



Variation of thermal conductivity and heat flux at the Earth's core mantle boundary



Michael W. Ammann^a, Andrew M. Walker^{b,c,*}, Stephen Stackhouse^c, James Wookey^b, Alessandro M. Forte^d, John P. Brodholt^a, David P. Dobson^a

^a Department of Earth Sciences, University College London, Gower Street, London, WC1E 6BT, UK

^b School of Earth Sciences, University of Bristol, Wills Memorial Building, Queen's Road, Bristol, BS8 1RJ, UK

^c School of Earth and Environment, University of Leeds, Leeds, LS2 9JT, UK

^d GEOTOP – Dépt. Sci. Terre & Atmosphère, Université du Québec à Montréal, CP 8888, succursale Centre-Ville, Montréal, QC H3C 3P8, Canada

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ABSTRACT

The two convective systems that dominate Earth's internal dynamics meet at the boundary between the rocky mantle and metallic liquid core. Energy transfer between processes driving plate tectonics and the geodynamo is controlled by thermal conduction in the lowermost mantle (D''). We use atomic scale simulations to determine the thermal conductivity of MgSiO₃ perovskite and post-perovskite under D'' conditions and probe how these two convective systems interact. We show that the thermal conductivity of post-perovskite (~12 W/mK) is 50% larger than that of perovskite under the same conditions (~8.5 W/mK) and is anisotropic, with conductivity along the *a*-axis being 40% higher than conductivity along the *c*-axis. This enhances the high heat flux into cold regions of D'' where post-perovskite is stable, strengthening the feedback between convection in the core and mantle. Reminiscent of the situation in the lithosphere, there is potential for deformation induced texturing associated with mantle convection to modify how the mantle is heated from below. We test this by coupling our atomic scale results to models of texture in D'' and suggest that anisotropic thermal conductivity may help to stabilise the roots of mantle plumes over their protracted lifetime.

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1. Introduction

Thermal interaction between the core and mantle is central to our understanding of the Earth's energy budget (Gubbins, 2003; Lay et al., 2008). In the absence of substantial chemical mixing heat is only transported across the core mantle boundary (CMB) by conduction in the lowermost mantle (D''). The rate of cooling of the top of the core and heating of the base of the mantle is therefore controlled by the temperature difference between the core and the interior of the mantle and the thermal conductivity of materials such as (Mg, Fe)SiO₃ perovskite and post-perovskite found in D''. However, the thermal conductivity of these materials under high pressure ($P \sim 135$ GPa) and temperature ($T \sim 2000$ – 4000 K) conditions is unknown. Historically, estimates of thermal conductivities at the CMB from low pressure or low temperature experiments, theoretical considerations and extrapolations are 4–29 W/mK (e.g. Osako and Ito, 1991; Hofmeister, 1999, 2008). Ongoing experimental work is aimed at refining these estimates but, as yet, it is still not possible to mea-

sure thermal conductivity under the conditions of simultaneously high *P* and *T* found at the CMB. Manthilake et al. (2011) performed measurements on MgSiO₃ perovskite, at 26 GPa, and MgO to 14 GPa and 1273 K in a multi-anvil cell. Goncharov et al. (2009) and Dalton et al. (2013) measured the thermal conductivity of MgO at 300 K to 32 GPa and 60 GPa, respectively, using a diamond anvil cell to generate pressure. Goncharov et al. (2010) performed a similar experiment on perovskite at 125 GPa and 300 K. The latest experimental results (Ohta et al., 2012) reach 144 GPa and include both MgSiO₃ perovskite and post-perovskite but are limited to near-ambient temperatures (300–436 K). These results reveal that post-perovskite has ~60% larger conductivity than perovskite and that the conductivity of perovskite increases from 8 to 37 W/mK as pressure increases from 8 to 144 GPa.

