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Evaluating post-perovskite as a cause of D'' anisotropy in regions of palaeosubduction

Andy Nowacki, Andrew M. Walker, James Wookey and J.-Michael Kendall

School of Earth Sciences, University of Bristol, Wills Memorial Building, Bristol, BS8 1RJ, UK. E-mail: andy.nowacki@bristol.ac.uk

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SUMMARY

Seismic anisotropy in the Earth’s lowermost mantle (D'') is often attributed to the alignment of MgSiO$_3$ post-perovskite (ppv) by the movement of dislocations in response to mantle flow. However, ppv’s plastic yield surface is not known; nor do we know if this is the main deformation mechanism. We make use of a heterogeneous, generally anisotropic model of elasticity in D'' derived from a three-dimensional model of mantle flow, which is obtained by inversion of geophysical observables. Unlike previous approaches, completely general, three-dimensional flow and full anisotropy are permitted, yielding more information to compare with observations than has been possible before. We model observations of anisotropy in D'' by calculating the shear wave splitting predicted in ScS waves for a series of models of ppv plasticity. We find that observations in regions of the lowermost mantle beneath subduction zones are best fit by a model which accommodates slip on (010). Our results show that, within one standard deviation, slip on (010)—or a mechanism giving the same style of anisotropy—explains D'' anisotropy beneath these regions.

Key words: Mantle processes; Creep and deformation; Seismic anisotropy; Dynamics of lithosphere and mantle; Rheology: mantle.
1 INTRODUCTION

Observations of seismic anisotropy in the Earth’s lowermost mantle (D’’ layer) are numerous (e.g., Lay et al. 1998; Kendall & Silver 1998; Nowacki et al. 2011), yet at present it is difficult to ascribe this anisotropy to any particular causative mechanism, limiting the further utility of these observations. In this study we assess one hypothesis regarding the cause of anisotropy in the lowermost mantle: that lattice-preferred orientation (LPO) in post-perovskite is created in response to mantle motion. We do so using the least ambiguous observations of anisotropy in D’’: shear wave splitting of the seismic phase ScS, which traverses the D’’ region.

Recent advances in computational and experimental mineral physics are providing new insights into the elasticity and rheology of lower mantle minerals (e.g., Shieh et al. 2011; McCormack et al. 2011; Niwa et al. 2012; Cordier et al. 2012). Tomography models can now be combined with constraints from mineral physics to predict models of mantle flow (Forte & Mitrovica 2001; Simmons et al. 2009, 2010). Finally, the proliferation of seismic networks is providing unprecedented coverage of anisotropy in the lowermost mantle (e.g., Nowacki et al. 2010). Nevertheless, a few studies have previously tried to link flow models, mineral physics and observations of seismic anisotropy in the lowermost mantle (e.g., Wenk et al. 2006; Merkel et al. 2007; Walker et al. 2011; Wenk et al. 2011). However, all previous attempts have either made the simplifying assumption that the style of anisotropy is transversely isotropic with a vertical symmetry axis (VTI), or imposed 2D flow, also limiting the types of anisotropy permitted. Here, for the first time, we compare seismic observations with predictions of D’’ anisotropy that are based on 3D state-of-the-art flow models with no assumptions about the style of anisotropy. In other words we allow the anisotropy to be general in form and arbitrary in orientation.

The post-perovskite polymorph of MgSiO\textsubscript{3} (ppv) has been proposed as a potential cause for anisotropy in D’’, as it exhibits stronger single-crystal anisotropy than the perovskite (pv) phase (Tsuchiya et al. 2004; Oganov & Ono 2004; Iitaka et al. 2004; Murakami et al. 2004; Wookey et al. 2005b), and pv is believed to transform into the ppv structure at depths near to the observed D’’ discontinuity (Oganov & Ono 2004; Iitaka et al. 2004; Murakami et al. 2004). Attention has focussed on ppv because it is more abundant than ferro-periclase ((Mg,Fe)O, fpc) in the assumed
lower mantle composition, thus a weaker LPO in ppv can cause the same strength of anisotropy than for other D'' phases. Ppv may be observed through its seismic anisotropy, provided it develops a sufficient LPO, and it is deformed enough whilst stable within the lowermost mantle. Some convection simulations with Earth-like parameters have indeed suggested that strain rates are high enough in D'' for dislocation creep to dominate (e.g., McNamara et al. 2003), which would allow LPO to form.

