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Thermo-chemical constraints on the interior structure and composition of the lunar mantle

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Based on a self-consistent thermodynamic-geophysical approach, we convert the recent seismic models of the lunar mantle to the temperature-depth profiles using Gibbs free energy minimization and petrological constraints in the $Na_2O–TiO_2–CaO–FeO–MgO–Al_2O_3–SiO_2$ system. Our calculations are unable to explain the reasonable distribution of temperature for a single homogeneous composition throughout the entire lunar mantle with concentrations of CaO and Al_2O_3 in the range of 2–6.5%, and FeO content between 8.5% and 13%. The results lend support to the chemically stratified lunar mantle with a change in composition from predominantly pyroxenite upper mantle depleted in Ca and Al to predominantly fertile lower mantle enriched in Ca and Al with larger amounts of garnet. Such a zoned structure places significant constraints on any theory of lunar origin. Unlike the Earth's mantle, compositional effects play a dominant role in determining the lunar mantle temperatures of the same observational model. Seismically derived temperatures allow us to constrain thermal structure of the lunar mantle and estimate the upper mantle heat flow (3.8–4.7 mW m^{-2}), which is not consistent with that found from the Apollo heat flow and thorium abundance measurements. Lower mantle temperatures are well below the probable solidus condition and can be evaluated at the level of 1420–1550 °C at the core-mantle boundary without requiring a melt layer. We find that regardless of the composition, the positive *S*-wave velocity gradient in the lunar mantle leads to a negative temperature gradient, which has no physical basis. The resulting temperature profiles provide an effective independent tool that allows us to discriminate between the available seismic and petrological models.

1. Introduction

The internal structure of the Moon depends strongly on its composition and thermal regime. However, geochemical studies of returned lunar samples place weak constraints on the composition and physical properties of the mantle whereas the current electromagnetic, seismic and surface heat-flow observations provide only indirect information about the composition and temperature of the lunar interior. In spite of the fact that a lot of works have been concerned with the thermal history of the Moon (Basaltic Volcanism Study Project, 1981; Konrad and Spohn, 1997; Shearer et al., 2006; Ziethe et al., 2009; Laneuville et al., 2013; Zhang et al., 2013; Evans et al., 2014), the present temperature of the lunar interior remains one of the most speculative and uncertain physical parameters.

Previous reviews (Taylor, 1982; Ringwood, 1977; Hood, 1986) summarized geochemical and geophysical constraints derived from Apollo-era measurements on lunar composition and thermal history. A comprehensive review of the constitution and structure of the lunar interior has recently been made by Lognonné (2005), Wieczorek et al. (2006), Khan et al. (2013). There have been numerous previous studies that have exhaustively discussed some unresolved differences existing among the geophysical, compositional and thermal models (Hood and Jones, 1987; Mueller et al., 1988; Williams et al., 2001; Khan et al., 2006a,b; Kronrod and Kuskov, 2011; Grimm, 2013; Zhang et al., 2013; Gudkova and Raevskii, 2013). However, several key aspects of the thermal structure and chemical composition of the lunar mantle are uncertain and merit further investigation. Quantitative estimation of the temperature distribution remains a key problem in lunar petrology and geophysics.

This study is motivated by the availability of improved models of the seismic structure of the deep interior based on both *P* and *S*

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wave velocity models (Khan et al., 2000, 2007; Lognonné et al., 2003; Lognonné, 2005; Gagnepain-Beyneix et al., 2006; Weber et al., 2011; Garcia et al., 2011). In this paper, we consider the potential of these models to estimate the temperature in the lunar mantle. The method we propose, allow us to take a critical look at the present state of the Moon and to find out whether the seismic models are consistent with thermal and compositional constraints.

2. Data and method

Thermodynamic basis for modeling of the phase equilibria and physical properties in the Earth's and lunar mantle and various databases have been discussed in a series of papers (e.g., Saxena and Eriksson, 1983; Stixrude and Lithgow-Bertelloni, 2011; Kuskov, 1997). Here, we use a thermodynamically self-consistent approach described in detail in our previous publications (Kuskov and Kronrod, 1998, 2009; K&K98, K&K09) where the isotropic seismic velocities are converted to temperatures based on a method of Gibbs free energy minimization combined with a Mie–Grüneisen equation of state (EOS) of minerals, and incorporating phase transformations, anharmonicity (thermal expansion and compressibility), and attenuation effects (anelasticity of mantle material at high temperatures). The aggregate elastic properties were estimated by Voigt–Reuss–Hill averaging.

The phase composition and physical properties of the mantle were modeled within the dry Na_2O–TiO_2–CaO–FeO–MgO–Al_2O_3–SiO_2 (NaTiCFMAS) system including the non-ideal solid solution phases. Chemical reactions in this system are independent of oxygen fugacity. Addition of Al_2O_3, Na_2O and TiO_2 is important for stability of garnet, two aluminous pyroxenes, and Ti-bearing phases (Wieczorek et al., 2006; Thacker et al., 2009; Sakamaki et al., 2010; van Kan Parker et al., 2011).

