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The anisotropic signal of topotaxy during phase transitions in D''

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ABSTRACT

While observations and modelling of seismic anisotropy in the lowermost mantle offers the possibility of imaging mantle flow close to the core-mantle boundary, current models do not explain all observations. Here, we seek to explain a long-wavelength pattern of shear wave anisotropy observed in anisotropic tomography where vertically polarised shear waves travel faster than horizontally polarised shear waves in the central Pacific and under Africa but this pattern is reversed elsewhere. In particular, we test an explanation derived from experiments on analogues, which suggest that texture may be inherited during phase transitions between bridgmanite (perovskite structured MgSiO₃) and post-perovskite, and that such texture inheritance may yield the long-wavelength pattern of anisotropy. We find that models that include this effect correlate better with tomographic models than those that assume deformation due to a single phase in the lowermost mantle, supporting the idea that texture inheritance is an important factor in understanding lowermost mantle anisotropy. It is possible that anisotropy could be used to map the post-perovskite stability field in the lowermost mantle, and thus place constraints on the temperature structure above the core-mantle boundary.

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1. Introduction

Recognising patterns of flow in the lowermost mantle (D'') is critical to our understanding of the evolution and dynamics of the Earth. Heat flow through this region is believed to control core cooling, the generation of the Earth's magnetic field and the growth of the inner core, while the related generation of thermal instabilities can lead to the formation of mantle plumes (e.g. Lay et al., 2008). These processes are modified by the arrival of subducted slabs at the core mantle boundary, which are also believed to sculpt heterogeneity concentrated at the base of the mantle into large scale structures (e.g. Garnero et al., 2016). The prospect that observations of seismic anisotropy can be used to probe flow in the deepest mantle has motivated the wide range of seismological, mineralogical and geodynamical studies that are needed to advance this idea and reveal the flow patterns (e.g. McNamara et al., 2002; Panning and Romanowicz, 2004; Hall et al., 2004; Wookey et al., 2005a; Long and Becker, 2010; Nowacki et al., 2011). While measurements of shear wave splitting from ScS, SKS and Sdiff phases unambiguously identify seismic anisotropy in the lowermost mantle (e.g. Lay and Young, 1991; Vinnik et al.,

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http://dx.doi.org/10.1016/j.pepi.2017.05.013 0031-9201/© 2017 Elsevier B.V. All rights reserved. 1995; Kendall and Silver, 1996; Wookey et al., 2005b; Rokosky et al., 2006; Long, 2009; He and Long, 2011) and show that in some places the elastic symmetry must be at most orthorhombic (Nowacki et al., 2010; Ford et al., 2015), our most spatially complete observations come from tomographic inversion of global seismic anisotropy where higher symmetry is often assumed.

Anisotropic tomographic models of global shear-wave velocities such as SAW642AN (Panning and Romanowicz, 2006), S362WMANI (Kustowski et al., 2008), SAW642ANb (Panning et al., 2010), S362WMANI + M (Moulik and Ekström, 2014), and SEMUCB-WM1 (French and Romanowicz, 2014, 2015) assume radial anisotropy compatible with material with hexagonal elastic symmetry and a vertical rotation axis (called vertical transverse isotropy, VTI). While this requires five elastic parameters for a full description, the use of empirical scaling relations reduce the description of shear wave anisotropy to two parameters, such as the velocity of a horizontally propagating shear wave with horizontal, V_{SH} , and vertical, V_{SV} , polarised particle motion, or a single shear wave velocity and an anisotropic parameter, $\xi = V_{sH}^2/V_{sV}^2$. Even with this simplification, the degree to which anisotropy is resolved in the lowermost mantle is typically lower than the resolution of isotropic inversions and anisotropic tomographic models, using different methods and parameterisations, are in less good agreement with each other at these depths than collections of

