

UNIVERSITY OF LEEDS

DOCTORAL THESIS

Simulating the thermal conductivity of lower mantle minerals

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for the degree of Doctor of Philosophy
in the*

**Institute of Geophysics and Tectonics
School of Earth and Environment**

April 27, 2018

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...

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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

Introduction

1.1 Why is thermal conductivity important?

1.1.1 Man-made applications

1.1.2 In the context of the Earth

1.2 What is thermal conductivity?

1.2.1 What affects it?

1.2.2 Mechanisms of heat transport

1.3 Previous work - geophysics

1.3.1 Mantle/core dynamics

1.3.2 Thermal conductivity of the lower mantle

1.4 Thesis outline

1.4.1 Aims

1.4.2 Objectives

Chapter 2

Intro/Background/Theory 2

2.1 Main Section 1

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2.1.1 Subsection 1

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Chapter 3

Constraining the finite-size effects of molecular dynamics methods to compute thermal conductivity

3.1 Introduction

3.1.1 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 (Snyder2008).

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. Lay2008), but uncertainty in the extrapolation of results made at low pressures and temperatures gives a range of $4 - 16 \text{ Wm}^{-1}\text{K}^{-1}$ (Brown1986; Osako1991; Goncharov2009; Hofmeister (1999), Manthilake et al. (2011), and Ohta et al. (2012)).

Chapter 4

Modelling the thermal conductivity of lower mantle minerals

4.1 Main Section 1

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4.1.1 Subsection 1

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4.2 Making the model

4.2.1 Fitting the data

Temperature dependence

Okuda et al., 2017

Compositional dependence

Ohta et al., 2017

Chapter 5

Modelling the lower mantle with variable thermal conductivity

5.1 Main Section 1

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5.1.1 Subsection 1

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Chapter 6

Summary/Discussion/Conclusion

6.1 Main Section 1

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6.1.1 Subsection 1

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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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