Although the presence of fluids, particularly water, provide an important role in resolving the thermal and magmatic evolution of the Moon (Shearer et al., 2006; Saal et al., 2008; Evans et al., 2014) and have an important impact on velocities (Kuskov et al., 1996) and electrical conductivity (Karato, 2013; Grimm, 2013), we will consider the dry (water-free) lunar interior in agreement with high *Q* and seismic velocities (Lognonné, 2005; Gagnepain-Beyneix et al., 2006; Garcia et al., 2011). Kuskov et al. (1996) have shown that the coexistence of ultramafic rocks with water-containing phases in the lunar mantle would lead to a strong decrease in velocity (and accompanying decrease in density) that is not consistent with the present seismic models (Gagnepain-Beyneix et al., 2006). However petrologic modeling suggests that the lunar mantle may contain about 10–100 ppm water (Elkins-Tanton and Grove, 2011; Tartèse et al., 2013; Khisina et al., 2013; Robinson and Taylor, 2014). A direct effect of the presence of such an amount of water in the mantle on seismic velocities and densities is negligible (Karato, 2011). We ignore also the effect of grain size (Nimmo et al., 2012; Karato, 2013) on anelasticity due to the large uncertainty and lack of experimental data on multicomponent solid solutions. We assume that the lunar mantle remains in a conductive heat transport regime or, strictly speaking, a dry model of the lunar mantle is predominantly conductive.

Input data for the thermodynamic quantities are summarized in the THERMOSEISM database (Fabrichnaya and Kuskov, 1991; Kuskov, 1997; Kuskov et al., 2014). The database was established by supplementing the calorimetric data for low-pressure phases and the EOS for low- and high-pressure phases with data calculated from high-*P-T* experiments. The output *P-T* results contain self-consistent information on the phase assemblage (the mineral phases, their proportions and individual chemical compositions), the total density and seismic velocities. The pressure distribution is approximated by the simplified expression $P = P_o\{1 - [(R - H)/R]^2\}$, where $P_o \sim 5$ GPa is the pressure at the center of the Moon, $R = 1738$ km, and H is the depth (K&K09; Garcia et al., 2012).

Sources of uncertainty involved in thermodynamic calculations, which are common to all of the compositions are discussed elsewhere (Fabrichnaya and Kuskov, 1994; Kuskov et al., 2002). For a given chemical composition, the effect on density and both velocities of temperature variations of ±150 °C is not higher than ±0.02 g cm^{-3} (0.6%) and ±0.07 km s^{-1} for V_P (0.9%) and ±0.06 km s^{-1} for V_S (1.3%). According to Gagnepain-Beyneix et al. (2006), the reported uncertainties in V_S and V_P are 1–1.5% at depths of 40–500 km and ~2.5% at depths of 500–1000 km. These uncertainties do not allow us to constrain temperatures from seismic models any tighter than ±100–150 °C.

Temperature dependence of seismic velocities comes both from anharmonicity and anelasticity. The lunar upper-mantle $Q_{P,S}$-values are around 1500–9000 (Nakamura and Koyama, 1982; Garcia et al., 2011), implying temperatures well below the solidus and absence of volatiles. This means that the uncertainties resulting from the anelastic correction are negligible in this depth range. However seismic observations argue for a warmer, more ductile lower mantle (Lognonné and Johnson, 2007). Thus, anelasticity can have an important effect on seismic properties, particularly when temperatures approach the solidus in the deep mantle (Khan and Mosegaard, 2005; Nimmo et al., 2012). We estimate the anelastic correction using the method described in the recent papers (e.g., Cammarano et al., 2003; Khan et al., 2007; K&K09). The solidus temperature of pyroxenite (Ringwood and Essene, 1970) is close to that for peridotite (Hirschmann, 2000). The solidus of harzburgite is situated at higher temperatures than the solidus for peridotite (Maaløe, 2004). The velocity conversion yields a temperature profile that is consistent with the equilibrium phase composition and density of the mineral assemblage at a given depth.

3. Seismic context

Since the publication of earlier works (e.g., Goins et al., 1981; Nakamura, 1983) additional results have become available (Khan et al., 2000, 2006a,b, Khan et al., 2007; Lognonné et al., 2003; Lognonné, 2005; Gagnepain-Beyneix et al., 2006; Garcia et al., 2011; Weber et al., 2011). In spite of different inversion results and physical interpretation, these models describe with increasing accuracy the internal structure of the lunar mantle. Despite the agreement between these various models is not perfect (Fig. 1), we use some of them for the assessment of thermal state of the lunar mantle.

A complete independent analysis of the Apollo data by Lognonné (2005), Gagnepain-Beyneix et al. (2006) presented new seismic models and shown a fair agreement in *P*-, *S*- velocities with those from earlier studies at depths of the upper mantle but found a significant difference in the middle and lower mantle where several discontinuities were found. The GB06 model is an improvement over the preliminary model of L05 and possesses somewhat smaller error bars. A model of Weber et al. (2011) at depths shallower than ~740 km is derived mainly from previous studies (L05; GB06) with a jump of a *P*-velocity value up to 8.5 km s^{-1} at greater depths.

Khan et al. (2000) found a uniform distribution of seismic velocities up to 500 km depth, which differs from other seismic models (Fig. 1). In the subsequent papers, Khan and coworkers (Khan et al., 2006a,b, 2007) presented a general approach to an integrated inversion of a priori unrelated geophysical data to constrain internal structure of the Moon; no substantial velocity changes were found, reflecting the implicit homogeneity of V_P and V_S in the lunar mantle. Kronrod and Kuskov (2011) using a