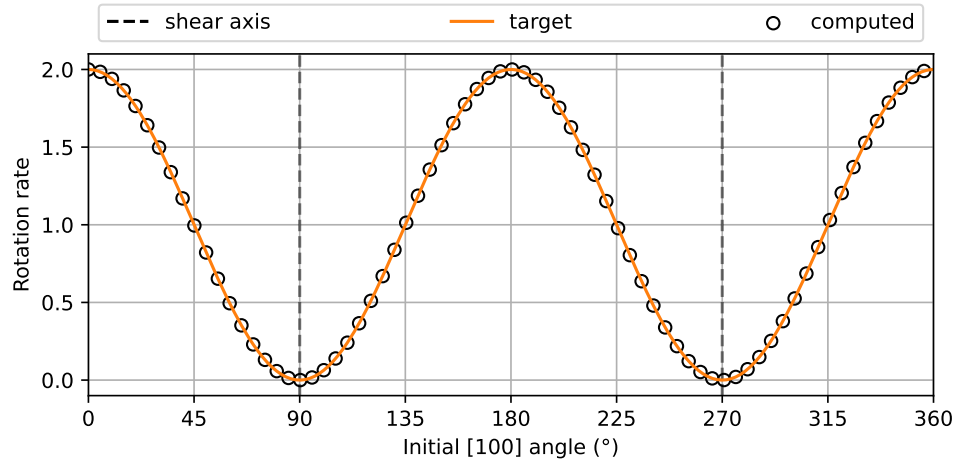
The numerical rotation rates for a single crystal of A-type olivine deforming on the (010)[100] system is presented in the main text. Here, we show that the rotation rates for the three

remaining slip systems of olivine follow the theoretical predictions (for the A-type case). Our test suite also checks for activation of the expected slip systems in these cases. These are the simplest validation checks of the PyDRex code and can be run on a personal computer.

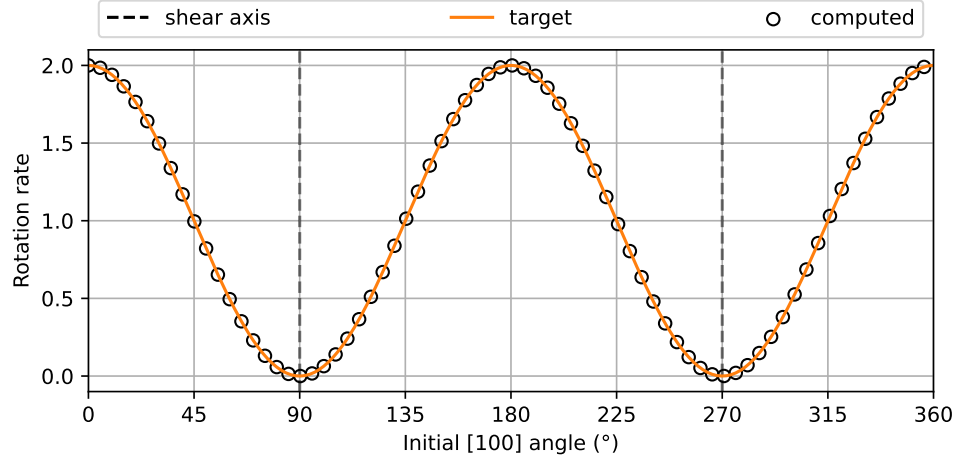
7 Supplementary Material



(a) slip on (010)[100]



(b) slip on (001)[100]



(c) slip on (010)[001]

Figure 7.1: Numerical rotation rates (empty circles) for a single crystal of A-type olivine deforming via dislocation creep in simple shear with (a) $L_{13} = 2D_0$, (b) $L_{31} = 2D_0$, (c) $L_{23} = 2D_0$ for D_0 the largest eigenvalue of the rate-of-deformation tensor. The initial [100] angle is measured from the shear axis in the shear plane. Computed values follow the theoretical relationships derived in Section 7.2. The rotation rate, like the strain rate, is measured per unit time.

7.4.2 Rotation and growth rates for an ideal girdle in the shear plane

A similar benchmark, for the case of a polycrystal exhibiting an ideal girdle texture in the *deformation plane*, is presented in the main text, where our geometrical terminology is also clarified. For completeness, we include here the result of an equivalent test run for an initial texture that is girdled in the shear plane, for which we do not derive analytical results (the activation of an additional slip plane makes analytical calculation rather tedious in this case). Note the somewhat unintuitive result that (surrogate) grains whose $[100]$ vectors lie in or near the shear plane will align more quickly towards the shear direction compared to those whose $[100]$ vectors lie in or near the deformation plane.

