Earth and Planetary Science Letters ••• (••••) •••–•••

Contents lists available at ScienceDirect

Earth and Planetary Science Letters

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Composition versus temperature induced velocity heterogeneities in a pyrolitic lower mantle

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ARTICLE INFO

Article history:
Received 18 March 2016
Received in revised form 22 August 2016
Accepted 7 October 2016
Available online xxxx
Editor: P. Shearer

Keywords:
spin transition
elasticity
first-principles calculations
bridgmanite
mantle composition
sound velocity

ABSTRACT

Interpretation of lateral velocity heterogeneities is essential for our understanding of Earth's interior. Ferropericlase's (Fp) spin crossover (FSC) fundamentally changes their interpretation in the mid lower mantle. In a typical pyrolitic aggregate, FSC induces an unusual increase in bulk sound velocity (V_ϕ) with increasing temperature at mid-lower-mantle depths. This reduces the sensitivity of longitudinal velocity (V_P) to lateral temperature variations around 1700 km. Here we show that FSC also dramatically impacts the manifestation of two important types of compositional heterogeneities: i) variations in iron concentration in Fp, e.g., caused by changes in iron partitioning; ii) variation in molar fraction of Fp, as expected in slab subduction regions. FSC enhances the sensitivity of V_ϕ and V_P to these compositional variations by several-fold at similar depths. The opposite effects of lateral variations of temperature and composition on V_P is critical for distinguishing the possible physical origin of heterogeneities in tomographic P-models. Temperature and composition variations also produce opposite types of correlation between V_ϕ and shear velocity (V_S) heterogeneities and between V_S and density (ρ) heterogeneities. Only lateral temperature variations can produce anti-correlation between V_ϕ and V_S at mid lower mantle depths, while only these compositional variations can produce anti-correlation between V_S and ρ in the spin crossover region and at greater depths. Together these effects suggest that heterogeneities in V_P in the mid lower mantle common to multiple seismic models could originate in simultaneous lateral temperature and compositional variations in this region.

1. Introduction

(Mg, Fe)O ferropericlase (Fp) is the second most abundant mineral in the lower mantle. Knowledge of its thermoelastic properties is fundamental for interpretation of seismic tomography models of Earth's lower mantle. Since the discovery of high spin (HS) to low spin (LS) crossover in iron in Fp (Badro et al., 2003), extensive studies have been carried out on the effect of the spin state of iron on the elasticity of Fp (e.g. Lin et al., 2013; Muir and Brodholt, 2015; Wu et al., 2013; Yang et al., 2015). The effect of Fp' spin crossover (FSC) on its elastic properties is unusual at least in two aspects: (1) in comparison to other phase transitions in the Earth's mantle, this state change is remarkably broad and smooth, spanning a pressure/temperature (PT) range that covers most of the lower mantle (Kantor et al., 2006; Komabayashi et al., 2010; Lin et al., 2010, 2007; Lin and Tsuchiya, 2008; Mao et al., 2011; Speziale et al., 2005; Sturhahn et al., 2005; Tsuchiya et al., 2006; Wentzcovitch et al., 2009; Wu et al., 2009; Holmstrom and Stixrude, 2015). (2) As indicated by several mineral physics studies (Crowhurst et al., 2008; Marquardt et al., 2009; Wentzcovitch et al., 2009; Wu et al., 2013; Yang et al., 2015) Fp's bulk modulus exhibits a dramatic softening in the spin crossover region. This softening leads to complex anomalies in Fp's thermoelastic properties in the spin crossover region (Wu et al., 2013), most notably, a positive isobaric temperature gradient in Fp's bulk modulus at certain PT conditions of the lower mantle, resulting in an insensitivity of V_P to lateral temperature variations at depths of ∼1730 km (Fig. 1a and Tables S1 and S2) for aggregates with compositions and elastic properties well constrained by the PREM model (Wu and Wentzcovitch, 2014; Wu, 2016). These anomalies produce a well-defined behavior that might be identified in

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http://dx.doi.org/10.1016/j.epsl.2016.10.009

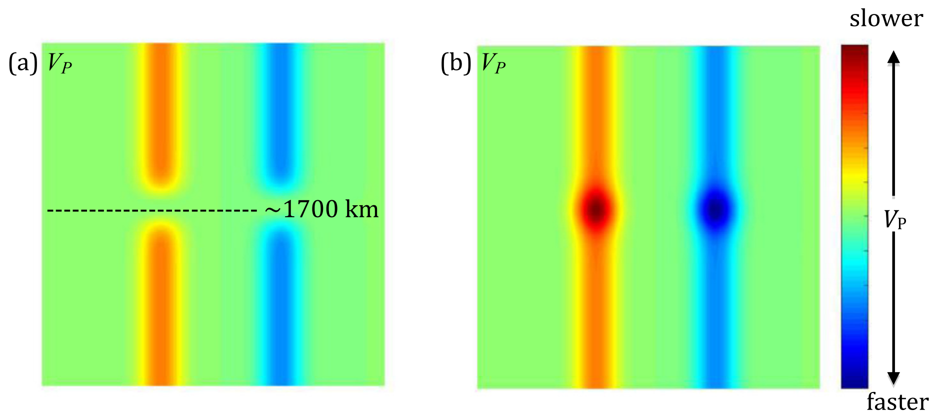

Fig. 1. Schematic representation of the nature of V_P heterogeneity in the lower mantle caused by depth independent temperature (a) and compositional (b) variations between 1000 km (top) and 2600 km (bottom). (a) Faster (slower) regions are caused by lower (higher) temperatures than those of ambient mantle. P-velocity structures are disrupted because of insensitivity of V_P to temperature variations at depths around 1750 km. (b) Faster (slower) regions are caused by less (more) $Mg_{1-x}Fe_xO$ or same amount of $Mg_{1-x}Fe_xO$ with smaller (larger) x than those in the ambient mantle. In contrast to the insensitivity of V_P to temperature variation at ~1750 km, V_P is highly sensitive to these compositional variations at similar depths.