Despite predictions of the presence of ppv in D'', so far no data have confirmed that another cause, such as LPO in another phase, or shape-preferred orientation (SPO) of seismically distinct material above the CMB (e.g., Kendall & Silver 1996), is inadequate to explain D'' anisotropy. Hence we attempt to test ppv LPO as a candidate mechanism. Because the pv–ppv transition has a positive Clapeyron slope, it is most likely to be found in colder regions, such as where subducted slabs have most recently reached the core-mantle boundary (CMB). We therefore focus on observations which sample seismically fast regions, which are believed to correspond to areas of palaeosubduction.

2 METHODS AND DATA

2.1 Observations

We consider nine previous measurements of differential S–ScS shear wave splitting in D'' in regions of palaeosubduction (Lithgow-Bertelloni & Richards 1998), shown in Figure 1. (For details of the method, see Wookey et al. 2005a; Nowacki et al. 2010). These give coverage beneath North and Central America, the northwest Pacific, and Siberia. Each result is a stack of shear wave splitting measurements, incorporating several seismic stations, and in some cases more than one earthquake. All measurements correct for upper mantle (UM) seismic anisotropy beneath the station using previous measurements of SKS splitting there, assuming that any contribution to SKS splitting from the lower mantle is negligible or would be detected as periodic variation in splitting parameters with backazimuth. Some measurements which use shallow earthquakes also correct for anisotropy in the UM near the source. The data are used because a series of rigorous tests of the quality of the measurements is applied in all cases: good signal to noise ratio, clear ellipti-
Figure 1. Previous multi-azimuth observations of shear wave splitting in D′, beneath North and Central America, the northwest Pacific and Siberia. Background colour and arrows show vertical and horizontal components respectively of flow 200 km above the CMB in the TX2008 model of Simmons et al. (2009). Circles with bars show shear wave splitting observations in ScS phase from Nowacki et al. (2010) (lower left), Wookey et al. (2005a) (upper left) and Wookey & Kendall (2008) (right). Orientation of bar corresponds to fast orientation in ray frame, $\phi$; length of bar corresponds to delay time, $\delta t$ (see legend). Thick black lines are representative ray paths in the bottom 250 km of the mantle along which the splitting measurements are made; arrows show sense of direction.

2.2 Elasticity Calculation From Mantle Flow

We calculate the elasticity for a wholly-ppv D′ in the regions of interest on a 5°-by-5° longitude-latitude grid at several radii spaced 50 km apart, starting at a radius of 3505 km (giving ‘layers’ at 25, 75, 125 and 175 km above the CMB). The procedure, similar to that of of Merkel et al. (2007) and Wenk et al. (2011), is described in detail by Walker et al. (2011). Briefly, for each point where the elasticity is required we trace pathlines from the pv to ppv phase transition to the point through a mantle flow field derived from the joint inversion of seismological and geodynamical data (model TX2008.V2, Simmons et al. 2009; Forte 2000; Mitrovica & Forte 2004). We use...
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the values of the Clapeyron slope of the pv–ppv transition given by Oganov & Ono (2004), as this relatively large value will maximise the topography of the transition. On regular time steps along the pathlines we accumulate velocity gradient tensors and use these to drive a viscoplastic self-consistent model (Lebensohn & Tomé 1993) of texture development in a sample of 500 ppv crystals. Finally, we convert the crystal orientations to an estimate of the bulk elasticity making use of the single crystal elasticity (Stackhouse & Brodholt 2008; Stackhouse et al. 2006; Wentzcovitch et al. 2006). The end result is a set of heterogeneous, generally anisotropic elastic constants where no symmetry on the style of elasticity is imposed. The three output models are named P100, P010 and P001, the three digits giving the Miller indices of the primary crystallographic plane on which slip is accommodated (Merkel et al. 2007; Metsue et al. 2009; Miyagi et al. 2010) in the VPSC calculation—for more details, see Walker et al. (2011). The elasticity, shown by strength of anisotropy, is summarised in Figure 2. We use the universal elastic anisotropy index, 
\[ A^U = 5G^V/G^R + K^V/K^R - 6 \] (Ranganathan & Ostoja-Starzewski 2008), where \( G \) is the shear modulus, \( K \) the bulk modulus, and the \( V \) and \( R \) superscripts denote the Voigt and Reuss bounds on these properties respectively. It is a measure from 0 upwards of the strength of anisotropy of a set of elastic constants, but does not capture the variation in shear wave splitting along any particular orientation.