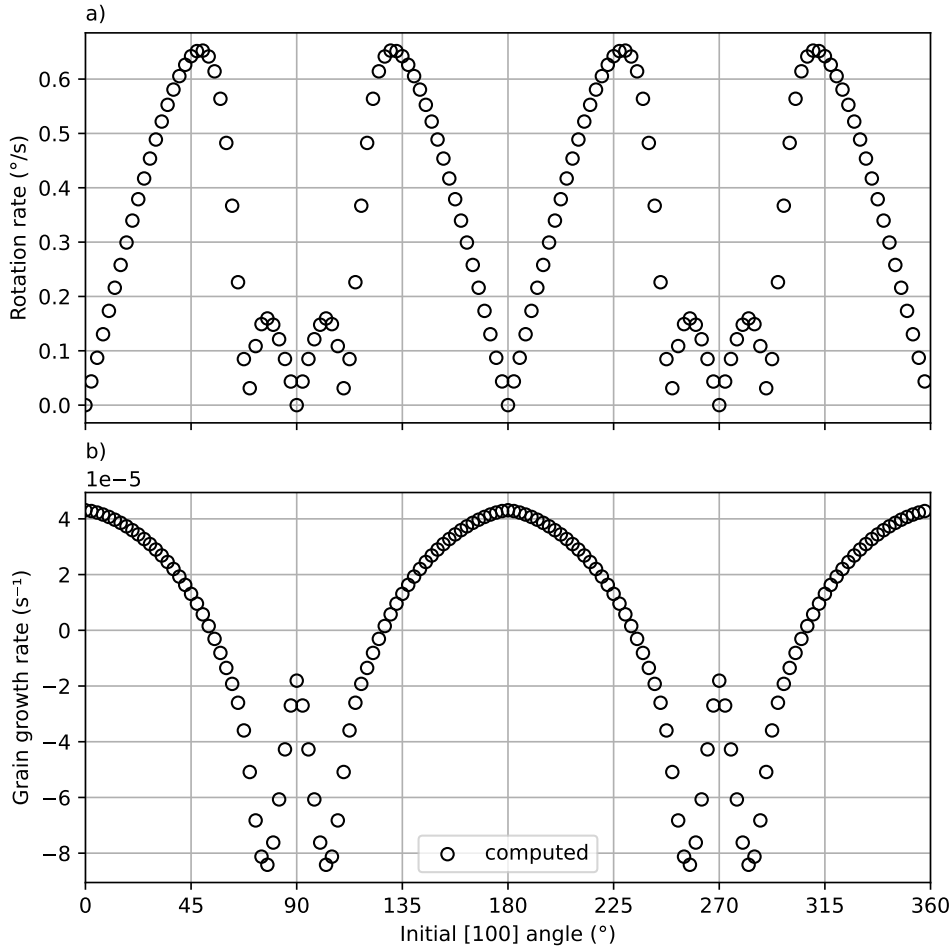


Figure 7.2: Numerical rotation rates (a) and grain growth rates (b) for an A-type olivine polycrystal, with an ideal girdle texture in the shear plane. Compared to the equivalent values computed for an ideal girdle texture in the deformation plane (presented in the main text), the evolution of crystallographic preferred orientation (CPO) is more complex due to activation of a second slip system. Rotation rate and grain growth are measured in units of inverse time.

7.5 Comparison of PyDRex ensemble outputs and Fortran 90 D-Rex outputs

In this section we compare crystallographic preferred orientation (CPO) computed with PyDRex to that computed with core Fortran 90 D-Rex routines adapted (no more than necessary) from the original implementation (Kaminski & Ribe, 2001; Kaminski et al., 2004). The main change to the Fortran code was removal of the pathline solver, and setting up the main loop such that simulated polycrystals experience simple shear deformation without moving through the prescribed flow. This removes any spurious discrepancies in output that could arise due to differences in pathline solvers, meshing techniques, or similar.

