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Mantle dynamics with pressure- and temperature-dependent thermal expansivity and conductivity

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ABSTRACT

In numerical simulations of mantle convection it is commonly assumed that the coefficients of thermal expansion α and thermal conduction k are either constant or pressure-dependent. Pressure changes are generally computed using parametrizations that rely on extrapolations of low-pressure data for a single upper-mantle phase. Here we collect data for both the pressure and temperature dependence of α from a database of first-principles calculations, and of k from recent experimental studies. We use these datasets to construct analytical parametrizations of α and k for the major upper- and lower-mantle phases that can be easily incorporated into exisiting convection codes. We then analyze the impact of such parametrizations on Earth's mantle dynamics by employing two-dimensional numerical models of thermal convection. When α is the only variable parameter, both its temperature and pressure dependence enhance hot plumes and tend to inhibit the descent of cold downwellings. Taking into account a variable k leads to a strong increase of the bulk mantle temperature, which reduces the buoyancy available to amplify bottom boundary layer instabilities and causes mantle flow to be driven primarily by the instability of cold plates whose surface velocity also tends to rise. When both parameters are considered together, we observe an increased propensity to local layering which favors slab stagnation in the transition zone and subsequent thickening in the lower mantle. Furthermore, the values of k near the core-mantle boundary ultimately control the effect of this physical property on convection, which stresses the importance of determining the thermal conductivity of the post-perovskite phase.

1. Introduction

The coefficients of thermal expansion α and thermal conduction k control the way heat is transported in the interior of solid planets by advection and diffusion, thereby affecting the dynamics and thermal evolution of the mantle. From laboratory experiments, it is well known that both parameters exhibit significant variations with pressure and temperature whose magnitude varies among different mineral phases (e.g. Fei, 1995; Xu et al., 2004; Katsura et al., 2009a,b; Manthilake et al., 2011a). Nevertheless, in most numerical simulations of mantle convection in the Earth and terrestrial planets, α and k are either assumed constant or their pressure (i.e. depth) dependence only is taken into account according to simplified parametrizations (e.g. Leitch et al., 1991; Hansen et al., 1993; Naliboff and L.H., 2006; Zhong, 2006; Foley and Becker, 2009; Schuberth et al., 2009; Nakagawa et al., 2010; Phillips and Coltice, 2010; Tan et al., 2011). A few attempts have been made to describe in a more detailed way the dynamical impact of variable α and k on mantle dynamics. Schmeling et al. (2003) and Ghias and Jarvis (2008) accounted for the pressure and temperature dependence of the thermal expansivity using a Birch–Murnaghan equation of state and the experimental data of Fei (1995) for olivine only in simple models of isoviscous convection. Matyska and Yuen (2005) discussed the effects of the strongly temperature-dependent radiative part of the thermal conductivity on the dynamics of the lower mantle. Tosi et al. (2010) presented global convection models with multiple phase transitions that incorporated experimental constraints on the thermal and transport properties of lower-mantle minerals. Hunt et al. (2012), in conjunction with measurements of the thermal conductivity of a post-perovskite low-pressure analog, showed simple simulations of isoviscous convection including a phase-dependent jump in thermal

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conductivity across the perovskite to post-perovskite interface. Maierová et al. (2012) reported results from kinematic models of subduction incorporating variable thermal conductivity associated with a detailed upper mantle phase-diagram.

Important efforts have also been made to account for a self-consistent treatment of mantle mineralogy and thermodynamics in numerical models of mantle convection on the base of pre-compiled look-up tables from which physical properties derived from thermodynamic databases can be interpolated (e.g. Nakagawa et al., 2010; Jacobs and van den Berg, 2011). Nevertheless, simple and up-to-date parametrizations for the major mantle minerals of key parameters such as α and k would facilitate their incorporation into existing numerical convection codes. Here we make use of data of thermal expansivity derived from the thermodynamic database of first-principles simulations of the Virtual Laboratory for Earth and Planetary Materials of the University of Minnesota (VLab, www.vlab.msi.umn.edu). In addition, we collect recent thermal conductivity data based on experiments performed on both the upper and lower-mantle major mineral phases (Xu et al., 2004; Manthilake et al., 2011a).

We first employ these data sets to construct analytical parametrizations that describe both the pressure and temperature dependence of α and k for forsterite and its high-pressure phases, as well as for perovskite and periclase. After describing the setup of our numerical model, we discuss the impact of the above parametrizations on the dynamics of the Earth's mantle using 2D numerical convection simulations in Cartesian geometry featuring a rheology which can mimic plate-like behavior and three major phase transitions covering the entire mantle.