We also performed similar calculations with a mixture of ppv and MgO with ratio 80%:20% (supporting information), but find that the main effect of this is to reduce the strength of anisotropy without affecting the pattern.

2.3 Shear Wave Splitting Calculation

Rays are traced through the 1D Earth model AK135 (Kennett et al. 1995) along the great circle paths of the observations, and followed from their entry into the anisotropic region. Whilst in the anisotropic region, they are repeatedly propagated forward along their 1D raypaths by a small increment, \( \delta s \). At each step, \( i \), the local elastic constants and the ray’s orientation are used to calculate the shear wave splitting for that step, \( \Gamma_i = (\phi_i, \delta t_i) \). The elastic constants from the texture calculation are regridded onto a 50 km cartesian grid of nodes which determine the local
Figure 2. Strength of anisotropy of elastic constants in $D''$ calculated at a radius of 3505 km (25 km above the CMB), shown with the universal elastic anisotropy index, $A^U$. The values for each of the plasticity models (P100, P010 and P001) are given for each of the three regions. Darker colours indicate stronger anisotropy. Black squares in NW Pacific region show points where pv and not ppv is not stable at this radius (temperature and pressure) for our Clapeyron slope, and where we therefore assume isotropy.

elastcity at each calculation point. Provided $\delta s$ is less than $\sim 10\%$ of the node spacing, we find no reduction in the total amount of splitting due to incomplete traversal of cells. Here, we use a value of 1 km for $\delta s$.

The splitting at each step is used as the input for the subsequent procedure. A synthetic waveform is created with the source polarisation predicted by the Global CMT solution for the event used in the observation. In some cases more than one event is used in a stacked measurement, in which case a representative polarisation is used; however, events for one path typically share a common tectonic mechanism, so the source polarisations do not vary much. In any case, tests showed varying the source polarisation had very little effect on the results. White noise is added to the trace with amplitude 0.1 of the signal to stabilise the splitting analysis.

The synthetic waveform is then split in turn by each local value of $\Gamma_i$. This is done in the frequency domain to reduce numerical noise and avoid the necessity of using very small sampling intervals, which would increase the computational cost. Tests showed the shape of the waveform has no effect on the predicted splitting. A waveform of period 100 s is used, because along some
paths the total amount of splitting is very large. This violates the assumption of the minimum-eigenvalue (Silver & Chan 1991) shear wave splitting measurement technique, which is that $\delta t$ is somewhat less than the period of the wave. In practice, we retrieve similar results using a wave of period 10 s, but the uncertainties are larger, hence we retain the long-period results for further study.

We then analyse the split waves using the minimum-eigenvalue method (Silver & Chan 1991) to find the splitting parameters $\phi'$ and $\delta t$ accrued along the ray. Pre- and post-analysis waveforms were manually inspected to check the quality of the result and find any null measurements. In some cases the waveforms are especially complicated and the splitting analysis cannot give a set of parameters which adequately linearises the particle motion, and in this case the result is noted but not used in the further analysis.

3 RESULTS AND DISCUSSION

3.1 Shear Wave Splitting Predictions

Figure 3 and the supporting information show the results for the nine paths considered and three plasticity cases, compared to the previous observations. The modelled splitting times are between 1.1 and 23.0 s, with the strongest variation between raypaths, and secondarily between plasticity models. Mean delay times, $\langle \delta t \rangle$, are largest for P100 (7.5 s) and smallest for P010 (3.2 s). This reflects the strength of the texture for the different models. For P010, individual slip system activities are more similar to each other, implying texture development should be weaker, and thus we might expect that this model should produce much smaller $\langle \delta t \rangle$ than the other models: this is not the case. One explanation may be that in regions of palaeosubduction, the flow is dominantly downward (Figures 3, S1 and S2), hence texture has not had much time (pathline distance) to develop. The S1, W1 and Siberian paths cross the regions with the strongest textures (Figures S1 and S2), and here the values of $\delta t$ are indeed much larger for the P001 case.

