

UNIVERSITY OF LEEDS

DOCTORAL THESIS

Simulating the thermal conductivity of lower mantle minerals

Author:

Ben TODD

Supervisor:

Dr. Stephen STACKHOUSE

Dr. Andrew WALKER

Dr. Jon MOUND

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Declaration of Authorship

I, Ben TODD, declare that this thesis titled, “Simulating the thermal conductivity of lower mantle minerals” and the work presented in it are my own. I confirm that:

- This work was done wholly or mainly while in candidature for a research degree at this University.
- Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.
- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- I have acknowledged all main sources of help.
- Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself.

Signed:

Date:

“Thanks to my solid academic training, today I can write hundreds of words on virtually any topic without possessing a shred of information, which is how I got a good job in journalism.”

Dave Barry

UNIVERSITY OF LEEDS

Abstract

Faculty of Environment
School of Earth and Environment

Doctor of Philosophy

Simulating the thermal conductivity of lower mantle minerals

by Ben TODD

The Thesis Abstract is written here (and usually kept to just this page). The page is kept centered vertically so can expand into the blank space above the title too...

Acknowledgements

The acknowledgments and the people to thank go here, don't forget to include your project advisor...

Contents

| | |
|---|------------|
| Declaration of Authorship | iii |
| Abstract | vii |
| Acknowledgements | ix |
| 1 The Chapter formerly known as Paper 1 | 1 |
| 1.1 Introduction | 1 |
| 1.1.1 Intro Intro (remove this subsection header later) | 1 |
| A Frequently Asked Questions | 3 |
| A.1 How do I change the colors of links? | 3 |

List of Figures

List of Tables

List of Abbreviations

LAH List Abbreviations **Here**
WSF What (it) Stands For

Physical Constants

Speed of Light $c_0 = 2.997\,924\,58 \times 10^8 \text{ m s}^{-1}$ (exact)

List of Symbols

| | | |
|----------|-------------------|------------------------|
| a | distance | m |
| P | power | W (J s ⁻¹) |
| ω | angular frequency | rad |

For/Dedicated to/To my...

Chapter 1

The Chapter formerly known as Paper 1

1.1 Introduction

1.1.1 Intro Intro (remove this subsection header later)

Knowledge of the thermal conductivity of solids is key in a wide range of technological applications and for our understanding of natural systems. For example, in the Earth's lower mantle thermal conductivity controls the nature of planetary convection (Tosi et al. (2013)), and the heat flux out of the core which powers the geotherm. Low thermal conductivities are required in thermoelectric materials, to maximise the efficiency of heat-electricity conversion (Snyder and Toberer (2008)).

A range of atomic scale simulation methods are available to determine the lattice thermal conductivity of materials. These are invaluable for calculating thermal conductivity at conditions of which experiments are difficult, e.g. the extreme conditions found in the Earth's lower mantle (pressures and temperatures up to 136 GPa and 4000 K at the core-mantle boundary).

(MOVE - to where though?) Many studies assume lowermost mantle thermal conductivity to be $10 \text{ Wm}^{-1}\text{K}^{-1}$ (e.g. Lay, Hernlund, and Buffett (2008)), but uncertainty in the extrapolation of results made at low pressures and temperatures gives a range of $4 - 16 \text{ Wm}^{-1}\text{K}^{-1}$ (Brown and McQueen (1986), Osako and Ito (1991), Hofmeister (1999), Goncharov et al. (2009), Manthilake et al. (2011), and Ohta et al. (2012)).

Appendix A

Frequently Asked Questions

A.1 How do I change the colors of links?

The color of links can be changed to your liking using:

```
\hypersetup{urlcolor=red}, or  
\hypersetup{citecolor=green}, or  
\hypersetup{allcolor=blue}.
```

If you want to completely hide the links, you can use:

```
\hypersetup{allcolors=.}, or even better:  
\hypersetup{hidelinks}.
```

If you want to have obvious links in the PDF but not the printed text, use:

```
\hypersetup{colorlinks=false}.
```


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