2. Parametrization of the thermal expansivity and conductivity

2.1. Thermal expansivity based on VLab data

The VLab service-oriented cyberinfrastructure (da Silva et al., 2007) consists of a portal, web services (da Silveira et al., 2008), workflows for first-principles computations of elastic and thermodynamic properties of materials (Wentzcovitch et al., 2010; da Silveira et al., 2012) in distributed environments (da Silveira et al., 2008, 2011), databases of raw inputs/outputs of successful calculations, and internet applications for obtaining thermodynamic properties of minerals (da Silveira et al., 2008, 2011). The latter are the source of the thermodynamic data utilized in this paper and are freely accessible online (VLab-ThoM, www.vlab.msi.umn.edu/resources/thermodynamics). These applications run interactive quasiharmonic (QHA) calculations (Wallace, 1972) using as input pressure-dependent vibrational density of states (VDoS) generated by first-principles calculations for a collection of minerals (Wentzcovitch et al., 2010). All VDoSs were obtained using codes of the Quantum ESPRESSO distribution (Giannozzi et al., 2009). The Thermodynamics of Minerals (ThoM) application produces volume, thermal expansion coefficient, specific heat (at constant pressure or volume), bulk modulus (isothermal or adiabatic), enthalpy, Gibbs free-energy and Grüneisen parameter, all on user-defined pressure–temperature grids, viewed as tables onscreen, to be downloaded, or analyzed visually as 2D plots through an interactive graphical interface (da Silveira et al., 2011).

Among these thermodynamic properties, the thermal expansivity exerts a first-order impact on the dynamics of the mantle as it controls the thermal buoyancy that drives convection. QHA expansivities for Mg_2SiO_4-forsterite (Li et al., 2007; Yu et al., 2008), -wadsleyite (Wu and Wentzcovitch, 2007), -ringwoodite (Yu and Wentzcovitch, 2006), MgO-periclase (Karki et al., 2000a; Umemoto et al., 2006) and $MgSiO_3$-perovskite (Karki et al., 2000b; Umemoto et al., 2006) were then regenerated using the ThoM application. As the thermodynamic properties of perovskite and post-perovskite phases of $MgSiO_3$ are very similar at CMB conditions (Tsuchiya et al., 2005), we have used the same expansivity for both. The expansivity values employed in the simulations that we carried out were obtained within the limit of validity of the QHA (Carrier et al., 2007) and for pure Mg end-member compositions. Regarding the latter assumption, it should be mentioned that the presence of Fe impurities is not expected to have a strong effect on the thermal expansivity (Wu et al., 2009; Metsue and Tsuchiya, 2012). First-principles simulations conducted on ferropericlase ($(Mg_{1-x}Fe_x)O$, $x = 0.1875$, Wu et al., 2009) agree extremely well with experimental measurements, at zero-pressure, of the expansivity of both periclase ($x = 0$, Touloukian et al., 1977) and ferropericlase ($x = 0.36$, Westrenen et al., 2005). Nevertheless, spin transitions would affect the thermal expansion and other properties of the aggregate with possible consequences for mantle convection (Bower et al., 2009; Shahnas et al., 2011). According to Metsue and Tsuchiya (2012), the spin state would also influence the expansivity of ferrosilicate perovskite ($(Mg_{1-x}Fe_x)SiO_3$, $x = 0.0625$). The effect however would not be large and would decrease upon compression.

Panels a–d in Fig. 1 show the corresponding distributions of α as a function of pressure and temperature. To obtain Fig. 1d, we assumed a standard lower-mantle assemblage consisting of 80% perovskite and 20% periclase. Fig. 1e depicts the radial profile of the thermal expansivity along a reference adiabat with potential temperature of 1600 K and two 100 km thick thermal boundary layers (TBL) (black lines); the blue and red lines show the profile of α along 200 K colder and hotter adiabats, respectively, while the green line is associated with a linear increase of temperature throughout the mantle without boundary layers. The surface and CMB temperatures are set to 300 K and 4000 K, respectively. The variability of the thermal expansivity is mostly evident in the uppermost part of the mantle. Here the strong increase of temperature across the top TBL determines a significant growth of α, which reaches almost twice the reference surface value for the hottest geotherm. Below the TBL, a steady decrease throughout the upper mantle is observed, with a pronounced jump across the olivine–wadsleyite transition where α decreases abruptly. A second, albeit less pronounced, jump is observed at the wadsleyite–ringwoodite transition. At the top of the lower mantle, another discontinuity is evident, with perovskite and periclase having a slightly higher expansivity than ringwoodite. Throughout the lower mantle, the value of α steadily diminishes apart from a minor increase due to temperature across the bottom TBL. Apart from a small increase in the uppermost mantle, the expansivity profile resulting from a linearly increasing temperature (green line) resembles the distribution used in previous studies in which only a depth-dependent and steadily decreasing α was taken into account (e.g. Tosi et al., 2010). Although this assumption appears to be reasonable for the lower mantle, it leads to an underestimation of α by up to $\sim 40\%$ in the upper mantle.

In order to facilitate the incorporation of the pressure and temperature dependence of the thermal expansivity in mantle convection codes, we used the Levenberg–Marquardt algorithm (e.g. Moré, 1978) to fit the VLab data to the following four-parameters function:

$$\alpha(T,P) = (a_0 + a_1 T + a_2 T^{-2}) \exp(-a_3 P), \quad (1)$$

where T is absolute temperature in K, P is hydrostatic pressure in GPa, and $a_i, i = 0,\ldots,3$ are phase-dependent coefficients obtained from the inversion of the data. Since the governing equations of thermal convection are generally discretized in terms of depth instead of hydrostatic pressure, we also provide a formula for the temperature and depth dependence of α that we obtained by integrating numerically the PREM density profile together with the associated gravity (Dziewonski and Anderson, 1981):