Earth and Planetary Science Letters 492 (2018) 35–46

Contents lists available at ScienceDirect

Earth and Planetary Science Letters

www.elsevier.com/locate/epsl

Deformation, crystal preferred orientations, and seismic anisotropy in the Earth's D″ layer

Andréa Tommasi [a,*], Alexandra Goryaeva [b], Philippe Carrez [b], Patrick Cordier [b], David Mainprice [a]

[a] Geosciences Montpellier, CNRS & Université de Montpellier, F-34095 Montpellier cedex 5, France
[b] Univ. Lille, CNRS, INRA, ENSCL, UMR 8207 – UMET – Unité Matériaux et Transformations, F-59000 Lille, France

ARTICLE INFO

Article history:
Received 27 November 2017
Received in revised form 2 March 2018
Accepted 16 March 2018
Available online 10 April 2018
Editor: J. Brodholt

Keywords:
mantle convection
D″ layer
post-perovskite
ferropericlase
deformation modeling
seismic anisotropy

ABSTRACT

We use a forward multiscale model that couples atomistic modeling of intracrystalline plasticity mechanisms (dislocation glide ± twinning) in $MgSiO_3$ post-perovskite (PPv) and periclase (MgO) at lower mantle pressures and temperatures to polycrystal plasticity simulations to predict crystal preferred orientations (CPO) development and seismic anisotropy in D″. We model the CPO evolution in aggregates of 70% PPv and 30% MgO submitted to simple shear, axial shortening, and along corner-flow streamlines, which simulate changes in flow orientation similar to those expected at the transition between a downwelling and flow parallel to the core–mantle boundary (CMB) within D″ or between CMB-parallel flow and upwelling at the borders of the large low shear wave velocity provinces (LLSVP) in the lowermost mantle. Axial shortening results in alignment of PPv [010] axes with the shortening direction. Simple shear produces PPv CPO with a monoclinic symmetry that rapidly rotates towards parallelism between the dominant [100](010) slip system and the macroscopic shear. These predictions differ from $MgSiO_3$ post-perovskite textures formed in diamond-anvil cell experiments, but agree with those obtained in simple shear and compression experiments using $CaIrO_3$ post-perovskite. Development of CPO in PPv and MgO results in seismic anisotropy in D″. For shear parallel to the CMB, at low strain, the inclination of ScS, Sdiff, and SKKS fast polarizations and delay times vary depending on the propagation direction. At moderate and high shear strains, all S-waves are polarized nearly horizontally. Downwelling flow produces Sdiff, ScS, and SKKS fast polarization directions and birefringence that vary gradually as a function of the back-azimuth from nearly parallel to inclined by up to 70° to CMB and from null to ∼5%. Change in the flow to shear parallel to the CMB results in dispersion of the CPO, weakening of the anisotropy, and strong azimuthal variation of the S-wave splitting up to 250 km from the corner. Transition from horizontal shear to upwelling also produces weakening of the CPO and complex seismic anisotropy patterns, with dominantly inclined fast ScS and SKKS polarizations, over most of the upwelling path. Models that take into account twinning in PPv explain most observations of seismic anisotropy in D″, but heterogeneity of the flow at scales <1000 km is needed to comply with the seismological evidence for low apparent birefringence in D″.

1. Introduction

The thin shell of the Earth's mantle just above the core, named D″ by Bullen (1949), is an essential feature of the mantle convection system. It forms its lower thermal boundary layer, controlling the thermal, chemical, and mechanical interactions with the core. D″ is expected to be mainly composed of (Mg,Fe)SiO_3 (∼70%) and (Mg,Fe)O – ferropericlase (Hirose et al., 2015). Experimental results, atomistic modeling, and seismological observations converge to (Mg,Fe)SiO_3 being present as bridgmanite, with an orthorhombic perovskite (Pv) structure in hot zones of D″, but acquiring a post-perovskite (PPv) structure in colder regions (cf. review in Hirose et al., 2015).

Seismic velocities in D″ show strong lateral variations at both small and large wavelengths, indicating thermal and chemical heterogeneity (e.g., Lay et al., 1998; van der Hilst et al., 2007). Seismological observations also point to changes in D″ thickness from <100 km to >350 km, which may occur over short lateral distances (e.g., Thomas and Kendall, 2002; van der Hilst et al., 2007). Last but not least, D″ is characterized by spatially

* Corresponding author.
E-mail address: andrea.tommasi@umontpellier.fr (A. Tommasi).

https://doi.org/10.1016/j.epsl.2018.03.032
0012-821X/

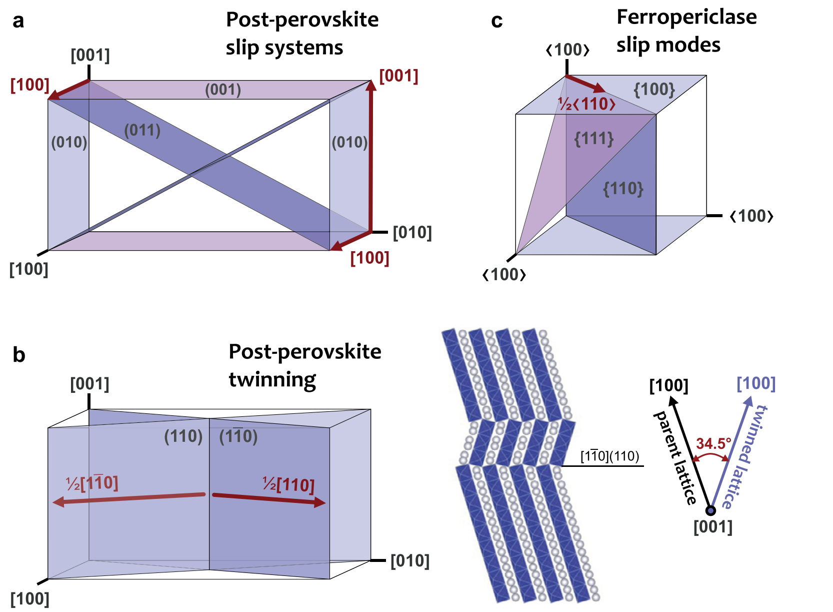

Fig. 1. (a) Slip systems and (b) twinning in $MgSiO_3$ PPv and (c) slip modes in MgO. Note that due to the cubic symmetry of ferropericlase the 3 slip modes displayed in Fig. 1c result in 24 slip systems.

