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7 **Mid-mantle heterogeneities and iron spin transition in the lower**
8 **mantle: Implications for mid-mantle slab stagnation**
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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.

Keywords: Iron spin transition, solid-solid phase transition, mantle mixing, slab stagnation.

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 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 ferropericlasite 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; Catalli et al., 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)SiO₃] 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; Catalli et al., 2011]. The volumetric contribution of these minerals in the lower mantle, are approximately 62% and 33%, respectively. The calcium silicate perovskite (CaSiO₃) 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_ϕ) 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 [Kellog et al., 1999]. Recent studies reveal that the spin change in ferropericlasite 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 ferropericlasite 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 residual magnetic moment in the Al-bearing perovskite is significantly higher than that in its Al-free counterpart. However, some other studies [e.g., Glazyrin et al., 2014] suggest that the ferric iron does not enter the octahedral site B and that there is no spin crossover in the ferric iron in (A) site. The high pressure experimental study of Ballaran et al. (2012) found that the bulk modulus of MgSiO₃-perovskite is insensitive to the maximum pressure (up to 75 MPa). Octahedral tilting in their (Mg,Fe)SiO₃-perovskite sample (with 4 mol% of the Fe²⁺SiO₃) in the process of the compression is referred to as the high spin to intermediate spin transition in Fe²⁺. However, they find that there is almost no significant change in the bulk modulus and density. For (Mg,Fe)(Al,Si)SiO₃-perovskite (containing 37 mol% of the Fe³⁺AlO₃) their results did not show any effect arising from spin transition in iron [Ballaran et al., 2012].

High pressure experimental studies [e.g., Catalli et al., 2010] reveal that ferric iron in MgSiO₃-perovskite occupies both the dodecahedral (A) and octahedral (B) sites with almost equal weighting and the portion in the (B) site transitions to a fully LS state in the range of pressures

50–60 GPa. This transition causes hardening in the elastic moduli in perovskite resulting in a negative density anomaly in the transition depths in Al-free perovskite. However, since the presence of aluminum in the lattice of perovskite expands the volume of perovskite at low pressures, due to the higher compressibility of Al-bearing perovskite, the volume of Al-bearing perovskite approaches the volume of magnesium perovskite by 50 GPa [Catalli et al., 2011]. X-ray emission spectroscopy and synchrotron Mossbauer spectroscopy measurements up to 95 GPa reveal that the spin transition in Fe^{3+} in Al-bearing perovskite occurs faster than Al-free perovskite and with no spin transition in Fe^{2+} in Al-free perovskite [Catalli et al., 2011]. Present experimental results [e.g., Catalli et al. 2010, 2011] provide rough estimates for the radial variations in density and bulk modulus of perovskite and the details of the (P-T)-dependence of the spin transition-induced effects are yet to be discovered. The degrees of the impact of Al in perovskite, as well as the spin transition effects on the molar volume variations in perovskite and the pressure- and temperatures dependence of this variation need to be investigated.

3. Numerical Setup

In the mixed spin state the volume (or density), the thermal expansivity and the bulk modulus of ferropericlasite may be approximated by:

$$V(n) = nV_{LS}(P, T) + (1 - n)V_{HS}(P, T) \quad (1)$$

$$\alpha(n)V(n) = nV_{LS}\alpha_{LS} + (1 - n)V_{HS}\alpha_{HS} + (V_{LS} - V_{HS})\left.\frac{\partial n}{\partial T}\right|_P \quad (2)$$

$$\frac{V(n)}{K_T(n)} = n\frac{V_{LS}}{K_{LS}^T} + (1 - n)\frac{V_{HS}}{K_{HS}^T} - (V_{LS} - V_{HS})\left.\frac{\partial n}{\partial P}\right|_T \quad (3)$$

[Wu et al., 2009] where $n \equiv n(P, T)$ is the fraction of LS states in the mixture [see Wu et al., 2009 for details Wentzcovitch et al., 2009]. It should be noted that the last terms in equations (2) and (3) have significant contribution to the thermodynamic properties of ferropericlasite in the MS state. While the density (or volume) depends only on n linearly, the thermal expansivity and the bulk modulus terms are sensitive to the variations in the fraction of LS variable n with the temperature and pressure in the mixture.