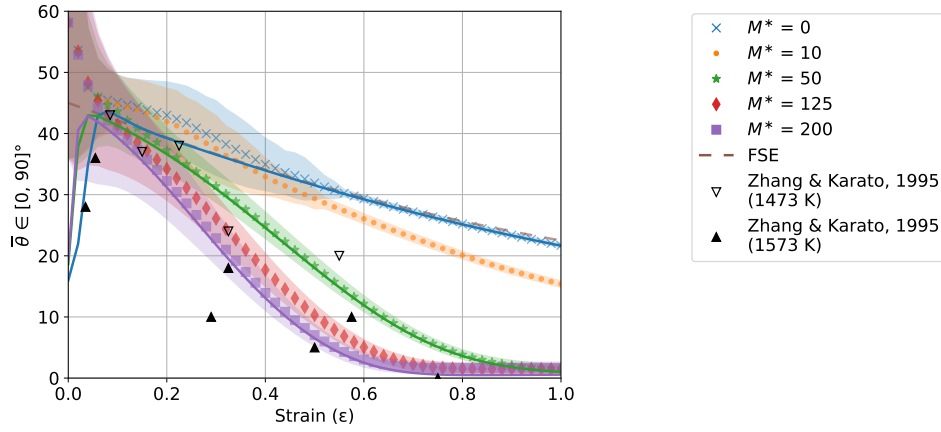


Figure 7.3: A-type olivine CPO results for a stationary polycrystal experiencing 2D simple shear. Both Fortran 90 outputs (solid lines) and PyDRex outputs (markers) are calculated as an average of 500 model runs with unique stochastic distributions of initial surrogate grain orientations. Shaded regions illustrate standard deviations of the PyDRex ensembles. Triangles are plotted at the location of CPO angles obtained from olivine deformation experiments performed by Zhang and Karato (1995) (angles between the shear direction and the peak intensity of a crystallographic pole figure). Ensembles were run for multiple values of the grain boundary mobility parameter M^* , which is a dominant control on CPO texture evolution in these kinematic models. Remaining model parameters are 1.5 for the stress exponent p , 3.5 for the deformation exponent n , 0 for the grain boundary sliding threshold, and 5 for the nucleation efficiency λ^* . In both PyDRex and the Fortran code, the polycrystal is discretised into ~ 3500 surrogate grains.

7.6 Planar corner flow using Fluidity

In the main text, we report CPO results in a planar (2D) corner flow velocity field. The analytical equations presented for velocity and velocity gradients were also used to prescribe a flow in the geodynamical framework Fluidity (Davies et al., 2011). Input files for this example are also included in the PyDRex online (git) repository. The outputs are nearly identical to those obtained by running the pure-Python (standalone) version of this simulation. Small discrepancies may arise due to differences in pathline solvers. Furthermore, in standalone mode, the pathlines are calculated based on the final locations of the ‘Mineral’ instances, whereas in Fluidity, particles are advected forwards from their initial locations. However, the fact that outputs remain consistent proves that PyDRex can be successfully coupled to larger geodynamics software frameworks.

The results shown in Figure 7.4 were obtained for the same parameter values as used in the planar corner flow simulation presented in the main text. Both CPO vectors and CPO strengths are markedly similar, as expected. Due to the additional overhead in running a full Fluidity simulation, performance is worse by about a factor of 4, however this difference could be reduced by employing Fluidity’s parallelisation capabilities.

