Physics of the Earth and Planetary Interiors 188 (2011) 1–8

Contents lists available at ScienceDirect

Physics of the Earth and Planetary Interiors

journal homepage: www.elsevier.com/locate/pepi

The impact of variability in the rheological activation parameters on lower-mantle viscosity stratification and its dynamics

Ctirad Matyska[a], David A. Yuen[b], Renata M. Wentzcovitch[c], Hana Čížková[a,*]

[a] Department of Geophysics, Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, 180 00 Praha 8, Czech Republic
[b] Department of Geology and Geophysics and Minnesota Supercomputing Institute, University of Minnesota, 117 Pleasant Street, South East, 599 Walter Library, Minneapolis, MN 55455-0219, USA
[c] Chemical Engineering and Materials Science, University of Minnesota, 151 Amundson Hall, 421 Washington Ave. SE, Minneapolis, MN 55455-0219, USA

ARTICLE INFO

Article history:
Received 30 September 2010
Received in revised form 25 May 2011
Accepted 27 May 2011
Available online 7 June 2011

Keywords:
Lower-mantle dynamics
Activation parameters
Postperovskite (ppv) phase transition
Lower-mantle rheology
Radiative thermal conductivity
Plume clusters

ABSTRACT

The recently discovered spin-state crossover in iron in major mantle minerals at high pressures should exert dramatic influences on transport properties, such as the activation creep parameters in the deep mantle. Wentzcovitch et al. (2009) have computed the elastic parameter of ferropericlase that is affected by this crossover, the bulk modulus, at high realistic conditions, using first principles density functional theory plus Hubbard U. As a consequence of the spin crossover there is a significant softening of the bulk modulus and an attendant reduction of the activation energy in the creep law. Using a parameterized model capturing the basic physics, we have studied the dynamical consequences within the framework of a 2-D Cartesian convection model. Our models reveal a series of asthenospheres and are characterized first by a low-viscosity channel below the 670 km boundary ('second asthenosphere') caused by an increase of temperature and decrease in grain size reduction (superplascity) with the post-spinel transition, which results in partially layered convection. Further, the variability of the rheological parameters leads to the prevalent formation of viscosity minimum at a depth of about 1600 km ('third asthenosphere') caused by spin crossovers followed by a 'viscosity hill' in the bottom half of the lower mantle, the latter due to the increase of the activation energy in some low spin irons at the bottom of the mantle. Our numerical simulations reveal a tendency to the formation of small-scale convection below the 670 km boundary and bigger stabilized plumes – and/or plume clustering in the deep lower mantle. Other material properties at the bottom of the mantle (decrease of thermal expansivity, radiative thermal conductivity) also exert significant influence on the multi-scale lower-mantle plume dynamics.

1. Introduction

The dynamics of the lower mantle depends a great deal on material properties that are not well known but are generally believed to be greatly dependent on the pressure. These lower-mantle transport and thermodynamic properties – such as increased viscosity, increased lattice thermal conductivity, reduction in thermal expansivity due to increased pressure and also the radiative component of thermal conductivity (Matyska et al., 1994) are fundamental physical quantities, which result in the generation of superplumes and also, at the same time, other smaller scale dynamical features in the lower mantle (Hansen et al., 1993; Yuen et al., 1996; van Keken and Yuen, 1995; Matyska and Yuen, 2001, 2005, 2006, 2007; Deschamps et al., 2007; Tackley et al., 2007). Since the first attempt by McKenzie (1966), where a very high viscosity was predicted for the lower mantle based on the Earth's rotational shape, the viscosity stratification of the lower mantle has been fraught with some uncertainties. For over three decades the lower mantle was thought to have a relatively constant viscosity (Cathles, 1975; Peltier and Andrews, 1976; Hager et al., 1985; King and Masters, 1992), until the issue of multiplicity of lower-mantle viscosity solutions was raised concerning the rotational data (Sabadini et al., 1982; Yuen and Sabadini, 1985) in which a higher lower-mantle viscosity of 10^{22} to 10^{23} Pas was allowed. The notion of a 'viscosity hill' in the middle of the lower mantle was first developed by Ricard and Wuming (1991) from modeling the dynamic geoid and topography. This idea was further reinforced from both geoid and post-glacial rebound inversion by Forte and Mitrovica (2001) and Mitrovica and Forte (2004), Tosi et al. (2005) or recently by Soldati et al. (2009). However, a real physical explanation still remained elusive for a long time.

