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Iron-spin transition controls structure and stability of LLSVPs in the lower mantle

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ABSTRACT

Seismic tomography models have revealed that there exist two large low shear velocity provinces (LLSVPs) beneath Africa and the Pacific Ocean in the Earth's lower mantle. Waveform modeling results suggest both LLSVPs have steep sharp side boundaries, which imply that they probably are compositionally heterogeneous from the ambient mantle. When applying the surface plate motion history in the last a few hundred million years (Ma) as the driving mechanism, numerical modeling has successfully reproduced the geographical distribution of the two LLSVPs in thermochemical mantle convection. However, two prominent seismic features of the LLSVPs, the steep side boundaries and the high elevation, can hardly be obtained in previous geodynamic models. Here, we include in our mantle convection model the effects of iron-spin transition of ferropericlase which substantially change physical properties of the mantle. Our results show that iron-spin transition plays a dominant role in controlling the structure and stability of LLSVPs. Large chemical blocks with steep side boundaries and high elevations up to ∼1200 km above core–mantle boundary (CMB) emerge in our models with the volume content of ferropericlase ∼20%. Such blocks cause a shear wave velocity decrease of ∼3.5% which is consistent with the seismic observations. Our results also show that these LLSVPs are transient structures in the lower mantle, which can typically last for a few hundred million years before destroyed by large-scale mantle motion.

1. Introduction

Two large low shear velocity provinces (LLSVPs) in the Earth's lower mantle have been identified from seismic tomography studies for their rapidly decreased shear wave velocity compared with the ambient mantle (Grand et al., 1997; Ritsema et al., 1999). The two LLSVPs are located nearly antipodal beneath Africa and the central Pacific Ocean, both with high elevations and steep side boundaries based on seismic waveform modeling studies (Ni et al., 2002; Ni and Helmberger, 2003; He and Wen, 2009). The African one extends 1200–1500 km upward from the core–mantle boundary (CMB) with steep and sharp side boundaries (Ni et al., 2002; Wang and Wen, 2007). The structure of LLSVP beneath the Pacific Ocean is less clear. It has been suggested that there exist two separated parts with ∼700 km and ∼300 km in height respectively (He and Wen, 2009). Similar to the Africa block, both Pacific parts have steep and sharp side boundaries (He and Wen, 2009). Besides the decreased shear wave velocity, the two LLSVPs also show anti-correlations between shear velocity and bulk sound velocity near the CMB (Ishii and Tromp, 2004). These seismic observations together suggest a chemical origin for the LLSVPs, possibly from the accumulation of recycled slabs or from the remnant material of dense melt formed in early evolution history of the Earth (Christensen and Hofmann, 1994; Labrosse et al., 2007).

Studying the formation and stability of these two LLSVPs is one of the key issues in understanding the evolutionary history of the Earth's lower mantle. Thermochemical geodynamic modeling has been employed to investigate the evolution of the two LLSVPs in large-scale mantle convection (McNamara and Zhong, 2005; Zhang et al., 2010; Tan et al., 2011). With the imposed plate motion history in the last 120 million years (Ma) as the surface boundary condition, McNamara and Zhong (2005) successfully reproduced the antipodal geographical distribution of the two LLSVPs beneath Africa and the Pacific Ocean. However, it is rather subtle to produce a chemical block with structures similar to the seismic observations, i.e. structures with high elevations and steep side boundaries. The structure of the LLSVPs is sensitive to their chemical density contrast compared with the

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ambient mantle (Ni et al., 2002; McNamara and Zhong, 2005; Tan and Gurnis, 2007). A small density contrast leads to quick mixture of the chemical composition with the ambient mantle. On the other hand, a large density contrast forms a flat layer without large topography at the base of the mantle (e.g. Tan and Gurnis, 2007). One possible way to form a stable chemical structure with high elevation and steep side boundaries is by assigning a different compressibility for the chemical composition compared with the ambient mantle (Tan and Gurnis, 2005). This setting leads to two distinct density profiles for the chemical material and the ambient mantle. The elevation of the chemical block is then controlled by a "height of neutral buoyancy" where two density profiles intersect each other (Tan and Gurnis, 2005, 2007). However, how to determine the neutral buoyancy height remains a difficult question.

The geographical stability of the two LLSVPs is another issue under great debate. Based on the reconstruction of large igneous provinces (LIPs), some studies propose that these two LLSVPs have been geographically stable since 300 Ma (Torsvik et al., 2008) or existed even much longer as an old isolated reservoir (Burke et al., 2008). But geodynamic modeling results indicate that these two LLSVPs may be transient structures which can only last for several hundred million years in large-scale mantle convection (Zhang et al., 2010; Tan et al., 2011).