Recently, to avoid the formidable experimental challenges in determining thermal conductivity to high pressure and temperature, considerable effort has been expended in the development of tools to make use of atomic scale simulations to calculate the thermal conductivity of lower mantle phases. Much of this work, reviewed by Stackhouse and Stixrude (2010), has focused on MgO where a range of different techniques have been used. For example, Cohen (1998) made use of equilibrium molecular dynamics (MD), interatomic potentials and Green-Kubo

* Corresponding author at: School of Earth and Environment, University of Leeds, Leeds, LS2 9JT, UK.

E-mail address: a.walker@leeds.ac.uk (A.M. Walker).

theory, [Tang and Dong \(2009\)](#) used anharmonic lattice dynamics (LD) truncated to third-order and density functional theory (DFT), [de Koker \(2009, 2010\)](#) combined DFT, MD and LD in the harmonic approximation, and [Stackhouse et al. \(2010\)](#) used DFT and non-equilibrium molecular dynamics (NEMD). Importantly, results of these studies are broadly in agreement with each other, and with the available experimental data (see [Stackhouse and Stixrude, 2010](#), Fig. 6).

There has been less attention focused on MgSiO_3 perovskite or post-perovskite, despite these phases dominating the mineralogy of the lower mantle and D'' , respectively. As discussed below [Stackhouse et al. \(2009\)](#) reported preliminary results for perovskite using DFT and NEMD. Very recently [Haigis et al. \(2012\)](#) used an interatomic potential model, MD and Green–Kubo theory to predict the thermal conductivity of MgO and the two MgSiO_3 phases to CMB conditions while [Dekura et al. \(2013\)](#) made use of anharmonic LD and DFT to probe the conductivity of perovskite. At low temperature the results of [Haigis et al. \(2012\)](#) give thermal conductivities substantially higher than the available experimental data and these authors appeal to an isotopic correction to reduce their calculated conductivities to values in better agreement with experiment (phonon scattering by atoms with a mass different to their replicas in adjacent unit cells will reduce the thermal conductivity). However, an isotopic correction is not applied by [Cohen \(1998\)](#), [de Koker \(2009, 2010\)](#) or [Stackhouse et al. \(2010\)](#) but their results for MgO are in reasonable agreement with the experiments (although the focus is not always on the low temperature properties where isotopic effects are most important). The LD calculations ([Dekura et al., 2013](#)) give good agreement with experiment at low temperature but the results deviate from the experiments of [Manthilake et al. \(2011\)](#) at higher temperatures. There is clearly further work needed to fully understand these methods at low temperature where the conductivity is most difficult to predict (e.g. where the effect of isotopic disorder is maximised). Work reported by, e.g. [Sellan et al. \(2010\)](#), [Hu et al. \(2011\)](#) and [Beck et al. \(2013\)](#) is a significant step in this direction. Nevertheless, under the high temperature conditions interesting for core–mantle interaction the various computational approaches are in good agreement and this motivates the current study, which has the aim of using atomic scale simulation to probe the variation of thermal conductivity in D'' .

Before outlining our approach it is important to note that all these calculations only capture the portion of heat transport caused by interactions between lattice vibrations (phonons). This lattice conductivity is believed to dominate in insulating solids like the mantle silicates and we neglect the electronic conductivity (important in metals, see [Pozzo et al., 2012](#)) and radiative heat transport, which is expected to be altered by the iron spin transition at high pressure (see [Lin et al., 2013](#), for a recent review). The importance of the radiative heat transport is disputed ([Hofmeister, 1999](#); [Keppler et al., 2008](#); [Goncharov et al., 2008](#)), but this process will contribute a maximum of 50% of the total conductivity (5 W/mK, [Keppler et al., 2008](#)), and probably much less (0.5 W/mK, [Goncharov et al., 2008](#)) in perovskite, and certainly in post-perovskite ([Goncharov et al., 2010](#)).

