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Viscosity undulations in the lower mantle: The dynamical role of iron spin transition

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ABSTRACT

A proper determination of the lower-mantle viscosity profile is fundamental to understanding Earth geodynamics. Based on results coming from different sources, several models have been proposed to constrain the variations of viscosity as a function of pressure, stress and temperature. While some models have proposed a relatively modest viscosity variation across the lower mantle, others have proposed variations of several orders of magnitude. Here, we have determined the viscosity of ferropericlase, a major mantle mineral, and explored the role of the iron high-to-low spin transition. Viscosity was described within the elastic strain energy model, in which the activation parameters are obtained from the bulk and shear wave velocities. Those velocities were computed combining first principles total energy calculations and the quasi-harmonic approximation. As a result of a strong elasticity softening across the spin transition, there is a large reduction in the activation free energies of the materials creep properties, leading to viscosity undulations. These results suggest that the variations of the viscosity across the lower mantle, resulting from geoid inversion and postglacial rebound studies, may be caused by the iron spin transition in mantle minerals. Implications of the undulated lower mantle viscosity profile exist for both, down- and up-wellings in the mantle. We find that a viscosity profile characterized by an activation free energy of $G^*(z_0) \sim 300$–400 kJ/mol based on diffusion creep and dilation factor $\delta = 0.5$ better fits the observed high velocity layer at mid mantle depths, which can be explained by the stagnation and mixing of mantle material. Our model also accounts for the growth of mantle plume heads up to the size necessary to explain the Large Igneous Provinces that characterize the start of most plume tracks.

1. Introduction

Lower mantle viscosity has been the subject of great debate over the last decades (Sammis et al., 1977; Ricard and Wuming, 1991; Forte and Mitrovica, 2001), and its determination would be fundamental to address a number of questions on the mantle, such as its composition, heterogeneity, and geodynamics. Interpretation of data, coming from geoid inversion and postglacial rebound studies, indicated undulations in the viscosity profile, with peaks around 1300 and 2000 km deep and a valley around 1600 km (Mitrovica and Forte, 2004). If viscosity is considered as controlled by thermally activated microscopic mechanisms (Sammis et al., 1977; Ellsworth et al., 1985), this viscosity profile could not be easily reconciled with a single diffusion creep mechanism taking place in the lower mantle. Those variations in the lower mantle viscosity suggest that several microscopic competing diffusion mechanisms could be taking place in the mantle. On the other hand, the recent discovery of the iron spin transition in major mantle minerals (Badro et al., 2003, 2004; Lin et al., 2005, 2007; Speziale et al., 2005; Tsuchiya et al., 2006; Fei et al., 2007), and the corresponding anomalies in their elasticity (Crowhurst et al., 2008; Wentzcovitch et al., 2009; Marquardt et al., 2009; Wu et al., 2009; Antonangeli et al., 2011; Wu and Wentzcovitch, 2014), could reconcile the description of viscosity with a single thermally activated mechanism by using the available information from simultaneous inversion of geoid and post-glacial rebound data (Mitrovica and Forte, 2004).

Van Keken et al. (1992) found that some radial viscosity profile would produce a pulsating diapiric rise. This work has simulated numerous investigations of the effects of non-monotonous

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viscosity profile in the lower mantle. Tomographic models of slabs that penetrated in the lower mantle show strong signals of large body lying between 1500 and 2000 km depth (Grand, 1994), such as the Farallon slab (Sigloch et al., 2008). This result has been confirmed by the analysis of a variety of global tomographic models, e.g. Tx2007 (Simmons et al., 2006), Rmsl-s06 (Li et al., 2007), Saw642an (Panning and Romanowicz, 2006), all finding a clear transition from fast to slow shear seismic velocities for degree up to ~16 at a less than 1500 km depth (Boschi et al., 2008). Morra et al. (2010) showed that a sinking plate might penetrate, reorganize or even stall when crossing a 200 to 500 km high viscosity region in the middle of the lower mantle. Shahnas et al. (2011) used global mantle convection models to demonstrate that the only effects on the density of the iron spin transition enhances the vigor of rising plumes below 2000 km depth and slightly increases the temperature of the lowermost region of the mantle. Peltier and Drummond (2010) used glacial isostatic adjustment observations to infer a modest increase of the viscosity at mid mantle depths. Overall, those investigations have shown that a non-monotonic lower mantle viscosity profile would create substantial complications to the dynamics of sinking slabs and rising plumes. Here, we employ a standard scaling for plume head size evolution (e.g., Griffiths and Campbell, 1990; Ribe et al., 2007) integrating it along a one-dimensional vertical profile to calculate a broad range of solutions for the dynamics of a plume rise through a variety of physically based lower mantle viscosity profiles, obtained by first principles calculations of mineral elasticity.

We used the elastic properties of ferropericlase (Fp), $Mg_{1-x}Fe_xO$ with $x = 0.1875$, computed by a combination of first principles calculations and quasiharmonic approximation (Carrier et al., 2008; Wentzcovitch et al., 2009; Wu et al., 2013), to determine its viscosity under lower mantle conditions. Fp was treated as a solid solution in a mixed spin state, with the concentration of material with iron in high and low spin determined by the respective free energies. Although Fp is only the second most abundant lower mantle mineral, it is likely controlling deformation in the lower mantle (Zerr and Boehler, 1994; Yamazaki and Karato, 2001). This is justified by the fact that Fp is softer than the more abundant ferrosilicate perovskite under the same thermodynamic conditions. The viscosity of Fp was described within the elastic strain model (Sammis et al., 1977; Ellsworth et al., 1985), in which the activation energy parameters were computed along adiabatic (0.3 K/km) (Boehler, 2000) and superadiabatic (1.2 K/km) (da Silva et al., 2000) geotherms. The manuscript explores the role of dilatation and shear microscopic mechanisms (Ellsworth et al., 1985), variations in activation energies at the top of the lower mantle, and the Newtonian character of the mantle. The results show that the variations in Fp elasticity due to the iron spin transition can explain the undulations in the mantle viscosity, such as the viscosity hill about 800 km above the core–mantle boundary (Mitrovica and Forte, 2004).