In previous thermochemical mantle convection models, they did not consider an electronic reconfiguration of iron under temperature–pressure conditions of the lower mantle: spin transition. Spin transition of iron has been observed in both ferropericlase [(Mg, Fe)O] and bridgmanite (Tschauner et al., 2014) [(Mg, Fe)(Si, Al, Fe)O_3] which volumetrically take up ~17% and ~79% of the lower mantle, respectively (Badro et al., 2003; Lin et al., 2013). Iron in bridgmanite is more complex than iron in Fp: it can exist in Fe^{2+} and Fe^{3+} states and can occupy the A site and B site. First-principles calculations show that the extremely high quadruple splitting value of Fe^{2+} in bridgmanite above ~30 GPa, which has been interpreted as the high-spin to the intermediate-spin transition (Lin et al., 2008; McCammon et al., 2008), results from the change of local structure of A site Fe^{2+} (Bengtson et al., 2009; Hsu et al., 2011), whose effect on density and bulk modulus are much smaller than the effect of spin transition on density and bulk modulus of ferropericlase (Lundin et al., 2008). The experimental and theoretical studies show that only B site Fe^{3+} experiences high spin to low spin transition at lower mantle pressure (Stackhouse et al., 2007; Hsu et al., 2011; Fujino et al., 2012). The abundance of B site Fe^{3+}, however, is still under debate. Some experiments show that (B site Fe^{3+})/(total Fe) is negligible at lower mantle pressure (e.g. Glazyrin et al., 2014). For this reason, we only focus on the effects of iron-spin transition in ferropericlase.

When the transition in ferropericlase occurs, the number of unpaired d electrons of Fe^{2+} decreases from four to zero, leading to the reduction of volume of iron atom, which significantly changes the physical properties of ferropericlase (e.g. Lin et al., 2013). The spin transition of iron causes anomalous softening of the bulk modulus of ferropericlase (Marquardt et al., 2009; Wentzcovitch et al., 2009; Wu et al., 2013) which produces an unusual effect: P wave of pyrolitic lower mantle becomes temperature insensitive at the depth of ~1750 km (Wu and Wentzcovitch, 2014). This effect provides reasonable explanations to most of the unusual results disclosed by seismic tomography at middle lower mantle such as the disruption of P wave image below some hot spots (Zhao, 2007) and the global disruption of P wave structure (van der Hilst and Kárason, 1999), which suggest that spin transition of iron in ferropericlase indeed occurs at lower mantle, although the spin transition is not visible in one-dimensional seismic velocity profile (Masters, 2008). The anomalous thermodynamics properties of ferropericlase caused by spin transition (Wu et al., 2009) inspire investigations of their effects on mantle convection. It has been shown that iron-spin transition enhances the vigor of plumes in numerical simulations of purely thermal mantle convection (Bower et al., 2009; Shahnas et al., 2011). However, the influence of iron-spin transition on thermochemical convection has not been discussed yet.

The purpose of this work is to investigate the influence of the iron-spin transition of ferropericlase on thermochemical mantle convection, particularly on the formation and stability of LLSVPs in the lower mantle. We first provide the governing equations and parameterization of iron-spin transition in our model. Then we show that iron-spin transition may significantly influence the structure and stability of LLSVPs.

2. Methods

We construct our model in a spherically axisymmetric geometry with a modified extended Boussinesq approximation (King et al., 2010). The non-dimensional conservation equations of mass, momentum and energy for thermochemical convection are as below,

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$-\nabla p + \nabla \cdot \left[\eta\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)\right] - \left[Ra\rho\alpha(T - T_r) - Ra_c C\right]\mathbf{g} = 0, \tag{2}$$

$$\frac{DT}{Dt} - Di\alpha \mathbf{g}\mathbf{u}(T + T_s) = \nabla \cdot (\kappa \nabla T) + \frac{Di}{Ra}\Phi + H. \tag{3}$$

Here, the variables are the velocity vector $\mathbf{u}$, dynamic pressure p, viscosity η, density ρ, thermal expansivity α, temperature T, horizontally averaged temperature T_r, chemical composition C (varying between 0 and 1), gravitational acceleration vector $\mathbf{g}$, surface temperature T_s, thermal diffusivity κ, viscous diffusivity Φ and heat production rate H. Each of these variables is non-dimensional. Rayleigh number Ra and chemical Rayleigh number Ra_c in Eq. (2) are defined as:

$$Ra = \frac{\rho_0 \alpha_0 g_0 \Delta T R^3}{\kappa_0 \eta_0}, \tag{4}$$

$$Ra_c = Ra \frac{\Delta \rho_c'}{\rho_0 \alpha_0 \Delta T}, \tag{5}$$

where ρ_0 is surface density; α_0 is surface thermal expansivity; g_0 is surface gravitational acceleration; ΔT is temperature contrast between surface and CMB; R is radius of the Earth; κ_0 is surface thermal diffusivity; η_0 is reference viscosity and $\Delta \rho_c'$ is chemical density anomaly. They are all dimensional variables. The physical constants used in our models can be found in Table 1. In all of our models, Ra is fixed at 10^8 (except for Cases 14–20, see Table S1 in supplementary materials), corresponding to a reference lower mantle viscosity of $\sim 9 \times 10^{21}$ Pa s. Di is the dissipation number which can be expressed as:

$$Di = \frac{\alpha_0 g_0 R}{C_{p\_0}}, \tag{6}$$

where C_{p_0} is the dimensional surface specific heat (Table 1).

We add a depth-dependent density profile in the buoyancy term. The non-dimensional density profile can be expressed as

$$\rho(z) = \exp(\chi z). \tag{7}$$

Here, χ is the mantle compressibility and z is the non-dimensional depth normalized by the Earth's radius (Table 1). The parameters used lead to a factor of ~1.65 increase in density from surface to CMB, similar to the Earth's mantle density distribution.