2. Methodology

We use the so-called direct scheme ([Müller-Plathe, 1997](#); [Nieto-Draghi and Avalos, 2003](#); [Stackhouse and Stixrude, 2010](#)) and invoke non-equilibrium molecular dynamics to calculate the thermal conductivity of perovskite and post-perovskite. In this method, physical reality is inverted in the sense that one imposes a heat flux leading to a thermal gradient (instead of a thermal gradient leading to a heat flux). The single crystal thermal conductivity k is

then given by the ratio of the time-averages of the heat flux (J) across a unit area and the temperature gradient (dT/dx):

$$k = -\frac{\langle J \rangle}{\langle dT/dx \rangle}. \quad (1)$$

The heat flux is imposed by virtual elastic scatters between two atoms in separated sections of a long simulation cell. The atom with the highest kinetic energy in the designated cold section and the one with the lowest kinetic energy in the hot section swap their momenta, effectively transferring heat from the cold to the hot section (see [Stackhouse and Stixrude, 2010](#), for details). In order to avoid the high computational costs and system-size limitations one encounters using density functional theory (DFT), which are particularly heavy for the large unit cells of perovskite and post-perovskite, we primarily made use of the two established interatomic potential parameterisations of [Murakami et al. \(2004\)](#) and [Oganov et al. \(2000\)](#). The choice of interatomic potential is critical to the success of our calculations and we note that a recent appraisal of 27 possible choices found that the [Oganov et al. \(2000\)](#) model and similar parameterisations were the most successful ([Chen et al., 2012](#)). The [Murakami et al. \(2004\)](#) model was not included in the study of [Chen et al. \(2012\)](#). In order to undertake these calculations we modified the code GULP ([Gale and Rohlf, 2003](#)) to implement the direct scheme for arbitrarily complex systems. The use of interatomic potentials allowed us to perform simulations with up to 11,520 atoms while maintaining predictive power. System-size effects were corrected by extrapolating to infinite cell size ([Schelling et al., 2002](#)) and by checking convergence on the cross-sectional area (see below). We also perform DFT simulations of smaller supercells as a test of the interatomic potentials. These calculations were performed with a modified version of the VASP code ([Stackhouse and Stixrude, 2010](#)).

To determine the cell parameters as a function of pressure and temperature we first performed equilibrium molecular dynamics (MD) for both phases at a constant pressure and constant temperature using the modified Nosé–Hoover thermostat ([Melchionna et al., 1993](#)) in $3 \times 3 \times 3$ super-cells. We used a time-step of 1 fs and the thermo- and barostat parameters both set to 0.05. After equilibration for 5 ps the time averages over a production run of 20 ps were used. The resulting parameters (pressure, temperature, unit cell parameters) are tabulated in the Supplementary Information. These parameters were used to calculate cell volumes for the non-equilibrium molecular dynamics runs used to calculate the thermal conductivity.

NEMD simulations were performed at a constant volume and a constant temperature using a Nosé–Hoover thermostat ([Nosé, 1984, 1985](#)) with a thermostat parameter of 0.05 and time-step of 1 fs. After 5 ps equilibration with MD, we started the NEMD simulation which ran for 100 ps. Following convergence testing ([Fig. 1](#)) energy was swapped every 20 fs (i.e., every 20th time-step). This established a thermal gradient across the simulation cell, and the temperatures of the slices within our simulation cell reached a constant temperature after about 30 ps. To calculate k the simulation cell of dimensions $N \times D \times D$ was divided into $2N$ slices each containing an equal number of atoms. As shown in [Fig. 2](#) we fitted weighted straight lines following [York \(1966, 1967\)](#) and calculated errors of our time-averages of temperature and energy-flux with the blocking method ([Flyvberg and Petersen, 1989](#)). The thermal gradients in the simulation cells were fitted to the central 33% of all slices between the hot and cold slice. However, for the smallest cells ($N \times 3 \times 3$ when $N = 6$ and 8) we excluded only the hot and cold slice for the fitting procedure. The same weighted linear fitting method was used to extrapolate from finite cell length to infinite cell length ([Schelling et al., 2002](#)), see [Fig. 3](#) for examples, and to calculate the errors on the fitting parameters (slope and

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