seismic tomographic models, although the FSC might not generate an obvious signature in one-dimension velocity profiles (Wu and Wentzcovitch, 2014). Some seismic tomographic structures, e.g., the global disruption of fast P-wave velocities at ~1700 km depth (van der Hilst and Karason, 1999) and the gap displayed by slow P-wave heterogeneities beneath some hotspots (Zhao, 2007; Boschi et al., 2007) are consistent with the insensitivity of V_P to lateral temperature variations caused by FSC. It also produces anomaly in other thermodynamics properties such as thermal expansion and heat capacity in Fp (Wu et al., 2009) and plays an important role in generating the sharp boundaries and high elevations in large low shear velocity provinces (LLSVPs) (Huang et al., 2015).

Velocity heterogeneities can reveal details about mantle convection and composition variations but need to be properly interpreted. FSC fundamentally changes our interpretation of the origin of lateral heterogeneities in the mantle. In general, increasing temperature simultaneously decreases bulk (K) and shear (G) moduli and density (ρ). Thus, the anti-correlation between $V_S(\sqrt{G/\rho})$ and $V_\phi(\sqrt{K/\rho})$ in the deep lower mantle (Masters et al., 2000; Simmons et al., 2010) has suggested the existence of compositional heterogeneity in this region, though lateral variations in perovskite to post-perovskite ratio can also produce anti-correlation between V_S and V_ϕ (Wentzcovitch et al., 2006). However, anti-correlation between V_S and V_ϕ in the mid lower mantle is not necessarily produced by chemical heterogeneity. It can be induced by lateral temperature variations in the presence of FSC in aggregates with compositions well constrained by the PREM model (Wu and Wentzcovitch, 2014).

FSC should also change dramatically the manifestation of compositional heterogeneities involving variations of Fp molar fraction or iron content in Fp, or both, since Fp's bulk modulus becomes extremely sensitive to iron concentration in the spin crossover region. How these compositional heterogeneities manifest in the presence of a spin crossover in Fp is still unclear, but it is essential to address this issue to understand the origin of mantle velocity structures. Here we investigate how these compositional heterogeneities manifest in a pyrolitic mantle (Fig. 1b).

2. First principles results

The thermoelastic properties of Fp ($Mg_{1-x}Fe_xO$) with $x = 0$ and $x = 0.1875$ used here have been previously reported (Karki et al., 2000; Wu and Wentzcovitch, 2011; Wu et al., 2013). Results for both compositions ($x = 0$ and $x = 0.1875$) agree well

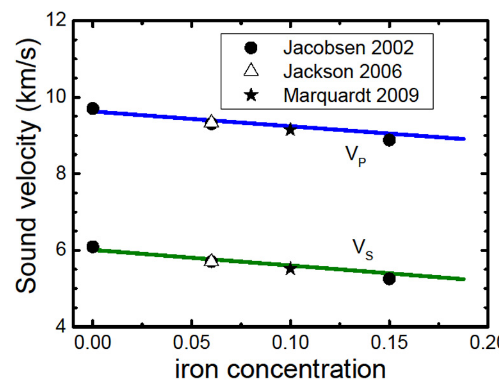

Fig. 2. Dependence of sound velocity of $Mg_{1-x}Fe_xO$ on x at 300 K and ambient pressure. The linear extrapolation of previous first-principles results (Wu and Wentzcovitch, 2011; Wu et al., 2013) is indicated by colored lines along with available experimental data (Jackson et al., 2006; Jacobsen et al., 2002; Marquardt et al., 2009). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

with available experimental data at high *PT* (see Karki et al., 2000; Wu and Wentzcovitch, 2011; Wu et al., 2013). Similar properties at intermediate compositions are linearly interpolated between those at $x = 0.1875$ and $x = 0$ (MgO). Such interpolation is justified by comparison of first-principles results and experimental data (Jacobsen et al., 2002; Wu et al., 2013), as shown in Fig. 2. Linearly interpolated results agree well with available experimental data (Jackson et al., 2006; Marquardt et al., 2009). As indicated by the last terms in Eqs. (4a) or (4b) in Wu et al. (2013), the magnitude of the anomalous depression in elasticity is determined by two factors: (1) the volume difference between high spin and low spin state, which is proportional to x and (2) the extent of the spin crossover, which is not affected by x at low concentration since the spin transition pressure is almost independent of x for $x < 0.1875$ (Tsuchiya et al., 2006). This suggests that the anomalous softening in elasticity caused by spin crossover is also proportional to x for $x < 0.2$. The linear interpolation w.r.t. composition can be used in the *PT* range of the spin crossover. We also use in this analysis the thermoelastic properties of Pv ($(Mg_{(1-x)},Fe_x)SiO_3$, with variable x) computed by first principles (Wentzcovitch et al., 2004; Kiefer et al., 2002) and properties of cubic $CaSiO_3$ perovskite (CaPv) fitted to a Mie–Debye–Grűneisen (MDG) model (Stixrude and Lithgow-Bertelloni, 2005). CaPv is not a major lower mantle component and despite still large uncertainties in its elastic properties this MDG model is adequate for the present purpose.