We employ an MPI-parallelized 3D-spherical control volume code with a modified Yin-Yang grid to solve the set of the thermo-mechanical equations [for details consult Shahnas and Peltier, 2015]. The difference in thermodynamic properties between the mixed spin state and the HS state introduce anomalies in the thermodynamic properties in the transition zone. The spin-transition induced density anomaly in the state equation is the superposition of three density anomaly terms:

$$\Delta\rho_{\text{STot}} = \Delta\rho_s + \Delta\rho_\alpha + \Delta\rho_K \quad (4)$$

where

$$\Delta\rho_\alpha = -\rho_0 \Delta\alpha_s (T - T_0), \quad (5)$$

$$\Delta\rho_K = \rho_0 \left[\left(\frac{1}{K_T + \Delta K_s} - \frac{1}{K_T} \right) (p - p_0) \right] \quad (6)$$

$\Delta\rho_\alpha$ and $\Delta\rho_K$ are pressure and temperature dependent spin transition-induced anomalies [Wu et al., 2009; Shahnas et al., 2011]. $\Delta\rho_s$, ΔK_s and $\Delta\alpha_s$ are the spin transition-induced anomalies calculated based on the density-functional perturbation theory [Wentzcovitch et al., 2009; Wu et al., 2009]. The zero subscripted quantities denote the reference values of the parameters.

Assuming the reference level at the surface of Earth; the density anomalies in equations (5) and (6) represent the total spin transition induced anomalies in the mineral at mantle temperatures at any depth. In the case of ferropericlasite to a large extent the spin-transition induced density anomaly arising from the variation in thermal expansivity ($\Delta\alpha_s$) eliminates the effect of the density anomaly arising from the variation in bulk modulus (ΔK_s), leaving a residual density anomaly effective in regions where the HS-LS transition occurs. The change in the buoyancy of the hot plumes and cold downwellings is therefore determined by the P-T dependence of $\Delta\rho_s$ and the residual density anomaly ($\Delta\rho_\alpha + \Delta\rho_K$). Figure 1 displays the total and components of the spin-induced density anomalies for a mantle geotherm occurring in the ferropericlasite phase of lower mantle minerals (assuming 33% volumetric contribution in this phase). While the $\Delta\rho_s$ -component increases smoothly from zero at mid-mantle depths to 80 kg/m³ at the core-mantle boundary, the $\Delta\rho_\alpha$ and $\Delta\rho_K$ -components, respectively negative and positive in sign, reach their highest magnitudes in the range of 1750-1850 km depth. The total impact of the density anomalies arising from the spin-transition induced variations in thermal expansivity and bulk modulus is such that the residual density ($\Delta\rho_\alpha + \Delta\rho_K$) on average increases at the upper levels of an effective transition zone, followed by a decrease in the lower depths and finally negligible variations in density in the deep mantle. According to the monotonic increase of the total density anomaly in ferropericlasite displayed in Figure 1, we expect that mixing in the lower mantle would increase.

In order to understand the influence of this T-P dependent lower mantle phenomenon on the buoyancy of hot plumes and cold sinking downwellings (“slabs” for geological context), we have

246 shown plots of the components of these spin-transition induced density anomalies for a sample
 247 temperature in Figure 2. The panels (b-d) in the first column of Figure 2 display the total and the
 248 components of the spin-induced density anomalies based on a sample temperature (a) for a spin-
 249 transition density model similar to the model M04 (Figure 3-a) in which the impact of the bulk
 250 modulus anomaly in perovskite due to the spin transitions has been mimicked by increasing the
 251 strength of the thermal expansivity anomaly as described below. In the second column, the
 252 spherically averaged value of each quantity has been subtracted from the relevant quantity. As it
 253 can be seen from the second row of Figure 2, owing to the density anomaly component $\Delta\rho_s$, the
 254 hot plumes become lighter (gaining positive buoyancy) and the cold downwellings become
 255 heavier (gaining negative buoyancy). This increases the mixing in the lower regions of the lower
 256 mantle. The density anomaly arising from the spin-transition induced variations in the thermal
 257 expansivity ($\Delta\rho_\alpha$) causes more complex features. Due to the spin transition-induced variations
 258 in the thermal expansivity, the hot plumes become heavier (gaining negative buoyancy) at the
 259 top of the spin-transition zone; however, in the most of the lower mantle region the hot plumes
 260 gain positive buoyancy. The impact of this component is such that the rising plumes become
 261 more vigorous in the lower regions of mantle but they are slowed down in a narrow region near
 262 mid-mantle levels. On the other hand the cold slabs approaching the transition zone first
 263 experience a velocity reduction due to the spin-transition induced positive buoyancy in a narrow
 264 region at mid-mantle depths, but after passing this narrow region, they gain acceleration (due to
 265 gaining a negative buoyancy). The effect of the spin-transition induced variations in the bulk
 266 modulus through $\Delta\rho_K$ in Fp is similar to the impact of $\Delta\rho_s$ except that unlike $\Delta\rho_s$ its maximum
 267 influence is not near the core-mantle boundary but is at about 1800 km depth (Figure 1). In sum,