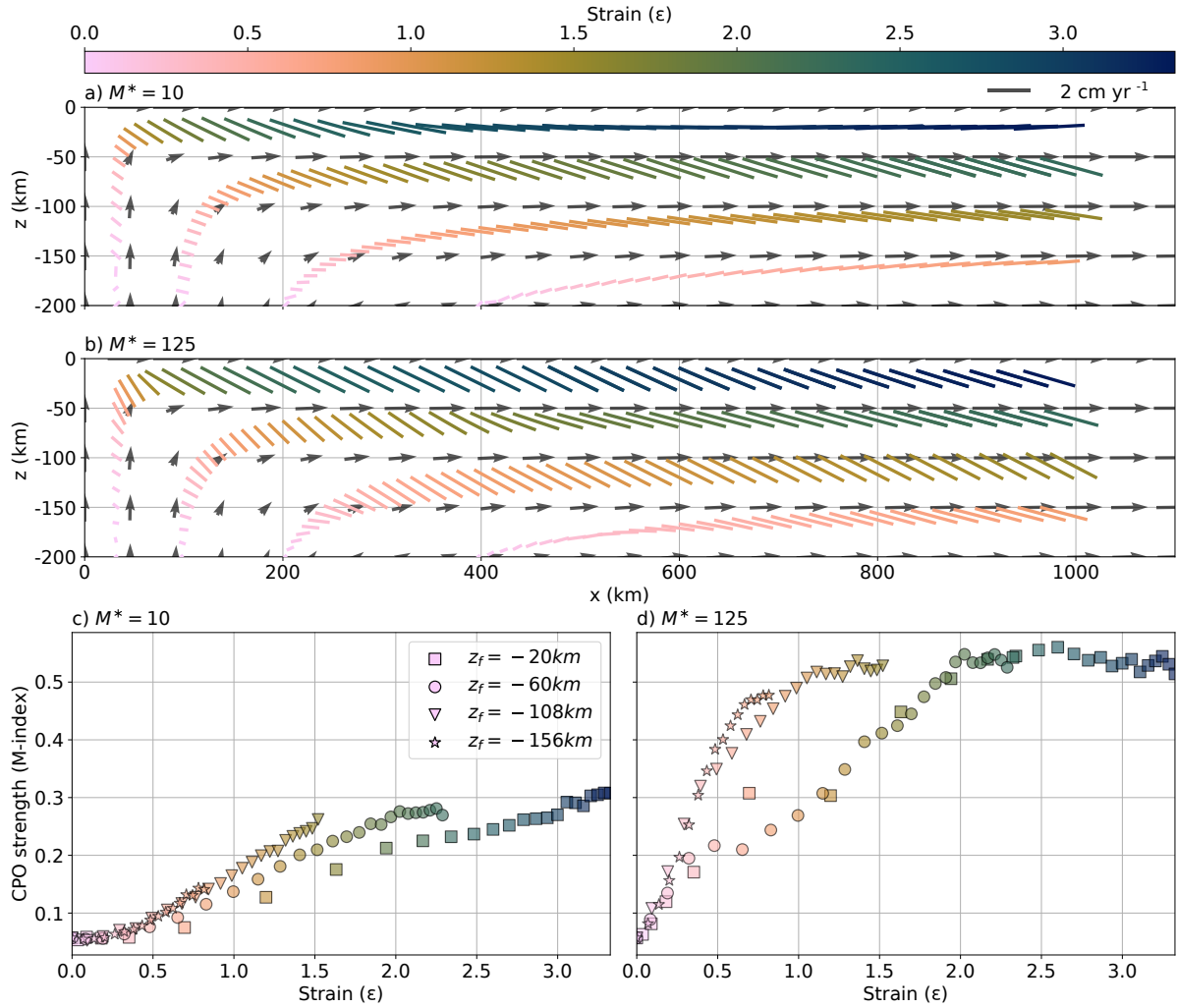


Figure 7.4: Texture evolution of A-type olivine in 2D corner flow, computed on-the-fly during a Fluidity simulation using PyDRex. Panels (a) and (b) show the *Bingham average* of the orientations at each step (i.e. the olivine a-axis), for $M^* = 10$ and $M^* = 125$ respectively, plotted as bars at locations that follow pathlines. These CPO bars are scaled by the texture strength (*M-index*); background arrows show the velocity field. Texture strength is plotted against accumulated strain in panels c and d. The color of the markers corresponds to the position along the pathline, according to the color in panels (a) and (b). Unique marker symbols are used for each pathline; the value of z_f shown in the legend is the final vertical position on the pathline.

