ARTICLE IN PRESS
EPSL:14157
Earth and Planetary Science Letters ••• (••••) •••–•••
Contents lists available at ScienceDirect
Earth and Planetary Science Letters
www.elsevier.com/locate/epsl

# Mid-mantle heterogeneities and iron spin transition in the lower mantle: Implications for mid-mantle slab stagnation

M.H. Shahnas [a,b,*], D.A. Yuen [b,c,d], R.N. Pysklywec [a]

[a] University of Toronto, Department of Earth Sciences, 22 Russell Street, Toronto, Ontario, M5S 3B1, Canada
[b] Department of Earth Sciences, University of Minnesota, Minneapolis, MN 55455, United States
[c] Minnesota Supercomputing Institute, Minneapolis, MN 55455, United States
[d] School of Environmental Studies, China University of Geosciences, Wuhan, 430074, China

ARTICLE INFO

*Article history:*
Received 12 February 2016
Received in revised form 12 September 2016
Accepted 25 October 2016
Available online xxxx
Editor: P. Shearer

*Keywords:*
iron spin transition
solid–solid phase transition
mantle mixing
slab stagnation

ABSTRACT

Recent high pressure experimental results reveal that the elastic and transport properties of mantle materials are impacted by the electronic spin transition in iron under lower mantle pressure and temperature conditions. The electronic transition in ferropericlase (Fp), the second major constituent mineral of the lower mantle material, is associated with a smooth increase in density starting from the mid-mantle depth to the core–mantle boundary (CMB). The transition also yields softening in the elastic moduli and an increase in the thermal expansivity over the transition zone in the lower mantle. Although there is not yet robust experimental evidence for spin-transition induced density change in the perovskite (Pv) phase (the major constituent mineral in the lower mantle), the spin transition in the octahedral (B) site in Al-free perovskite causes a bulk modulus hardening (increase in the bulk modulus) in the mineral. We have incorporated these physical processes into high resolution 3D-spherical control volume models for mantle convection. A series of numerical experiments explore how the electronic spin transition in iron modifies the mantle flow, and in particular the fate of sinking cold slabs. Such mid-mantle stagnations are prevalent globally in seismic tomographic inversions, but previous explanations for their existence are not satisfactory. Employing density anomalies from the iron spin transition in ferropericlase and density anomaly models for perovskite, we study the influence of the spin transition in the minerals of the lower mantle on mantle flow. Our model results reveal that while the spin transition-induced property variations in ferropericlase enhance mixing in the lower depths of the mantle, the density anomaly arising from the hardening in the bulk modulus of Al-free perovskite can be effective in slowing the descent of slabs and may cause stagnation at mid-mantle levels. A viscosity hill in the lower mantle may further enhance the stagnation effect. Cold descending slabs can stall in the mid mantle for tens of million years or even longer before penetrating to the lower mantle.


## 1. Introduction

The cooling of Earth and Earth-like planets is accomplished mainly by the circulation of mantle material in planetary interiors (McKenzie et al., 1974). The validity of the numerical models in mantle convection relies on our understanding about the processes occurring at mantle temperatures and pressures and on our knowledge about the parameters describing the physical and rheological properties of the mantle material.

Some enigmatic features in the lower mantle have not yet been well established or may be interpreted in different ways. For instance, mid-mantle fossil anomalies have been the subject of debate over the past decades and are not yet fully understood. Seismic tomographic imaging studies reveal the existence of thermal anomalies at mid-mantle depths below several fossil subduction zones which are usually interpreted as fossil sinking slabs (e.g., Fukao et al., 2001; van der Meer et al., 2012). However, based on the average velocity of mantle flow, most of these slabs are expected to have been fully recycled to the bottom of mantle by the present day. For example, seismic tomography of the mantle under India reveals the existence of several high P-wave regions at different depths, interpreted as the remnants of Tethyan subduction zones and Tertiary lithospheric delamination from the India–Asia collision (Van der Voo et al., 1999). Based on estimates for the cessation of different subduction zones (reaching to ∼130 Ma) the average sinking rate for these anomalies is estimated to be