while the density anomalies in ferropericlasite, $\Delta\rho_s$ and $\Delta\rho_K$, both have an enhancing impact on mantle circulation and mixing in the lower mantle, the density anomaly $\Delta\rho_\alpha$ may cause slab stagnation at about 1600 km depth. However, just like the other components this density anomaly enhances the circulation in the lower regions of the mantle based on the ferropericlasite phase. The relative strengths of these density anomaly components ($\Delta\rho_\alpha$ and $\Delta\rho_K$) play a crucial role in mid-mantle slab stagnation.

The details of this transition through its P-T dependence are important in understanding the dynamics of the lower mantle but are not yet well known. The P-T dependence of the total spin-transition induced anomaly arising from both major minerals of the lower mantle, Fp and Pv and the sign of this anomaly determine the behaviour of hot plumes and cold downwelling mantle material in the effective transition zone in the mid lower-mantle.

To study the conditions under which slab stagnation may occur at mid-mantle depths based on an iron spin transition in mantle minerals, we present a series of models as follows: **M01**) in which the spin transition is absent; **M02**) in which the spin transition occurs only in the ferropericlasite phase; **M03**) with spin transition in ferropericlasite but assuming that the impact of spin-transition induced bulk modulus in ferropericlasite is eliminated by the similar term in perovskite ($\Delta\rho_{K(Fp)} \approx -\Delta\rho_{K(Pv)}$); **M04**) the same as M03 but with stronger $\Delta\rho_K$ anomaly in the perovskite phase by a factor of two ($\Delta\rho_{K(Fp)} \approx -2\Delta\rho_{K(Pv)}$), which can be justified by the volumetric percentage of perovskite relative to ferropericlasite in the lower mantle; **M05**) the same as **M03** but with stronger $\Delta\rho_K$ anomaly in the perovskite phase by a factor of three

290 $(\Delta\rho_{K(Fp)} \approx -3\Delta\rho_{\alpha(Fp)})$. However, since $\Delta\rho_{K(Fp)} \approx -\Delta\rho_{\alpha(Fp)}$, we have included the influence of
 291 larger magnitude of the density anomaly in Pv by increasing the magnitude of $\Delta\rho_{\alpha(Fp)}$ (i.e.
 292 $\Delta\rho_{K(Pv)} \approx 2\Delta\rho_{\alpha(Fp)}$ and $\Delta\rho_{K(Pv)} \approx 3\Delta\rho_{\alpha(Fp)}$ in M04 and M05 respectively). The starting snapshot of
 293 these models for comparison purpose has been taken from model M03 in its quasi-statistically
 294 equilibrium state. The total spin transition-induced radial density profiles for these models have
 295 been displayed in Figure 3-a. The model names end with V1, V2, and V3 as explained below
 296 specifying the viscosity profile of the model.