7.7 Change in shear direction with $M^* = 10$

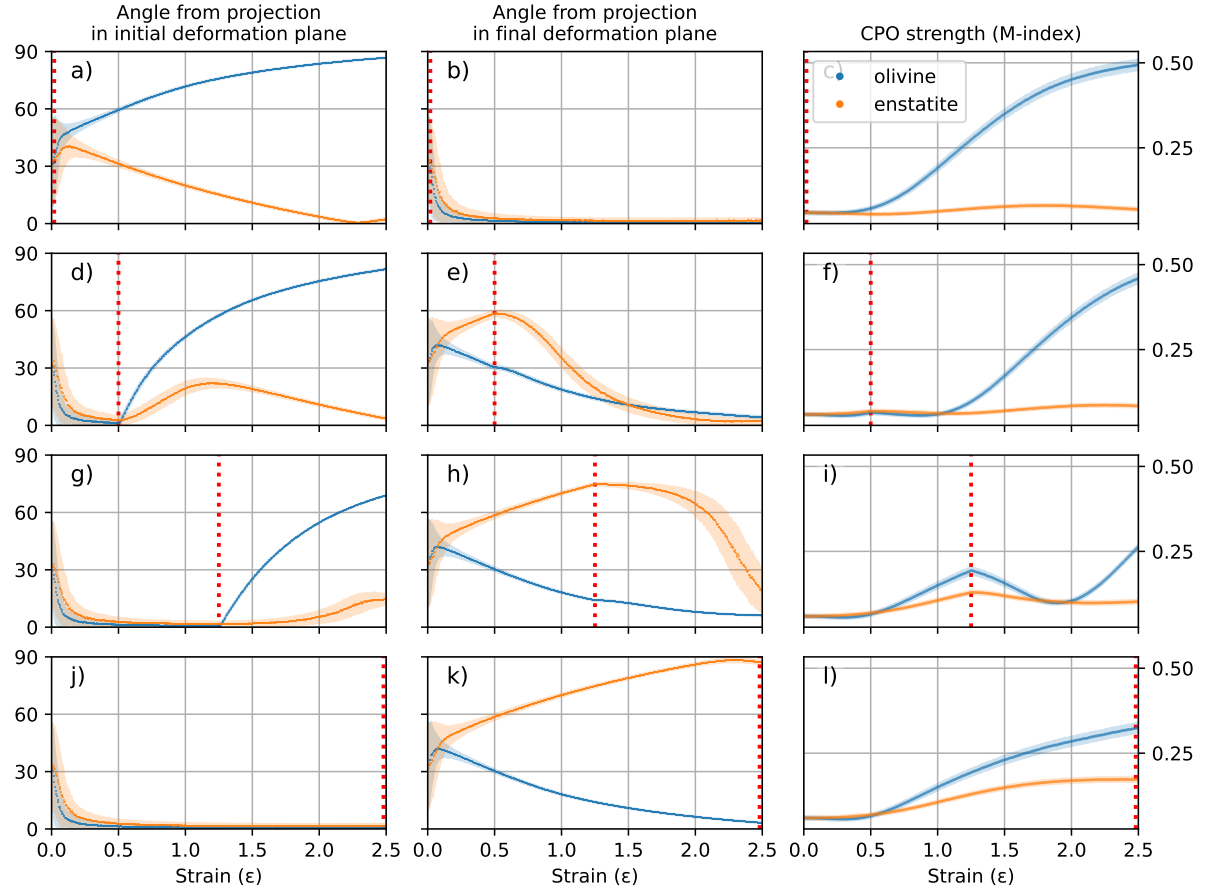


Figure 7.5: Angle in degrees (left and middle column) between a planar projection of the mean [100] axis, calculated by Bingham averaging, and a reference vector. Blue (orange) traces show the angles for olivine (enstatite), which are averages of 500 model runs. The figure is equivalent to Figure 4.8, but using $M^* = 10$ for the grain boundary mobility parameter.

7.8 Supplementary pole figures for olivine A-type in simple shear

These pole figures supplement Figure 9 in the main document and confirm that the CPO for $M^* = 0$, $M^* = 50$ and $M^* = 200$ indeed evolves to a point maximum texture for $M^* = 50$ and $M^* = 200$.

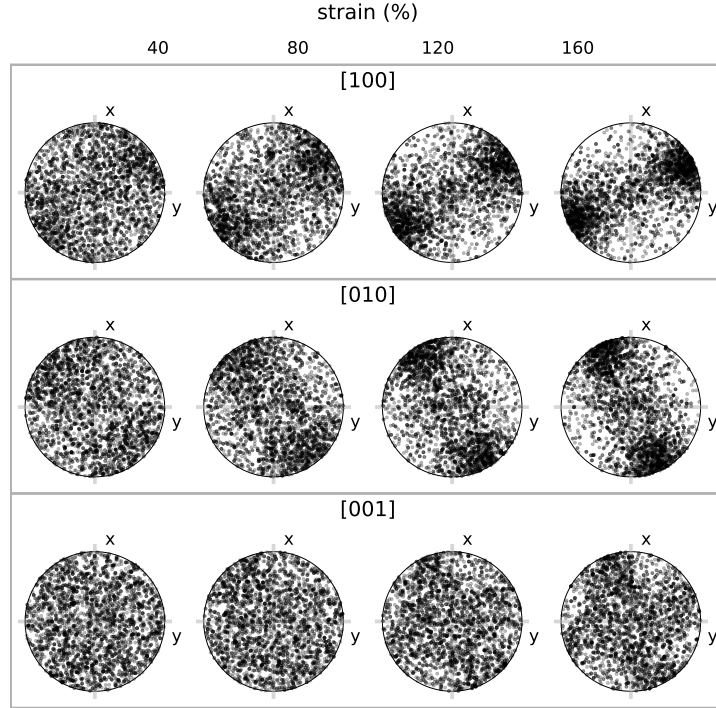


Figure 7.6: Pole figures (lower hemisphere projection) for A-type olivine textures resulting from simple shear for a grain boundary mobility of $M^* = 0$. Remaining simulation parameters are as in Figure 9.