* Corresponding author.
*E-mail addresses:* shahn004@umn.edu (M.H. Shahnas), daveyuen@gmail.com (D.A. Yuen), russ@es.utoronto.ca (R.N. Pysklywec).

http://dx.doi.org/10.1016/j.epsl.2016.10.052
0012-821X/

Please cite this article in press as: Shahnas, M.H., et al. Mid-mantle heterogeneities and iron spin transition in the lower mantle: Implications for mid-mantle slab stagnation. Earth Planet. Sci. Lett. (2016), http://dx.doi.org/10.1016/j.epsl.2016.10.052

1–2 cm/yr (Van der Voo et al., 1999). Similar mid-mantle heterogeneities have been detected by the application of the S-to-P converted waveform method that establishes mid-mantle scatterers under northern China and Japan (Li and Yuen, 2014). The heterogeneities, with lateral extent ∼800 km and detected between 930 km and 1120 km depth, have been interpreted to be related to the ancient subducted basaltic crust of the Izanagi plate. Seismic tomographic studies at a number of other locations reveal that the remnants of subducted slabs as old as 150 Myr or more may still exist in the lower mantle, apparently with slow rates of descent towards the bottom of the mantle. High-velocity seismic features in the lower mantle located to the west of Lake Baikal have been identified as slab remnants of Jurassic age from when the Mongol–Okhotsk and Kular–Nera oceans closed between Siberia with the collision of the Mongolia–North China blocks and the Omolon block (Zhao et al., 1990).

Interpreting these enigmatic mid-mantle thermal structures is essential for our understanding of mantle geodynamics and the surface tectonic processes. Some recent work suggests that the slab stagnation at shallower depths (∼1000 km depth) can be explained by compositional lower mantle layering (Ballmer et al., 2015). However, alternative mechanisms like a gradual viscosity increase may account for slab stagnation and slab flattening. A viscosity increase between 800–1200 km depths has been detected by the analysis of the long-wavelength non-hydrostatic geoid (Rudolph et al., 2015).

Attempts have been made to explain kinds of layering at about 1000 km depth by invoking a second endothermic phase transition at this depth. This could be supported by the existence of a low viscosity zone (LVZ) at some depths between 660 and 1000 km depth based on the results from the inversion of the oceanic geoid (Cserepes et al., 2000). Some contributions have invoked a local viscosity stratification or regional viscosity constraints to explain the presence of fossil remnants in the lower mantle (e.g., Shahnas and Jarvis, 2007; Li and Yuen, 2014). Estimates from these studies find that a slab descent rate of 1–2 cm/yr requires a viscosity increase from the middle mantle into the lower mantle of approximately three orders of magnitude (Shahnas and Jarvis, 2007). However, only a modest increase in viscosity at mid-mantle depths is supported by glacial isostatic adjustment observations (Peltier and Drummond, 2010).

The iron spin transition in the lower mantle presents a potential new explanation. Owing to the spin transition in ferropericlase a strong elasticity softening occurs in the range of depths in which the transition is effective, leading to a large reduction in the activation energies and consequently leading to significant viscosity undulations (Wentzcovitch et al., 2009; Justo et al., 2015). These viscosity undulations occur at a minimum depth of about 1600 km depth and a maximum of about 2500 km, consistent with the double peak viscosity model of Mitrovica and Forte (2004). Recent studies suggest that a descending slab in interaction with a viscosity and/or density discontinuity in the lower mantle may be stalled in the lower mantle depths (Morra et al., 2010). We use three-dimensional (3D) computational mantle convection models to explore the impact of the electronic transition in iron on mantle dynamics. In particular, we study how the physics of the iron spin transition can impact the behaviour of sinking cold slabs, as a way of considering how such features can stagnate in the mantle.