297
 298 In the first sequence of models we have employed a modified version of a VM3-depth
 299 dependent viscosity profile [Peltier and Drummond, 2010] with a low viscosity layer at an
 300 endothermic phase transition depth (660 km) to simulate the influence of transformational
 301 superplasticity at this region and a low viscous layer in the deep mantle region to represent the
 302 viscosity reduction in D'' layer [Shahnas and Peltier, 2015]. In order to study the impacts of the
 303 spin-transition induced density anomalies on the mantle dynamics, we have confined ourselves
 304 to radial viscosity profiles (Figure 3-d) in this study and have not included the influence of lateral
 305 viscosity heterogeneity. This viscosity profile is shown as V1 in Figure 3-d. Two more viscosity
 306 profiles have also been considered. The viscosity profile V2 is similar to V1 except for the lack
 307 of low viscosity layer at deep mantle. A comparison between the model results with V1-viscosity
 308 profile and V2-viscosity profile is useful in understanding of how a low viscosity layer at deep
 309 mantle may influence the descending of the cold slabs. The last viscosity model V3 is inferred
 310 from the spin transition consideration in ferropericlasite. We have assumed an activation energy of

200 kJ/mol and weighting shear-dilatation parameter of $\delta = 0.5$ (for details see [Justo et al, 2015](#)).

All models presented in this study include the influence of fluid compressibility in the anelastic fluid approximation. A free slip boundary condition is imposed at the surface and CMB. The models also include the solid-solid phase transitions at 410 km, 660 km, and 2700 km depths approximated by

$$\Delta\rho_{\text{Ph}(i)} = \Delta\rho_i (\Gamma_i - \Gamma_n), \quad i = 1, 2, 3 \quad (7)$$

in the state equation where $\Delta\rho_i$ is the density contrast between two solid phases across the divariant phase transition i and Γ_i is a phase density functional defined by:

$$\Gamma_i = \frac{1}{2} \left[1 + \tanh\left(\frac{d_i - d - \gamma_i(T - T_i)}{h_i}\right) \right], \quad (8)$$

The parameters d , d_i , h_i , T_i , and γ_i are depth, reference depth of phase boundary i , width of the i^{th} divariant phase transition, transition temperature at the reference depth d_i and the Clapeyron slope of the relevant phase transition, respectively. The latent heat of all transformations has been considered in the energy equation (for details see [Shahnas and Peltier, 2015](#)). The CMB temperature is kept at 3600° K. Most recent experimental studies reveal that the solidus temperature of a primitive (pyrolitic) mantle is as low as 3570 ± 200 K at CMB pressures [[Nomura et al., 2014](#)]. The Clapeyron slopes for the exothermic phase transition at 410 km depth and endothermic phase transition at 660 km depth are assumed to be 3.0 MPa/K and -2.8 MPa/K [[Ito and Takahashi, 1989](#)] with density contrasts of 200 kg/m³ and 440 kg/m³, respectively. For the endothermic Clapeyron slope other values as low as -1.3 MPa/K have been suggested [[Fei et](#)

al., 2004; Katsura et al., 2003], however, the slope considered here is the effective Clapeyron slope. Further to the transformation of the spinel phase to perovskite + ferropericlasite at 23-24 GPa, there exists a chain of phase transitions at about 660 km depth including the transformation of spinel + stishovite to ilmenite at ~20 GPa (for a system with Mg_2SiO_4 composition) and from ilmenite to perovskite at ~24 GPa. The second transformation has a strongly negative slope of -6 ± 1 MPa/K [Yu et al., 2011]. The Clapeyron slope and the density contrast for Pv-pPv phase transition are assumed to be 12 MPa/K [Hirose, 2006] and 80 kg/m^3 , respectively. The thermal expansivity and thermal conductivity are pressure and temperature-dependent [Schmeling et al., 2003; Hofmeister, 1999, see also Shahnas and Peltier, 2015 for details]. A uniform internal heating rate of 13 TW consistent with the requirement of chondritic meteorites is assumed for these models.

4. Results

We have employed control volume method to solve the set of thermal-mechanical equations on a high-resolution modified Yin-Yang grid [Shahnas and Peltier, 2015] ($2 \times \theta \times \phi \times r = 2 \times 130 \times 360 \times 201$) on the Mesabi supercomputer at the University of Minnesota. The snapshots of our 3D-models at 60 Myr, 80 Myr, and 100 Myr evolution time are shown in Figure 4 for the first sequence of models (M01V1-M05V1). Two downwelling plumes can be detected in all models. The blue isosurface contours represent -100° K temperature anomalies and a 2D-cross section of the temperature field has been shown to simplify visualization. The blue isosurface contours have been trimmed at 1000 km depth for clarity and the surface of the light gray sphere indicates the effective spin transition depth (1600 km).