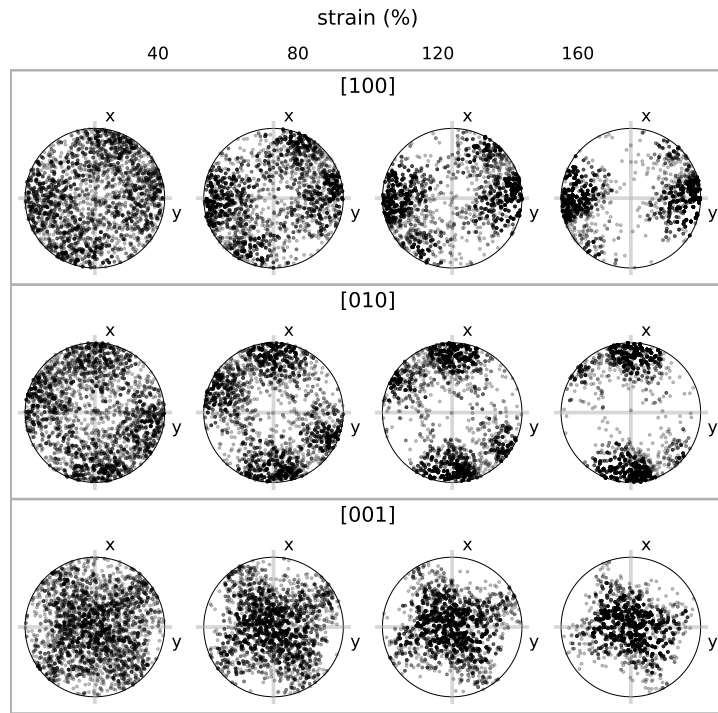


Figure 7.7: Pole figures (lower hemisphere projection) for A-type olivine textures resulting from simple shear for a grain boundary mobility of $M^* = 50$. Remaining simulation parameters are as in Figure 9.

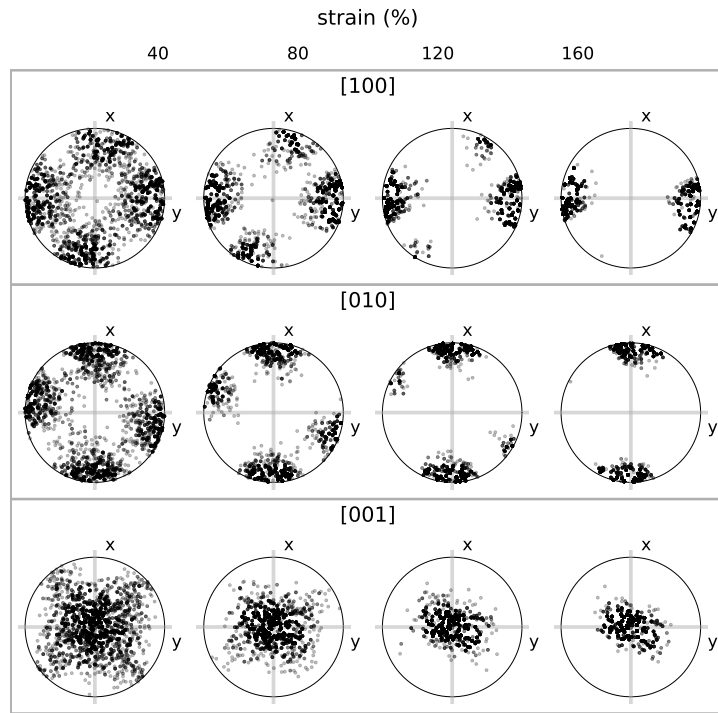


Figure 7.8: Pole figures (lower hemisphere projection) for A-type olivine textures resulting from simple shear for a grain boundary mobility of $M^* = 200$. Remaining simulation parameters are as in Figure 9.

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8 Appendix

8.1 Data Availability

The PyDRex package is published in the Python packaging index (PyPi) and available at <https://pypi.org/project/pydrex/>. Source code, including all benchmarks presented here, is available at the GitHub repository: <https://github.com/seismic-anisotropy/PyDRex>. Input data for the calibration benchmark is also available in the same repository. The version of the code used in this work is PyDRex version 0.0.1.

8.2 CRSS values for known olivine fabrics

Olivine fabrics are characterised by four CRSS values (τ_s^*) of the respective slip systems (indexed by s). The CRSS values are normalised to the activity of the softest slip system. In PyDRex, we use the CRSS values listed in Table 8.21 by default, which are identical to those used by Fraters and Billen (2021).

s	Slip system	A-type CRSS	B-type CRSS	C-type CRSS	D-type CRSS	E-type CRSS
1	(010)[100]	1	3	3	1	3
2	(001)[100]	2	2	2	1	1
3	(010)[001]	3	1	∞	3	2
4	(100)[001]	∞	∞	1	∞	∞

Table 8.21: Olivine CRSS values for known fabric types. Values are compiled from Kaminski et al. (2004) and Karato et al. (2008) and define the relative slip activities on all slip systems. Values are normalised to the CRSS of the softest slip system(s), which is always 1.

8.3 Convention for the matrix representation of grain orientations

In PyDRex, polycrystals are described by a set of orientations, and a corresponding set of scalar weights. Orientations are represented as passive (i.e. alias) rotations from a fixed Eulerian reference frame. Any single orientation can be described by a transformation matrix of the form

$$\mathbf{a} = \begin{bmatrix} \cos \phi \cos \varphi - \cos \theta \sin \varphi \sin \phi & \cos \theta \cos \varphi \sin \phi + \cos \phi \sin \varphi & \sin \phi \sin \theta \\ -\sin \phi \cos \varphi - \cos \theta \sin \varphi \cos \phi & \cos \theta \cos \varphi \cos \phi - \sin \phi \sin \varphi & \cos \phi \sin \theta \\ \sin \theta \sin \varphi & -\sin \theta \cos \varphi & \cos \theta \end{bmatrix}, \quad (8.1)$$

where $\{\varphi, \theta, \phi\}$ are the extrinsic ZXZ Euler angles (i.e. the component a_{ij} gives the direction cosine of the angle between the i -th grain axis and the j -th reference axis). This definition is identical to the one used in Kaminski and Ribe (2001).

