The Rise and Fall of the Lower Mantle: Modelling Thermal Conductivity in Earth's Interior

Stephen Stackhouse
email: s.stackhouse@leeds.ac.uk www: http://www.see.leeds.ac.uk/people/s.stackhouse
Andrew Walker
email: a.walker@leeds.ac.uk www: http://www.see.leeds.ac.uk/people/a.walker
Jon Mound
email: j.e.mound@leeds.ac.uk www: http://www.see.leeds.ac.uk/people/j.mound

1. Introduction

The Earth's lower mantle is convecting, with cold slabs subducting and hot plumes rising (Figure 1). Surface expressions of this large-scale convection include earthquakes, volcanism, oceanic trenches, mid-ocean ridges and island arc chains. The key role of heat transport means that thermal conductivity is a fundamental parameter in controlling mantle processes. In addition, as the thermal conductivity of the mantle mediates heat-loss from the core, it will also have significant implications for the thermoevolution of the Earth (Lay et al., 2008) and magnetic field generation (Gubbins et al. 2011).

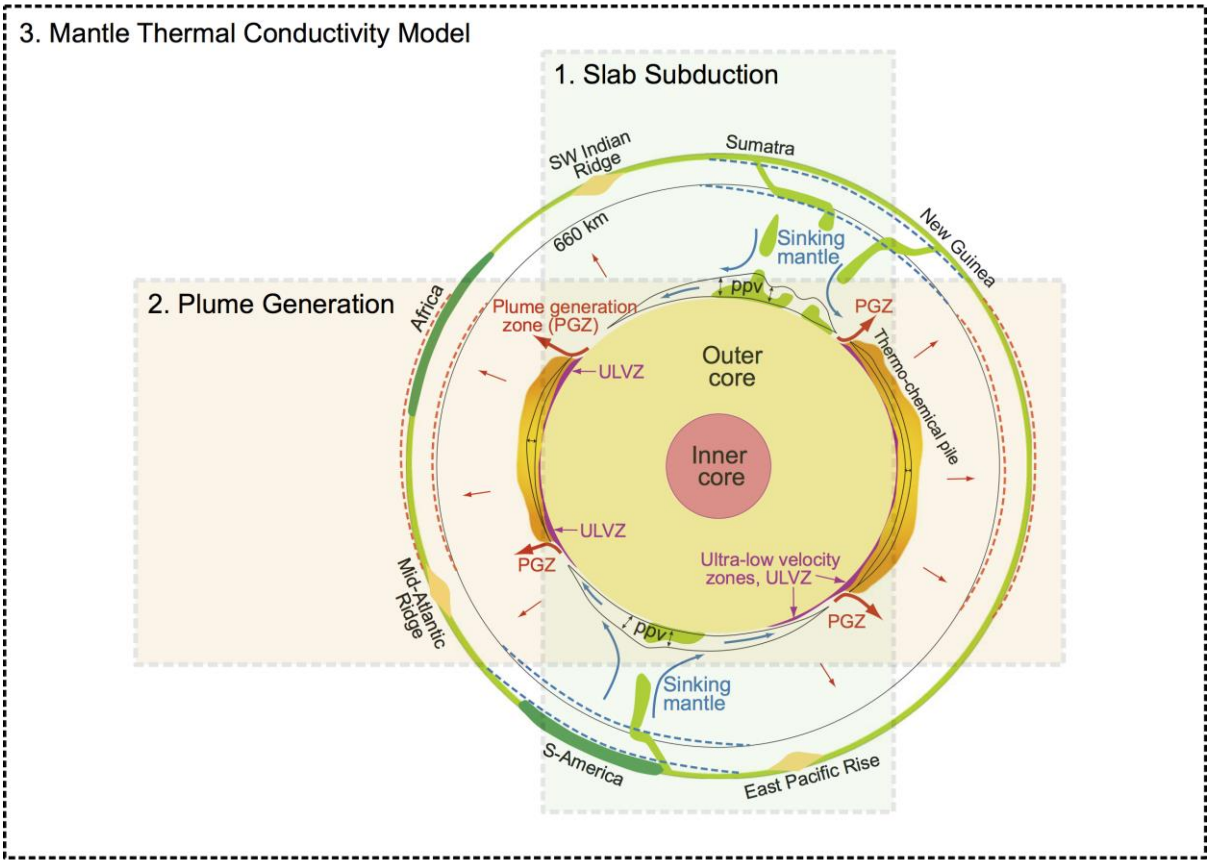

Figure 1. The dynamic lower mantle (adapted from Trønnes (2010)), with cold slabs sinking and hot plumes rising. Thermochemical piles, known as large low shear velocity provinces (LLSVPs) dominate the core-mantle boundary. Boxes correspond to proposed research areas (see below).

The importance of constraining the thermal conductivity of the mantle is reflected in the number of recent experimental investigations of major mantle phases (Hofmeister, 2008; Goncharov et al., 2010; Manthilake et al., 2011; Ohta et al., 2012). While these are of some interest, technical limitations mean that measurements are restricted to temperatures far below those in the deep Earth and long extrapolations must be made to estimate values at mantle conditions. Theoretical calculations offer an invaluable alternative and have been used to determine the thermal conductivity of major mantle phases at high temperature (de Koker, 2010; Haigis et al. 2012; Dekura et al. 2013; Tang et al., 2014; Amman et al., 2014; Stackhouse et al., 2015).