Inspection of the panels in the first column (at 60 Myr evolution time) reveals that the bottom of the left-cold downwelling flow in [M02V1](#) with spin transition in ferropericlasite, is closer to the core-mantle boundary than the bottom of the similar flow in [M01V1](#) with no spin transition. This is consistent with the propensity for spin transition to increase mixing and circulation of the mantle flow in the lower regions of the lower mantle [Bower et al., 2009; Shahnas et al., 2011]. The bottom of the same downwelling cold flow in the model [M03V1](#) (assuming that the density anomalies arising from spin-transition induced bulk modulus anomalies in F_p and P_v are identically cancelled out) resides at a higher level than the bottom of its counterpart in [M02V1](#). Part of the same cold downwelling patch in the model [M04V1](#) has been laminated over the transition depth which is partly due to the forcing acted on the patch from a rising plume. However, the cold downwelling flow also experiences a positive buoyancy force at the top of the spin transition zone which retards motion of the cold patch. The radial location of this descending flow also indicates that the descending rate of the patch has decreased. This can be better seen in model [M05V1](#) in which we have assumed higher degrees of contribution from the spin-transition induced anomaly in the bulk modulus of perovskite (or equivalently an increase in the magnitude of the anomaly in the thermal expansivity in the ferropericlasite phase). This results in higher degrees of positive buoyancy for the cold flow at the top of the transition zone. In model [M05V1](#) the downwelling flow has stagnated at the spin transition depth (~1600 km). While in [M04V1](#) part of the cold patch is in the process of penetrating to the lower region of the lower mantle (below 1600 km depth), in the model [M05V1](#) the penetration is in its early stages.

Inspection of the panels in the second column (at 80 Myr evolution time) provides insight into the evolution of these structures. In [M01V1](#) the same cold material is almost touching the core-

mantle boundary surface and from the top it is still connected to the cold material penetrating to the lower mantle from the 660 km depth endothermic phase transition boundary. In model [M02V1](#) the cold material has mainly sunk to the bottom of the mantle and has been disconnected from the sinking flow at the top. The similar cold downwelling material in [M05V1](#) is still in the process of penetrating to the lower regions of the spin transition zone. However, in all models the cold patch has touched the core-mantle boundary after 100 Myr evolution time. To a large extent the sinking mantle material at the right hand side of the models has passed the spin transition depth in the model [M01V1](#) and [M02V1](#). However, the degree of mid-mantle stagnation increases from [M03V1](#) to [M05V1](#) which can be seen from the snapshots at all times.

In [Figure 5](#) we show the temperature anomalies and the spin-transition induced density anomalies for the model [M05V1](#) for 100 Myr of evolution time in 20 Myr intervals. From the panels of the first column, it is evident that the cold downwellings are being arrested at mid-mantle spin transition depths. One can also see that the stagnated left-flow (for about 80 Myr) finally sinks to the bottom of mantle through an avalanche event (being initiated after 60 Myr, [panel d](#)) from the mid-mantle spin-transition boundary, a process termed as the Spin-transition Induced Mid-Mantle Avalanches (SIMMA) process [[Shahnas et. al, 2011](#)].

The panels of the second column of [Figure 5](#) display the total spin-transition induced density anomaly from which the spherically averaged value of the anomaly has been subtracted (i.e., $\Delta\rho_{STot} - (\Delta\rho_{STot})_{ave}$). We compare the hot rising plume in the [panels 5\(b\) and \(d\)](#). In [panel 5\(b\)](#) the rising hot plume has gained positive buoyancy from the spin transition in the mantle minerals in the lower mantle regions. At the top of this plume there exists a region with negative

buoyancy which is due to the cold region at the top of the plume. On the other hand, the negatively buoyant region at the top of the plume in [panel 5\(d\)](#) is a result of the head of the hot plume. This shows that the hot plume gains positive buoyancy in most of the lower mantle below the spin transition zone, but in a narrow layer near the top of the transition zone the plume gains negative buoyancy due to the P-T dependence of the spin-transition induced density anomalies. Inspection of [panel 5\(e\)](#) in the second column reveals that while the left cold downwelling material has gained positive buoyancy near the top of the spin transition zone, the section of this material which has penetrated into the lower region of the lower mantle has a negative buoyancy. This means that the cold slab approaching the spin transition boundary at about 1600 km depth first experiences an upward forcing which may slow down the descent rate of the slab or cause stagnation or deflection of the sinking slab. However, as soon as the slab does penetrate into the lower regions of the spin transition boundary, due to the spin-transition induced negative boundary, it accelerates and pulls the tail of the slab from the upper mantle into the deeper regions of the mantle.