8.4 Computational resources required for PyDRex simulations

A key result of this study is the need for a large number of grains in order to adequately resolve numerical CPO results, which bears a computational cost. The original DRex routines are implemented in Fortran, and Fortran compilers are known to produce programs with excellent computational performance, especially relative to Python, which is an interpreted language. To aid users in estimating the computational resources required for larger models, we present a table with some initial results for computational resource costs for a single olivine A-type polycrystal experiencing 2D simple shear. As PyDRex leverages established and actively developed Python libraries, such as SciPy (which provides easily configurable numerical solvers, with access to solver tolerances) and Numba (which generates just-in-time compilation of key PyDRex functions), we expect that the actual achievable performance can and will be further optimised, depending on the required accuracy.

The comparison presented in Table 8.41 suggests that, in its present state, PyDRex is about 8 times slower than the original Fortran routines. However, the performance scaling as a function of the number of grains remains roughly similar. An increase in the number of grains

N	D-Rex	D-Rex	PyDRex	PyDRex
	CPO solver	average elastic tensor	CPO solver	average elastic tensor
10^3	0.3 s	1.3 s	2.5 s	9.0 s
15^3	0.9 s	2.7 s	7.5 s	13.8 s
20^3	1.6 s	7.0 s	14.4 s	37.5 s

Table 8.41: Computation time for PyDRex and original Fortran routines, as a function of the number of surrogate grains N . For both DRex and PyDRex cases, a single simulated polycrystal of A-type olivine with initially isotropic grain orientations experienced a 2D simple shear for 200 timesteps until a strain of $\varepsilon = 1$ was reached. Grain boundary sliding processes were not included in these simulations. For PyDRex simulations, timings do not include Numba compilation time, which incurs a small transient performance cost at the beginning of the simulation. Averaged elastic tensors are computed for all 200 timesteps of all simulations. DRex routines were compiled with the GNU Fortran compiler version 11.4.0, using optional compiler optimisations (via the `-O3` command line flag).

incurs a nearly linear increase in required computation time. However, the required memory can increase significantly, most notably during calculation of the M-index diagnostic. To estimate the required RAM for this computation, note that the M-index routine (introduced in PyDRex) must be able to allocate a single-precision array of $\frac{N!}{(N-2)!} \times 4M$ values, for N the number of grains and M the number of symmetry operations for the lattice system of the mineral phase. Olivine belongs to the orthorhombic lattice system, which is defined by 7 symmetry operations (3 rotations by π , 3 reflections, and the identity operation). For a single polycrystal comprising 5000 surrogate grains, the M-index calculation therefore requires at least 21 GB of RAM (for a single timestep of the simulation — parallel computation will multiply this cost by the number of simultaneous processes or the size of a polycrystal stack). This is by far the highest memory requirement of the program, and omitting this diagnostic computation results in a base requirement of around 2 MB RAM per 1000 grains for each polycrystal at each timestep of a simulation. Currently, no automatic checkpointing features are provided, and avoiding extreme memory use during large, long-running simulations requires periodically saving the contents of the in-memory CPO store to a persistent storage (except the data for the most recent timestep, which is required for the calculations).

8.5 Numerical rotation rates for A-type olivine in pure shear deformation

To supplement the analysis of single-crystal rotation rates in simple shear presented in Figure 4.2, we include a demonstration of the computed rotation rates for pure shear deformation. The velocity gradient for this case is given by

$$L = \begin{bmatrix} 0 & 0 & D_0 \\ 0 & 0 & 0 \\ D_0 & 0 & 0 \end{bmatrix} \quad (8.2)$$