To date, almost all studies of the thermal conductivity of the lower mantle have focused on the pure magnesium end-members of major mantle phases (i.e. $MgSiO_3$ bridgmanite and MgO periclase), which comprise the bulk of the mantle. However, it is clear from Figure 1 that most interesting processes in the mantle (e.g. subduction and mantle upwelling), involve regions that are expected to differ in composition from the bulk (e.g. subducting slabs, large low shear velocity provinces (LLSVP) and ultra-low velocity zones (ULVZs)). The aim of this project is to determine the thermal conductivity of these regions, by performing atomistic simulations. The results will provide constraints on three important mantle processes (subduction of slabs, plume generation) and be integrated with previous results to construct a complete model of the thermal conductivity of the mantle, for use in mantle dynamics models.

Seismic tomography (e.g. Fukao and Obayashi, 2013) suggests that some subducting slabs stagnate just above the 660 km seismic discontinuity, while others penetrate through to the lower mantle (Figure 1 – Box 1). Several groups have investigated possible factors underlying slab stagnation using numerical simulations (e.g. Bina et al. 2001; Marquardt and Miyagi, 2015). Two important factors in slab subduction are the relative temperature of the slab and the viscosity of the surrounding mantle. Slabs sink since they are colder and denser than the surrounding mantle, meaning they have negative thermal buoyancy. The rate at which the temperature of slabs equilibrates with that of the surrounding mantle could have significant implications for their rate and depth of subduction and seismicity (Emmerson and McKenzie, 2007). This will depend on the thermal conductivity of both the slab and surrounding mantle. At present, there is only limited data for the thermal conductivity of the phases that comprise slabs at mantle conditions.

The Earth’s lowermost mantle acts as a lower boundary layer for convection. As such, it plays a very crucial role in controlling the style of convection and thermal and chemical evolution of the mantle. The largest-scale features of the lowermost mantle are two regions, located beneath central Pacific and Africa (Figure 1 – Box 2), where seismic velocities are observed to be depressed by a few percent compared to surrounding mantle. Interpreted as thermochemical piles, these areas are referred to as so-called large low shear velocity provinces (LLSVPs). Several theories regarding their origin and composition have been proposed, such as accumulated subducted slab material (Garnero et al., 2016).

In addition, recent studies (e.g. Steinberger and Torsvik, 2012; Austermann et al., 2014) have shown that mantle plumes tend to originate at the edges of LLSVPs. It has been suggested (Trønnes, 2010) that cold mantle material, including subducted slab material, warms up as it flows laterally along the core-mantle boundary (CMB), giving it thermal buoyancy. As the material is deflected at the margins of LLSVPs, it rises, but the majority of the denser basaltic material is thought to sink, forming piles. At present, the thermal conductivity of the denser basaltic material is unknown, but it could provide important constraints on convection processes in the thermal boundary layer. In addition, if the thermal conductivity of LLSVPs differs from that of normal mantle, it could lead to a heterogeneous heat-flux at the core-mantle boundary, influencing magnetic field generation.

The thermal conductivity of the mantle is an important parameter in mantle dynamics simulations. While models already exist for the thermal conductivity of the lower mantle (Ammann et al., 2014), these are based on values for major mantle phases alone and do not incorporate the more finer detail of slabs and LLSVPs, which could have a significant impact on convection (Figure 1 – Box 3).

2. Methods Overview

The lattice thermal conductivity of minerals will be calculated using non-equilibrium molecular dynamics simulations (Stackhouse et al., 2010; Stackhouse et al., 2015), recently implemented in the ab inito codes VASP (Kresse and Furthmuller, 1996a; Kresse and Furthmuller, 1996b) and cp2k (Vandevondle and Hutter, 2007; Krack, 2005, VandeVondele et al., 2005; Frigo and Johnson, 2005) at the School of Earth and Environment at the University of Leeds, and is already implemented in the classical code LAMMPS (In‘t Veld et al., 2008).

The method is intuitive, following the design of experimental techniques. The simulation cell is divided up into sections. One is designated the ‘hot section’ and another half a simulation cell away is designated the ‘cold section’. At regular intervals heat is transferred from the cold to hot section, generating a heat-flux. Over time, a temperature gradient develops between the hot and cold sections and once steady state is reached thermal conductivity can be calculated from Fourier’s law.

The Leeds Earth Modeling Apparatus (LEMA) will be used to predict the possible implications of the calculated lattice thermal conductivity values on heat-flow in the lower mantle.

3. Proposed Research

The aim of the project is to determine the thermal conductivity of mantle phases involved in subduction of slabs and plume generation, and their geophysical implications. This will be achieved using atomic scale simulations. In particular, you will:

1. Determine the thermal conductivity of slab minerals and upper mantle phases at mantle conditions, including garnet, olivine, wadsleyite and ringwoodite, and their influence on slab dynamics.
2. Determine the thermal conductivity of Bridgmanite and post-perovskite (incorporating Fe and Al), the α-PbO$_2$ phase of SiO$_2$ and aluminous phase and their impact on plume generation.

3. Combine the above results with those already in the literature for major mantle phase, to develop a complete thermal conductivity model of the mantle, and implement it in the Leeds Earth Modeling Apparatus (LEMA)..

4. Training

You will be trained in the application of atomistic simulations and high performance computing. In particular, you will be taught to perform density functional theory calculations, a method that is used widely in chemistry, physics, and materials science research. Alongside the transferable skills in communication and management this can open a range of career pathways. These skills will be developed by a mixture of hands on experience, attending external training courses, and taking part in the Leeds – York NERC doctoral training partnership programme. You will become a member of the University of Leeds Deep Earth Research Group, benefiting from interactions with other staff and students who have a range of interests and expertise.

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