Please cite this article in press as: Walker, A.M., et al. The anisotropic signal of topotaxy during phase transitions in D". Phys. Earth Planet. In. (2017), http:// dx.doi.org/10.1016/j.pepi.2017.05.013 isotropic models (e.g. Lekić et al., 2012). However, all models have some large scale features in common. In particular, in regions of the lowermost mantle around the central and western Pacific and under southern Africa V_{SV} is faster than V_{SH} while for much of the rest of the lowermost mantle V_{SH} is found to be faster than V_{SV} . This $V_{SH} > V_{SV}$ signal is also observed in the global average (Montagner and Kennett, 1996; de Wit and Trampert, 2015, but see Beghein et al., 2006).

Since the discovery of the phase transition from bridgmanite (perovskite structured MgSiO₃) to post-perovskite at conditions similar to those found in the lowermost mantle (Murakami et al., 2004; Oganov and Ono, 2004; Tsuchiya et al., 2004a) much attention has focussed on the ability of the alignment of post-perovskite crystals to explain the observed seismic anisotropy (Lay and Garnero, 2007; Wookey and Kendall, 2007; Nowacki et al., 2011). A key assumption is that flow in the lowermost mantle causes deformation of post-perovskite by the motion of dislocations. This deformation mechanism causes the rotation of the crystal lattices and the creation of a crystallographic (or lattice) preferred orientation (CPO). As single crystals are elastically anisotropic the rock aggregate develops an elastic anisotropy and this is the presumed cause of observed seismic anisotropy. In this case knowledge of the way that dislocations can move in lowermost mantle minerals can, in principle, be used together with seismic observations to infer flow patterns (e.g. Doornbos et al., 1986; Lay and Young, 1991; Karato, 1998a,b; McNamara et al., 2002; Panning and Romanowicz, 2004). In order to use this information to inform models of mantle flow it is necessary to know the elastic anisotropy of single crystal post-perovskite, the deformation mechanism and how this relates strain to the formation of CPO (e.g. knowledge of the critical resolved shear stress for each dislocation slip system, or the stress needed to form deformation twins), and to undertake measurements of seismic anisotropy in the lowermost mantle. However, thus far there have been few attempts to constrain lowermost mantle flow directly from observations of seismic anisotropy (e.g.Wookey et al., 2005b; Wookey and Kendall, 2008; Nowacki et al., 2010; Thomas et al., 2011; Ford et al., 2015).

For post-perovskite in D["], the single crystal elasticity is fairly well constrained from atomic scale simulations (litaka et al., 2004; Tsuchiya et al., 2004b; Caracas and Cohen, 2005; Stackhouse et al., 2005; Wentzcovitch et al., 2006; Stackhouse and Brodholt, 2007) and experiments (Murakami et al., 2007; Mao et al., 2010), but consensus on how post-perovskite deforms under lowermost mantle conditions remains elusive. Because it is only stable at very high pressure, deformation experiments on MgSiO₃ post-perovskite are limited to those that can be undertaken in the diamond anvil cell (DAC), which imposes limitations on the range of strains, strain rates, stresses, temperatures and grain sizes that can be investigated. Miyagi et al., 2010 showed that under achievable low-temperature, high-stress conditions deformation yielded a texture consistent with that expected from the movement of dislocations gliding on (001). DAC experiments with the MnGeO₃ and MgGeO₃ analogues give similar results (Hirose et al., 2010; Nisr et al., 2012). Earlier studies indicating dislocation glide on (100) or {110} (Merkel et al., 2006, 2007) seem to be explained as a transformation texture (see Walte et al., 2009; Okada et al., 2010; Miyagi et al., 2011). Additional information has been extracted from analogue materials with a lowerpressure perovskite to post-perovskite phase transition as deformation can then be undertaken at high temperature and with more control over, for example, strain rate and stress. Such experiments on CaIrO₃ and NaCoF₃ indicate that post-perovskite is weaker than perovskite (Hunt et al., 2009; Dobson et al., 2012) and that the dominant dislocation slip system for CaIrO₃ and CaPtO₃ postperovskite is [100](010) (Yamazaki et al., 2006; Niwa et al.,