heterogeneous seismic anisotropy, which has been measured using a variety of techniques, such as the analysis of: (i) waveforms anomalies (e.g., Lay and Young, 1991; Maupin, 1994; Cottaar and Romanowicz, 2013), (ii) splitting of shear waves traveling at low incidence angles through D″ (e.g., Kendall and Silver, 1996; Nowacki et al., 2010), (iii) differences between horizontally and vertically polarized shear waves in global tomography models (e.g., Panning and Romanowicz, 2006), (iv) the discrepancy in the residual splitting, after corrections for upper mantle anisotropy, of core shear waves (SKS and SKKS, e.g., Restivo and Helffrich, 2006; Long, 2009), and (v) changes in polarity of P-waves reflected at the top of D″ (e.g., Thomas et al., 2011). These data carry information on the convective flow in D″, but their exploitation depends on our ability to relate the seismic anisotropy observations to deformation-induced compositional layering or crystal preferred orientations of the main rock-forming minerals in D″: bridgmanite, post-perovskite, and ferropericlase. This led to a large number of forward models of development of seismic anisotropy in D″ based on mantle circulation or convection models, which tested different hypotheses on the $(Mg,Fe)SiO_3$ post-perovskite deformation or phase transition mechanisms (e.g., Wenk et al., 2006, 2011; Walker et al., 2011, 2017; Nowacki et al., 2013).

In this article, we also use a forward multi-scale modeling approach for exploring the contribution of deformation-induced crystal preferred orientations (CPO) of PPv and ferropericlase to seismic anisotropy in the D″ layer. We couple the most recent atomistic models of intracrystalline viscoplastic deformation in $MgSiO_3$ PPv and MgO (the pure Mg end-member of both solid solutions) at D″ conditions (Amodeo et al., 2011; Cordier et al., 2012; Goryaeva et al., 2015a, 2015b, 2016, 2017; Carrez et al., 2017) to polycrystal plasticity simulations of simple, end-member flow patterns. Potential effects of this CPO-induced anisotropy on P- and S-waves reflected at the top of D″ are analyzed in a companion article (Pisconti et al., in preparation).

2. Viscoplastic deformation of PPv and MgO at D″ conditions

Numerical modeling of the dislocation structures and glide properties in $MgSiO_3$ PPv and MgO at lowermost mantle strain rates, temperatures, and pressures (Amodeo et al., 2011; Cordier et al., 2012; Goryaeva et al., 2015b, 2016, 2017) constrain the active slip systems in the two minerals and their relative strengths under D″ conditions (Fig. 1 and Table 1). These models predict that the easiest slip systems for both minerals, namely $[100](010)_{PPv}$ and $[001](010)_{PPv}$ and $1/2\ \langle 110\rangle\{1\bar{1}0\}_{MgO}$ and $1/2\ \langle 110\rangle\{100\}_{MgO}$, have extremely low lattice frictions under lowermost mantle conditions, implying low strengths for mantle flow by dislocation creep in domains with high volume fractions of PPV in D″. In contrast, similar models for bridgmanite predict extremely high lattice frictions for all studied slip systems, implying that dislocation glide is not an effective deformation process for this phase in the lower mantle (Kraych et al., 2016). Dislocation dynamics models predict that bridgmanite should rather deform by pure climb (Boioli et al., 2017) and, hence, not develop strong CPO under lower mantle conditions. The corollary of these models is that PPv-rich domains in D″ should develop strong CPO of both PPv and ferropericlase, leading to a marked anisotropy of physical properties, whereas bridgmanite-rich ones should have much lower anisotropies, only controlled by the CPO of ferropericlase.

In PPv, if only dislocation glide is active, no strain parallel to the [100], [010], or [001] crystal axes can be accommodated. However, atomic-scale models for PPv also predict the development of $1/2\ \langle 110\rangle\{1\bar{1}0\}$ deformation twins (Carrez et al., 2017). {110} twinning should play a significant role in the evolution of the CPO in PPv, since it adds additional degrees of freedom for deformation (it may accommodate strain parallel to [100] and [010]), reducing strain incompatibility problems.

3. Modeling strain-induced CPO evolution and associated seismic anisotropy in D″

Development of CPO in PPv and MgO polycrystals deformed under D″ conditions is modeled by a viscoplastic self-consistent (VPSC) approach (Molinari et al., 1987; Lebensohn and Tomé, 1993), which considers each grain as a viscoplastic inclusion embedded in and interacting with a viscoplastic effective medium that represents the average behavior of the polycrystal. Each grain deforms by dislocation glide only (MgO) or by dislocation glide and twinning (PPv); these processes allow for shear in a finite set of crystallographic planes and directions (Fig. 1). Diffusive processes are only implemented in an implicit way. First, by assuming that they contribute to recovery mechanisms, such as climb, which