Recently, the high-to-low spin crossover in ferrous iron in ferropericlase (e.g. Badro et al., 2003; Lin et al., 2005, 2007a; Goncharov et al., 2006; Kantor et al., 2006; Tsuchiya et al., 2006a; Crowhurst et al., 2008; Lin and Tsuchiya, 2008; Wentzcovitch et al., 2009;

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* Corresponding author. Tel.: +420 2 21912544; fax: +420 2 21912555.
E-mail address: Hana.Cizkova@mff.cuni.cz (H. Čížková).

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doi:10.1016/j.pepi.2011.05.012

Wu et al., 2009; Hsu et al., 2010) and in ferrous and ferric irons in perovskite (McCammon, 1997; Badro et al., 2004; Frost et al., 2004; Li et al., 2004, 2006; Jackson et al., 2005; McCammon et al., 2008; Lin et al., 2008; Hofmeister, 2006; Zhang and Oganov, 2006; Stackhouse et al., 2007; Bengtson et al., 2008, 2009; Umemoto et al., 2008, 2010; Hsu et al., 2010, 2011; Catalli et al., 2010; Bower et al., 2009; Shahnas et al., 2011) have been extensively investigated by experiments, theory and dynamic modeling. Some of these studies have been able to address thermoelastic properties of these minerals at relevant pressure (P) and temperature (T) conditions (Lin et al., 2007b; Tsuchiya et al., 2006b; Wentzcovitch et al., 2009; Wu et al., 2009; Hsu et al., 2011) and there is clearly a bulk modulus softening during the spin crossover. Combining from first principles total energy calculations with classical elastic deformation theory Wentzcovitch et al. (2009) computed thermoelastic properties of ferropericlase. Preliminary results by Hsu et al. (2011) indicate similar effects along the spin crossover in perovskite in the same pressure range in the mantle. Shear and bulk sound wave velocities can be related to the activation energy G^* (e.g. Sammis et al., 1977), which has traditionally been taken to be a monotonically increasing function (e.g. Ranalli, 1995; Karato, 2008) and has been employed exclusively in mantle convection modeling (e.g. Schubert et al., 2001). Consequently, the viscosity η can be assumed as a thermally activated process in the Arrhenius sense

$$\eta = A \exp\left(\frac{G^*}{RT^*}\right), \tag{1}$$

where the prefactor A is a constant for a Newtonian fluid, R is the universal gas constant and T^* is the absolute temperature. Although ferropericlase is not the most abundant lower-mantle mineral, it probably controls lower-mantle deformations because of its relative softness (Zerr and Boehler, 1994; Yamazaki and Karato, 2001; Holtzman et al., 2005; Larkin et al., 2005; Wentzcovitch et al., 2009). The additional spin crossover in ferric iron in perovskite (Catalli et al., 2010; Hsu et al., 2011) should contribute to make the non-monotonicity in activation parameters even more a poignant issue.