The waveforms produced are generally simple. The supporting information shows examples where clear elliptical particle motion results from applying the modelled splitting, and a clear minimum in the eigenvalue surface is evident. In two cases (path W1 for P100 and W2 for P001),
Figure 3. Shear wave splitting predicted by each plasticity model along each path (red), and observed splitting (black). Bars within circles show observed (black) and synthetic (red) splitting parameters. Orientation of bars represents fast orientation in ray frame, $\phi^f$, and length shows delay time, $\delta t$, as for Figure 1. Legend to right indicates where dotted inner circles show increasing $\delta t$, from 1 s to 3 s (circle edge). $\delta t$ is scaled by 0.5 for all paths apart from Sib1 and Sib2 (where scaling is 0.2). W1 for P100 and W2 for P001 are excluded from analysis (see text).

the waveforms are too complicated to give a simple, single splitting operator which adequately recovers the initial, linear particle motion (supporting information). Therefore, these paths are rejected from further analysis.

3.2 Circular Misfit

In order to quantitatively assess the fit of each of the plasticity models, and noting that a linear misfit is not appropriate for periodic data, we propose a ‘circular misfit’ in analogy to the reduced $\chi^2$ misfit:

$$\chi^2_c = \frac{1}{\nu} \sum_i \frac{\sin^2(\phi_{i,\text{obs}} - \phi_{i,\text{syn}})}{\sin^2(\sigma_{i,\text{obs}})}$$

where $N$ is the number of data, $\nu = N - 1$ is the number of degrees of freedom, $\phi$ is the observed or synthetic fast orientation, and $\sigma$ is the uncertainty in the observed orientations. These are orientational rather than directional data, hence observed and synthetic angles of $-90^\circ$ and $90^\circ$ respectively should give a misfit of 0, as inspection of the form of $\chi^2_c$ shows. Although the values of $\phi_{\text{syn}}$ are themselves somewhat uncertain, incorporating these into the measure is difficult as the range in $\sigma_{\text{syn}}$ is very large (varying from 1.0° to 24.3°, with mean 7.3°).
This study

Figure 4. Misfit of synthetic shear wave splitting $\phi'$ compared to observations. The value of $\chi^2_c$ for each model is shown by circles. Dashed and dotted lines show 1$\sigma$ and 2$\sigma$ bounds respectively of 500,000 sets of random $\phi'$. The underlying shading shows histograms for the random $\chi^2_c$ by colour intensity and are normalised to have the same maximum frequency. Values of $\chi^2_c$ for three global anisotropic tomographic models are also shown, and vary between plasticity cases only because different paths are included in the calculation of $\chi^2_c$ between the plasticity models: Panning & Romanowicz (2004) (saw642an; triangles); Panning et al. (2010) (saw642anb; inverted triangles); Kustowski et al. (2008) (S362WMANI; squares).

The misfit intentionally does not include $\delta t$. This is because the texture in the models is unrealistically strong, hence none of the models can be reasonably compared to the observed $\delta t$. This strong texture may be for several reasons. Primarily we do not incorporate any effects to limit texture, such as recrystallisation, into the VPSC calculation. Any method to scale the values would also be arbitrary, and the subsequent fit would be entirely due to this. Therefore we include only $\phi'$: tests show that $\phi'$ is approximately independent of the scaling of the strength of anisotropy in our models, down to 10% of the maximum texturing.