Hot rising plumes in most of the deep mantle gain acceleration owing to the spin transition effect, but they experience deceleration in the region near the top of the spin transition boundary from spin-transition induced negative buoyancy. The hot regions below stagnated slabs can cause an additional upward forcing because the additional spin transition-induced positive buoyancy. This can increase the duration of the cold slab-stagnation or reduce the descending velocity of the slab. The horizontally extended hot material below the middle slab in [panel 5\(c\)](#) is an example.

Figure 6 shows the radial velocity fields in 20 Myr time intervals for the model M05V1. The total velocities have been superimposed on the radial velocity fields. Inspection of the panels of this figure shows that all three cold downwellings have not yet passed through mid-mantle depth after 40 Myrs evolution (panel 6c). The radial velocity fields also show that there is no significant radial flow below the head of these downwellings in the lower regions of mantle. In panel (d), the right most downwelling has entered to the lower mantle by an avalanche process but the velocity field indicates that the avalanche is not very intense. However, 20 Myr later the avalanche becomes more vigorous (panel e). The avalanche process for the middle downwelling at this time is in its triggering stage. The last panel shows that after 100 Myr part of the middle downwelling mantle flow has merged to the left downwelling and compared to the snapshot at 80 Myr, the radial velocity has increased. The triggering of the mid-mantle avalanche for the left most downwelling has started at ~60 Myr (panel d), similar to the other cases with increasing avalanche velocity in the next panels. As it can be seen from the last frame, part of the middle downwelling is still halted at mid-mantle depths even after 100 Myr evolution.

In the second sequence of models we eliminate the low viscosity layer at the bottom of mantle (V2-viscosity profile). The model results with and without a low viscosity layer in the deep mantle have been compared in Figure 7. A comparison between the snapshots of these two sequences of models reveals that the presence of a deep mantle low-viscosity layer facilitates the spreading of the slabs and development of plumes over the CMB. In the models with moderate hardening in the bulk modulus of Pv, M02V1 and M02V2, the influence of this viscosity reduction is extended to the mid-mantle depths. However, the increase in the bulk modulus in Pv and the associated negative density anomaly buffers the impact at shallower depths above the

mid-mantle horizon (~1600 km depth), which is evident in a comparison of the snapshots of the models [M05V1](#) and [M05V2](#). The absence of a deep mantle low viscosity layer can work in favour of mid-mantle stagnation. This effect may be further enhanced by employing lower values for the Clapeyron slope of the Pv-pPv phase transition. Our models assume a high-end value for the Clapeyron slope of deep mantle phase transition [e.g., [Hirose, 2006](#)], while some other studies suggest lower values [e.g., [Tsuchiya et al., 2004](#)].

In the last sequence of models we employ a viscosity profile ([V3](#)) inferred from the spin transition in ferropericlasite [[Justo et al, 2015](#)]. The high spin to low spin transition in ferropericlasite can cause viscosity undulations in the lower mantle as shown in [Figure 3-d](#) that may enhance the flow stagnation at mid-mantle depths or slow the descending slabs. The model results for the model [M02V3](#) with spin transition in [Fp](#) and the model [M03V3](#) with spin transition in [Fp](#) and a moderate increase in the bulk modulus of [Pv](#) due to the spin transition have been shown in [Figure 8](#). Tracking the slab close to the left, the slab in model [M02V3](#) at 100 Myr, is almost below 1600 km depth, which has been indicated by a white wireframe sphere. At the same time the radial center of the same slab in [M03V3](#) resides at about 1600 depth. The cyan and pink wireframe spheres at 2070 km and 2370 km depths respectively have been added to help visualize the structures. The situation at 120 Myr is similar, however, parts of the slab in [M03V3](#) are still above 1600 km mid-mantle horizon. Also, in the last snapshot at 140 Myr the bottom of the slab in [M03V3](#) is closer to the CMB than is the case in [M02V3](#), which reveals that the downward motion of the slab in [M03V3](#) has been accelerated compared to [M02V3](#) which can be interpreted as a very mild mid-mantle avalanche.