2. Theoretical models

The viscosity (η) of Fp was described as a thermally activated process, as a result of diffusion of atomic species (Saha et al., 2013),

$$\eta = f(\sigma)\exp\left(\frac{G_e^*}{RT}\right) \tag{1}$$

where G_e^* is the Gibbs free energy of activation and $f(\sigma)$ is a function of stress. For a Newtonian fluid, $f(\sigma)$ is a constant and $G^* = G_e^*$, where G^* is the activation energy of the appropriate dynamical mechanism (Ellsworth et al., 1985). On the other hand, the effective viscosity of a power law fluid of order n is equivalent to the viscosity of a Newtonian fluid with an apparent activation energy $G^* = 2G_e^*/(n+1)$ (Karato, 1981). Here we have considered the mineral as a Newtonian fluid, consistent with assumptions used to determine the lower mantle viscosity experimentally (Mitrovica and Forte, 2004). Therefore, the viscosity at a certain depth z, $\eta(z)$, is given by:

$$\eta(z) = \eta(z_0)\exp\left(\frac{G^*(z)}{RT(z)} - \frac{G^*(z_0)}{RT(z_0)}\right) \tag{2}$$

where $z_0 = 670$ km (the top of the lower mantle), $\eta(z_0)$ and $G^*(z_0)$ are respectively the viscosity and the activation free energy at that reference depth.

The activation energy $G^*(z)$ can be described as a linear combination of energies from pure shear, $G_s^*(z)$, and pure dilatation, $G_D^*(z)$, mechanisms:

$$G^*(z) = \delta G_s^*(z) + (1-\delta)G_D^*(z) \tag{3}$$

where δ is a free parameter ($0 \le \delta \le 1$) that weights the respective contributions. Using the elastic strain energy model, those activation energies for pure shear and dilatation can be calculated in terms of the seismic velocities (Ellsworth et al., 1985),

$$\frac{G_s^*(z)}{G_s^*(z_0)} = \left[\frac{V_s(z)}{V_s(z_0)}\right]^2 \quad \text{and} \quad \frac{G_D^*(z)}{G_D^*(z_0)} = \left[\frac{V_\phi(z)}{V_\phi(z_0)}\right]^2 \tag{4}$$

where $V_s(z)$ and $V_\phi(z)$ are respectively the shear and bulk sound wave velocities at a depth z, which were computed from the mineral elastic constants (Wentzcovitch et al., 2009; Wu et al., 2013).

This model has five free parameters: δ, n, $G_s^*(z_0)$, $G_D^*(z_0)$, and $\eta(z_0)$. We have assumed that $G^*(z_0) = G_s^*(z_0) = G_D^*(z_0)$. Earlier phenomenological considerations (Ellsworth et al., 1985) have suggested $G^*(z_0) = 680$ kJ/mol at the top of the lower mantle. However, recent investigations have indicated considerably lower values for this activation energy, around 300 kJ/mol (Stretton et al., 2001; Van Orman et al., 2003; Ito and Tomiuri, 2007). We considered several values for this parameter, ranging from 200 to 500 kJ/mol. The competition between shear and dilatation mechanisms in the lower mantle is still not fully understood, such that we considered values for δ ranging from pure shear to pure dilatation.

According to Eqs. (2)–(4), the viscosity can be computed knowing the shear and bulk sound wave velocities as a function of depth. First of all, we considered adiabatic (≈0.3 K/km) and superadiabatic (≈1.2 K/km) geotherms, allowing explore variations in viscosity for different mantle temperature profiles. In order to compute the seismic velocities, we need the adiabatic bulk $K_s(z)$ and shear $\mu(z)$ moduli and the density $\rho(z)$ of Fp as a function of depth along a geotherm, which requires those properties as a function of pressure and temperature: $K_s(P,T)$, $\mu(P,T)$ and $\rho(P,T)$. In order to obtain those properties, a thermodynamic model to describe the Fp in a mixed spin state was recently developed (Wu et al., 2009, 2013). Within that model, the material, at finite temperatures and pressures, was described as a solid solution in thermal equilibrium, composed of concentrations of iron atoms in low and high spins. The high temperature properties in pure spin states were computed by a combination of first principles calculations and the quasiharmonic approximation (Carrier et al., 2008; Wentzcovitch et al., 2009). The first principles calculations were performed using a plane-wave-pseudopotential methodology in which the electron–electron interactions were described by an invariant version of the local density approximation plus Hubbard potential (LDA+U) (Cococcioni and de Gironcoli, 2005).

In modeling plume upwelling, we follow a standard theory (e.g., Griffiths and Campbell, 1990; Ribe et al., 2007) which relates the mantle viscosity profile with plume rising speed, plume head volume and plume conduit size. The instability that initiates the plume rises with speed $V = g\Delta\rho a^2/3\eta_0$, where a is the radius