Figure 4 compares the misfit for the texture models. P010 appears to match the observations best, whilst the other two have similar $\chi^2_c$. We may test whether the fit of any model is significant by comparison with the case of random $\phi'_\text{obs}$. The means and standard deviations of $\chi^2_c$ for 500,000 random sets of orientations are used to compute the 1$\sigma$ and 2$\sigma$ limits (Figure 4), noting that not all paths are included for each model as discussed previously. This shows that, whilst none of the models vary significantly from the random case at the 2$\sigma$ level, all cases are significant at the 1$\sigma$ level, with P010 fitting better than random.
The $\chi^2$ of shear wave splitting predicted from three tomographic models with radial anisotropy in D'' are also shown. It is important to note that inversions for radially-symmetric shear wave anisotropy in D'' are still somewhat uncertain and the three models may be affected by similar biases. None of the tomography models differs significantly from random, which suggests that, in the regions for which we compare with observations, there is a stronger correlation between our P010 model than the currently available anisotropic seismic tomography models. This is likely due to the constraint of radial anisotropy in the inversions, which allows only two values of $\phi'$: 0° and 90°. The significant improvement offered by our models, by contrast, permits any orientation of $\phi'$, and allows the incorporation of more data than would otherwise be the case.

3.3 Discussion

Several causes of misfit between the predictions and observations are possible. Firstly, ppv LPO may not be the cause everywhere, or at all, of D'' anisotropy in regions dominated by subducted material. However, we show that at present, the data do not require this to be the case. Secondly, the flow model we use may not accurately represent the true flow field. The TX2008 model is smooth, hence does not include any effects of strain localisation such as strain-weakening rheologies (e.g., Yamazaki & Karato 2001), or weakening across the pv–ppv transition itself (e.g., Hunt et al. 2009). It also has no time dependence. Further, there is uncertainty in the viscosity profile, which may lead to different texturing, however previous work (Walker et al. 2011) suggests that the main effect of changing lower mantle viscosity in the flow inversions is to scale the velocity of the flow, not the pattern, which would change only the delay times in this study. Thirdly, it is possible that none of the three plasticity models are an adequate description of ppv’s behaviour. For instance, point defect motion (Ammann et al. 2010), which would not necessarily generate LPO, is a potential mechanism which cannot at present be excluded. Finally, the ray-theoretical approach of the shear wave splitting modelling may not fully incorporate the effects of finite wave sensitivity to CMB structure. With current methods, forward modelling these observations at the correct frequency is computationally challenging, however we expect that doing so would not yield significantly different results, as the texture model varies very smoothly.
To within $1\sigma$, our results suggest that one set of slip system activities in ppv predicts shear wave splitting in $D''$ better than random. At $2\sigma$ none of the models is significantly different, meaning we cannot rule out LPO in ppv as a cause of $D''$ anisotropy. The pattern of misfit—that one slip system matches observations whilst the other two do worse than random—is expected because of ppv’s orthorhombic symmetry and the fact that the three plasticity models mainly favour slip on each of the three primary crystallographic planes. Our result is in agreement with previous work (Walker et al. 2011), where the approximation of hexagonal symmetry was imposed in the comparison with global P and S wave anisotropic tomography. With the global approach, the P100 and P010 cases could not be distinguished, whereas in this work we can conclude that slip on (010) in ppv LPO—or a mechanism related to flow, such as SPO of inclusions, which produces the same style of anisotropy—is most likely.

4 CONCLUSIONS

A new model of ppv texture in $D''$ imposing no constraints on the style of anisotropy predicts shear wave splitting in ScS waves which is compatible with observations in regions of palaeosubduction to within one standard deviation. Three different plasticity cases for dislocation creep in ppv are considered, with that favouring slip on (010) matching best. This corresponds to the mechanism predicted by previous computational and experimental work. Our approach means that as emerging datasets become available and mineral physical measurements improve, further data may be incorporated.

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REFERENCES


Lithgow-Bertelloni, C. & Richards, M., 1998. The dynamics of Cenozoic and Mesozoic plate motions,
Anisotropy in $D''$ in regions of subduction


Panning, M. & Romanowicz, B., 2004. Inferences on flow at the base of Earth’s mantle based on seismic


Wentzcovitch, R. M., Tsuchiya, T., & Tsuchiya, J., 2006. MgSiO$_3$ postperovskite at D$''$ conditions, P Natl
Anisotropy in Dʰ in regions of subduction