5. Discussion and Conclusions

Recent high pressure laboratory experimental discoveries in mineral physics have provided us a better understanding of deep mantle features. The anticorrelation between the shear velocity (V_s) and bulk sound velocity (V_ϕ) in the shallower depths which commonly has been accepted to be the consequence of chemical heterogeneities [Masters et al., 2000; Ishii and Tromp, 2001; Kellogg et al, 1999], may also be explained by spin crossover in ferropericlase in the lower mantle [Wu and Wentzcovitch, 2014].

In this study we investigated the influence of the iron spin transition in lower mantle minerals on mid-mantle slab stagnation. Such mid-mantle stagnations are prevalent globally in seismic tomographic inversions, but previous explanations for their existence have not been robust. Our high resolution numerical models reveal that cold subducted slabs descending through the endothermic phase transition barrier at 660 km depth may be halted in the mid mantle before descending to the deep mantle and then being recycled. While the spin-transition induced property changes in ferropericlase enhances the mixing in the deep mantle, a possible hardening in the bulk modulus in Pv may slow down the descent rate of slabs or cause stagnation at mid-mantle levels.

Mid-mantle slab stagnation becomes robust in the models, which assume higher degrees of hardening in the bulk modulus of perovskite. The experimental results, however, support a moderate increase in the bulk modulus of this mineral at mid-mantle pressures [Catalli et al.,

2010, 2011]. Some other studies even find the impact of the spin transition on the bulk modulus of perovskite non-significant [e.g., Ballaran et al., 2012]. So the magnitude of the density anomaly arising from the bulk modulus of perovskite and even its sign are yet to be investigated fully. In our numerical models we have also assumed Al-free perovskite as the main constituent of the lower mantle material. This is an approximation since the mantle bridgmanite is expected to contain some amount of aluminum. However, this is not well constrained and our present notions about the properties of the mantle mineral may drastically change with future mineral physics studies that better resolve the role of the oxidation states of Fe (Fe^{2+} or Fe^{3+}), their populations in the dodecahedral and octahedral sites in the mixed-spin state, and the concentration of Al in perovskite which influence the spin transition effects. The pressure- and temperature dependence of the thermo-elastic properties in the presence of spin transition also plays a crucial role in the dynamics of convection in the lower mantle. The details of the changes in physical and rheological properties of perovskite due to the spin transition in iron at mantle pressures and temperatures are not yet well established and there are controversies among different experimental results [Catalli et al., 2010, 2011; Ballaran et al., 2012; Glazyrin et al., 2014]. More sophisticated experimental results for thermoelastic properties of perovskite in the mixed spin state at high pressure and temperature conditions are needed. The technical difficulty arises from the fact that in the case of perovskite, it is ferric iron in the B site which makes a transition from HS to LS at mid-mantle pressures, and there are uncertainties about the percentage of the ferric iron in B site.

Although the stagnation is weakened by decreasing the strength of the hardening in the bulk modules of perovskite, this may be compensated by other mechanisms including an appropriate

viscosity profile or an increase in the thermal expansivity of perovskite due to the spin transition. In the main sequence of our numerical models we assume a moderate increase in viscosity with depth (V1). The model results reveal that stagnation prevails more with the larger increase in the perovskite bulk modulus. However, the model with a viscosity profile inferred from the spin transition in ferropericlasite (V3) reveals signs of stagnation even with lower degrees of hardening in the bulk modulus of perovskite.

The processes occurring at high mantle pressure and temperature conditions may affect the spin states of iron oxides in the mantle as well as influencing their oxidation states and phase instabilities [Hu et al, 2016; Badro et al., 2003; Ono and Ohishi, 2005; Bykova et al., 2016]. New oxidation states such as Fe_4O_5 and Fe_5O_6 may develop at high pressure and mantle conditions with possible impacts on the mineralogy, chemistry, and physical properties of mantle constituents [Lavina and Meng, 2015], which could in turn change our notion about the Fp-Pv mantle. The contribution from new phases of mantle material and their property changes at extreme mantle pressure and temperature conditions particularly the changes in their thermoelastic properties under spin transition need to be incorporated in geodynamic models and considered in the interpretation of seismic images. Our results point to the importance of detailing a deeper understanding of the three-dimensional structure of the elastic moduli in the lower mantle, particularly under regions with a recent subduction history for the past 150 million years [e.g., van der Meer et al., 2012].