Further clarification of activation parameters behavior and related micro/meso scale mechanisms related with plasticity in the spin crossover regime at mantle conditions is desirable. In particular, a first principles calculation of diffusion rates of high-spin and low-spin ferrous iron in periclase (Ammann et al., 2011) does not confirm the notion of reduced activation parameters. Deformation at the high temperatures and low stresses typical of the lower mantle should occur by diffusion creep and this type of calculation generally offers good insights on activation parameters for diffusion creep. However, the phenomenon of spin crossover is essentially a state change in a broad pressure range in a certain sense, resembling the two phase loop of a structural transformation. It is well known that during phase changes involving volume reduction, the bulk modulus softens and longitudinal velocities decrease (Li and Weidner, 2008). Also, visco-plastic deformation is observed during the transformation if subjected to stress perturbations with periods comparable to the transformation relaxation time. In the case of the olivine-ringwoodite system in the two-phase loop regime, the Q factor reduces to 5 for cyclic loads with periods 1000 s. Although relaxation times for spin crossovers should be short, stress relaxation is not simply accommodated by diffusion creep, but also by a continuous change in spin populations and/or configurations. Therefore, the deformation mechanism during spin state change should be more complex than simple diffusion creep, very likely involving also an anelastic component unrelated with diffusion but related with elasticity. In this situation, the elastic strain energy model should capture the essence of this phenomenon. In fact, deformation experiments at room temperature up to 81 GPa in ferropericlase (Lin et al., 2009), indicate a reduction in the strength of ferropericlase in the regime of the spin crossover. Deformation at room temperature under relatively large stresses should occur by dislocation creep, as opposed to by diffusion creep, therefore these results do not translate directly to deformation in the deep mantle. Nevertheless the reduction in strength in the mixed spin regime observed by Lin et al. (2009), supports the notion of a reduction in strength and therefore viscosity during spin crossovers in the mantle.

The main purpose of this paper is to demonstrate the dynamical influences exerted by the viscosity variations due to the possible non-monotonic behavior of the activation energy with depth and also horizontal temperature variations in the lower mantle. The main idea of the viscosity behavior due to the variability of activation energy with depth is illustrated in Fig. 1 – viscosity variations are very sensitive to both the activation energy G^* and local temperature field and thus even a relatively shallow local minimum of G^* can result in a substantial minimum of viscosity. Temperature gradients in both the vertical and horizontal directions are then important control parameters in determining the viscosity structure in the lower mantle. In the rest of the paper we will also discuss the role played by potential changes of local properties in the D''-layer on lower-mantle dynamics.

2. Model description

We have employed a two-dimensional Cartesian model for thermal convection in which the dimensionless stream function and temperature in the extended-Boussinesq approximation (e.g. Steinbach et al., 1989) are employed. The details of this model can be found in (Matyska and Yuen, 2007). We note that the mantle phase changes are set at a given depth within the framework of the effective thermal expansivity formulation (Christensen and Yuen, 1985). The Rayleigh number $Ra \equiv \rho_s^2 c_p \alpha_s \Delta T g d^3/\eta_{ref} k_s = 10^7$, ($\rho_s$ is the surface density, α_s is the surface thermal expansivity, ΔT is the temperature drop across the mantle, g is the gravity acceleration, d is the depth of the mantle used in the non-dimensionalization, c_p is the specific heat under a constant pressure, η_{ref} is a reference viscosity and k_s is the surface thermal conductivity). The dimensionless internal heating $R \equiv Qd^2/k_s\Delta T = 3$, where Q denotes volumetric heat sources, which corresponds approximately to one fourth of the whole mantle chondritic heating (e.g. Leitch and Yuen, 1989) because of our Cartesian geometry (O'Farrell and Lowman, 2010). Finally, the surface dissipation number Di used for adiabatic and viscous heatings $Di = \alpha_s g d/c_p = 0.5$ was chosen.

At a dimensionless depth $z = 0.23$, corresponding to a depth of 670 km, endothermic spinel-perovskite phase change was incorporated into all models by means of the buoyancy parameter $P = (\Delta\rho/\alpha_s \rho^2 g d)(dp/dT)$ equal to -0.08(ρ is a reference mantle density, $\Delta\rho$ is the density jump due to the phase change under consideration and dp/dT is the Clapeyron slope). The post-perovskite phase change near the core-mantle boundary at a depth $z = 0.92$, corresponding to a depth of 2680 km, with $P = 0.05$ was considered in the cases, when the ppv phase transition in the D''-layer was taken into account. Computations have been performed in a wide box with an aspect ratio equal to ten. One hundred twenty-nine evenly spaced points were employed in the vertical direction and the same resolution was used in the horizontal direction.

The dimensionless thermal expansivity profile decreasing with depth has been parameterized to