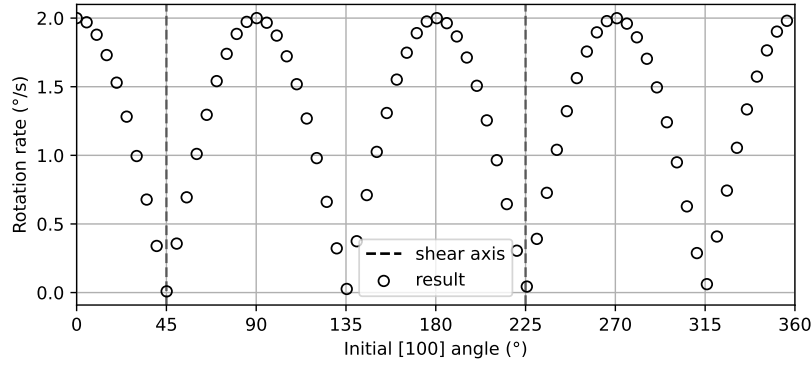


Figure 8.51: Numerical rotation rates (empty circles) for a single crystal of A-type olivine deforming via dislocation creep in pure shear with $L_{13} = D_0$. The initial [100] angle is measured from the X axis in the X-Z plane, so that at values of 45° and 225° (dashed lines), the [100] vector is aligned to the maximum extension axis and the crystal does not experience rotation. At 135° and 315°, the [100] vector is aligned to the maximum compression axis, and rotation is also not experienced. The rotation rate, like the strain rate, is measured per unit time.

where D_0 is the strain-rate scale. In this deformation, the axis of maximum extension is inclined at 45 degrees to the 2D coordinate axes, as indicated by the dashed line in Figure 8.51. The axis of maximum compression is orthogonal to this extension axis. Compared to the simple shear case, there are twice as many modes in the rotation rate distribution. Crystals aligned to either the maximum extension or maximum compression directions do not rotate, but those not aligned to either axis do. The texture of a polycrystalline aggregate deformed in pure shear will therefore be characterised not by a single point symmetry but rather by a combination of two distinct maxima in grain orientations.

8.6 Numerical rotation rates and grain growth for A-type olivine under uniaxial compression

Another type of deformation that has often been employed in laboratory experiments is uniaxial compression, where a (poly)crystal is compressed along one axis. The velocity gradient experienced by the samples in such an experiment is of the form

$$L = \begin{bmatrix} \nu D_0 & 0 & 0 \\ 0 & \nu D_0 & 0 \\ 0 & 0 & -D_0 \end{bmatrix} \quad (8.3)$$

where ν is the material constant known as Poisson's ratio, and D_0 is the strain-rate scale. In this example, the compression direction is along the Z-axis. Under such deformation, there are some grain orientations that prevent any slip activation (therefore, some grains may only change their shape via recrystallisation processes). The results presented in Figure 8.61 were obtained using a value of $\nu = 0.25$.

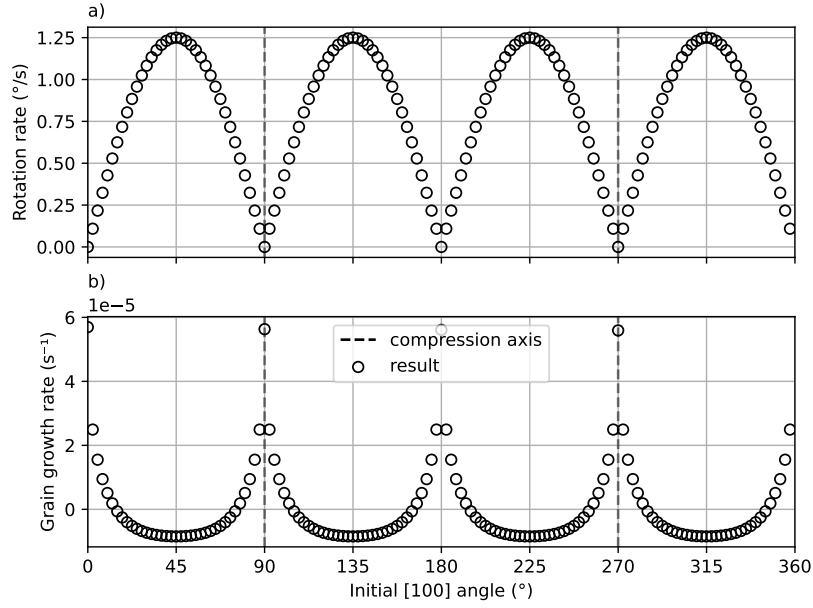


Figure 8.61: Numerical rotation rates and grain growth (empty circles) for an A-type olivine polycrystal, with grains oriented to form a perfect girdle texture in the X-Z plane, deforming via dislocation creep and dynamic recrystallisation under uniaxial compression along the Z-axis. The initial [100] angle is measured from the X axis in the X-Z plane, so that at values of 90° and 270° (dashed lines), the [100] vector is aligned to the compression axis and the crystal does not experience rotation. At 0° = 360° and 180°, the [100] vector is orthogonal to the compression axis, and rotation is also not experienced. Grain growth is significant for grains in both of these configurations, which correspond to the least and most favourable slip orientations, respectively. The rotation rate, like the strain rate, is measured per unit time.