In this study we restricted ourselves to using radial viscosity profiles [Peltier and Drummond, 2010; Wentzcovitch, et al., 2009; Justo et al., 2015], avoiding the lateral variations in viscosity

in the lower mantle. The effects from the lateral variation in viscosity were isolated in our numerical models to clearly demonstrate the impacts of the spin-transition induced density anomalies in the dynamics of mantle circulation. Additional study is required to incorporate the impact of the spin transition-induced viscosity undulations [Justo et al., 2015] with strong lateral variations in the lower mantle viscosity in the models to demonstrate the relative importance of the spin-transition dependent density anomalies and viscosity.

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Figure captions:

Figure 1- Spherically averaged spin transition-induced total density anomaly and its components for ferropericlase.

Figure 2- A sample test model demonstrating the spin-transition induced density anomaly and its components for the model in which we assume stronger $\Delta\rho_K$ anomaly in the perovskite phase by a factor of two (M04). The first column represents (a) sample temperature, (b) $\Delta\rho_s$, (c) $\Delta\rho_\alpha$ and (d) $\Delta\rho_{STot}$. In the second column, the radially averaged value of each quantity has been subtracted from the relevant quantity (e.g. $\Delta\rho_{STot} - (\Delta\rho_{STot})_{ave}$ in d').

Figure 3- a) Spherically averaged total spin-transition induced density anomaly ($\Delta\rho_{STot}$) for the models M01-M05, b) density anomaly models assumed in perovskite phase, c) bulk modulus anomaly models in perovskite phase, d) viscosity models employed in our numerical convection models.

Figure 4- Snapshots of five models (M01V1) no spin transition, (M02V1) with spin transition in ferropericlase, (M03V1) with spin transition in ferropericlase in which the density anomaly arising from the bulk modulus in ferropericlase identically eliminates the similar term in the perovskite phase, (M04V1) the same as M03V1 but with stronger $\Delta\rho_K$ anomaly in the perovskite phase by a factor of two, (M05V1) the same as M03V1 but with stronger $\Delta\rho_K$ anomaly in the perovskite phase by a factor of three. The blue isosurface contours represent -100° K temperature

anomalies which have been trimmed at 1000 km depth for clarity and the surface of the light gray sphere indicates the effective spin transition depth (1600 km depth). A 2D-cross section of the temperature field has also been shown. Temperature is in Kelvin and the density anomaly in kg/m^3 .

Figure 5- Snapshots of the temperatures anomalies and the spin-transition induced density anomalies for the model [M05V1](#). The first column displays the temperature profiles in 20 Myr intervals. The panels of the second column display the total spin-transition induced density anomaly from which the spherically averaged value of the anomaly has been subtracted (i.e. $\Delta\rho_{\text{STot}} - (\Delta b\rho_{\text{STot}})_{\text{ave}}$). Temperature is in Kelvin and the density anomaly in kg/m^3 .

Figure 6- The radial velocity fields (second column) corresponding to the snapshots displayed in [Figure 5](#) are shown for the 2D-section of the 3D-model shown in [Figure 5](#) (first column). The arrows represent the total velocities. Temperature is in Kelvin and the velocity in m/s.

Figure 7- The snapshots of the model with V1-viscosity profile have been compared with their counterparts with V2-viscosity profile. The white wireframe sphere represents 1600 km depth and the cyan and pink spheres at 2000 km and 2600 km depths are shown for better visualization of the slab displacements.

Figure 8- The snapshots of the model [M02V3](#) and [M03V3](#) with a viscosity profile inferred from the spin transition consideration in ferropericlase (V3) have been compared. The white

789 wireframe sphere represents 1600 km depth and the cyan and pink spheres at 2070 km and 2370
790 km depths respectively are shown for better visualization of the slab displacements.