2007; Walte et al., 2007; Miyagi et al., 2008; Miyajma and Walte, 2009; McCormack et al., 2011; Hunt et al., 2016). This contradicts the results found for MnGeO₃ and MgGeO₃. An alternative approach to avoid the limitations of DAC experiments is to make use of atomic scale simulation to investigate the way that postperovskite deforms. Simulations designed to probe atomic diffusion in post-perovskite indicate that diffusion is strongly anisotropic and, if deformation is influenced by atomic diffusion, support the idea that MgSiO₃ post-perovskite is weaker than bridgmanite (Ammann et al., 2010). Models of dislocation mobility within the Peierls-Nabarro framework suggest that deformation of MgSiO₃ post-perovskite in the dislocation controlled regime should be dominated by motion of dislocations belonging to the [100] (010) and [001](010) slip systems (Carrez et al., 2007a,b), that CalrO₃ should behave in a similar manner to MgSiO₃ but not $MgGeO_3$ (Metsue et al., 2009) and that the addition of Fe does should not dramatically alter this behaviour (Metsue and Tsuchiya, 2013). Recent calculations going beyond the Peierls-Nabarro approximations and incorporating thermal effects reinforce the importance of the [100](010) slip system in MgSiO₃ post-perovskite (Goryaeva et al., 2015a,b) and suggest the possibility of dislocation accommodated anelasticity (Goryaeva et al., 2016). As yet, the apparent disagreement between the DAC experiments, studies of analogues, and simulations remains unresolved.

There have been several attempts to use geodynamical modelling alongside simulations of the development of anisotropy parameterised by data from mineral physics to understand shear-wave splitting or long-wavelength anisotropy (e.g. Wenk et al., 2006; Wenk et al., 2011; Walker et al., 2011; Nowacki et al., 2013; Cottaar et al., 2014) and place inferences of mantle flow derived from observations of anisotropy on a stronger footing. The main differences between these studies are: (a) the choice of how to generate a mantle flow field that drives deformation, either by 2D (Wenk et al., 2006, 2011) or 3D (Cottaar et al., 2014) simulations of convection, or by using flow field generated by the inversion of geophysical observations (Walker et al., 2011; Nowacki et al., 2013): (b) whether they seek to compare predictions with observations of shear wave splitting making use of a ray theoretical calculation (Nowacki et al., 2013), with summary anisotropic parameters more comparable with tomography (Wenk et al., 2011; Walker et al., 2011), or both (Cottaar et al., 2014); and (c) the details of the model of texture evolution in post-perovskite or other deep mantle phases. Studies based on mantle flow derived from geophysical observation are set in the geographical reference frame of the Earth, and this allows a relatively direct comparison with observations of anisotropy. However, such approaches make use of models of mantle flow that are damped and are at relatively low spatial resolution: this may modify deformation experienced by rocks in the deep mantle. A further limitation is that such models do not vary with time. These limitations are not present when a forward simulation of mantle flow is used, which yield a time varying flow field at a spatial resolution only limited by the available computational resources, but at the cost of losing the ability to directly compare such models with specific geolocated observations. Comparison with shear wave splitting (e.g. Nowacki et al., 2013; Cottaar et al., 2014) is generally limited to regions close to the location where subducting slabs are expected to impinge on the core-mantle boundary (although Ford et al., 2015, combined observations of ScS and SK(K) S to explore anisotropy around the African LLSVP) and these studies tend to yield evidence for anisotropy consistent with post-perovskite deformation with glide on (010) or (001). However, an important caveat derived from recent finite-frequency simulation is that these ray-theoretical approaches may be inaccurate if lowermost mantle anisotropy is complex and spatially varying (Nowacki and Wookey, 2016). In contrast with the studies of shear wave splitting, results from

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