## 2. The electronic spin transition in iron

The spin transition in ferrous iron from high spin state (HS) to low spin state (LS) in mantle minerals was predicted more than five decades ago (Fyfe, 1960). The occurrence of this transition at high mantle pressures has also been supported by crystal field theory (Burns, 1993) and band theory (Cohen et al., 1997). However, direct evidence for this mid-mantle transition has been provided by the high pressure experimental results only in recent years. Recent advances in high pressure experimental techniques have provided the necessary means for researchers to conduct experiments closer to mantle pressure and temperature conditions (Badro et al., 2003; Murakami et al., 2004; Catalli et al., 2010, 2011; Hirose et al., 2015). The manner in which mantle material properties change under mantle high pressure and temperature conditions is fundamental to understanding mantle evolution, because they can directly influence mantle convective flow.

The two major constituent minerals of the lower mantle aluminous silicate perovskite [Al–(Mg, Fe)$SiO_3$] and ferropericlase [(Mg, Fe)O], undergo a spin transition in iron, starting mainly at ∼1600 km depth under lower mantle pressure and temperature conditions (e.g., Speziale et al., 2005; Catalli et al., 2010, 2011). The volumetric contribution of these minerals in the lower mantle, are approximately 62% and 33%, respectively. The calcium silicate perovskite ($CaSiO_3$) contribution is estimated to be about 5% of the volumetric composition (Ringwood, 1982).

The iron transition in these minerals may change both heat transport and elastic properties of the mantle minerals including radiative thermal conductivity, thermal expansivity, heat capacity, density, compressibility, seismic velocity, and elastic moduli (e.g., Badro et al., 2003; Wentzcovitch et al., 2009; Wu et al., 2009; Catalli et al., 2010; Wu and Wentzcovitch, 2014). As such, variations in these elastic and transport properties of these minerals due to their electronic transition may have significant impacts on the style of circulation in the Earth's mantle (e.g., Bower et al., 2009; Shahnas et al., 2011; Huang et al., 2015; Shahnas and Peltier, 2015) which in turn will be reflected in the surface tectonic evolution. Specifically, the spin-transition induced variations in these properties may enhance the mantle velocities and the advective heat transport (Bower et al., 2009; Shahnas et al., 2011).

The nature and origin of seismic heterogeneities in the mantle is crucial to the understanding of inferred mantle structures and their geodynamic evolution. The distribution of heterogeneities is not uniform varying from one depth to another. These lateral (isobaric) heterogeneities are commonly interpreted as compositional in origin (e.g., Ishii and Tromp, 2001). Seismic data from free oscillations reveals that in the shallower depths of the lower mantle, there exists an anticorrelation or decorrelation between the shear velocity ($V_s$) and bulk sound velocity ($V_\phi$) which is commonly interpreted as chemical heterogeneities (Masters et al., 2000; Ishii and Tromp, 2001). Attempts have been made to explain the phenomenon in terms of the compositional lower mantle layering by employing simple Cartesian models (Kellogg et al., 1999). Recent studies reveal that the spin change in ferropericlase may produce seismic velocity anomalies similar to the compositional anomalies (Wu and Wentzcovitch, 2014). Employing density functional theory-based computational methods Wu and Wentzcovitch (2014) showed that for the mixed spin state (MS) in ferropericlase the sign of the temperature gradient of the shear modulus and the density for a temperature range of 920–1850 °K remains negative. However, the temperature gradient of the bulk modulus changes sign at 1400°K from negative to positive. Their calculations also show that the spin change reduces thermally induced longitudinal velocity variations between ∼1,500- and 2,000-km depths which may be misinterpreted as compositional heterogeneity in the mantle. Recent studies reveal that the spin crossover in ferropericlase, the second major mineral in the lower mantle, may provide an alternative explanation for the observed anticorrelation (Wu and Wentzcovitch, 2014).

The spin state of perovskite in the lower mantle pressure and temperature conditions is still debated. The experimental evidence of Li et al. (2004) suggests that both Al-bearing and Al-free perovskite exhibit a mixed spin state at 100 GPa and that the resid-

Please cite this article in press as: Shahnas, M.H., et al. Mid-mantle heterogeneities and iron spin transition in the lower mantle: Implications for mid-mantle slab stagnation. Earth Planet. Sci. Lett. (2016), http://dx.doi.org/10.1016/j.epsl.2016.10.052