UNIVERSITY OF LEEDS

DOCTORAL THESIS

Simulating the thermal conductivity of lower mantle minerals

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A thesis submitted in fulfillment of the requirements for the degree of Doctor of Philosophy

in the

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School of Earth and Environment

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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

List of Figures

List of Tables

List of Abbreviations

LAH	**L**ist **A**bbreviations **H**ere
WSF	**W**hat (it) **S**tands **F**or

Physical Constants

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

List of Symbols

a	distance	m
P	power	W ($\mathrm{J\,s^{-1}}$)
ω	angular frequency	rad

For/Dedicated to/To my…

Chapter 1

Intro/Background/Theory 1

1.1 Main Section 1

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Chapter 2

Intro/Background/Theory 2

2.1 Main Section 1

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Chapter 3

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

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 (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 $\mathrm{Wm^{-1}K^{-1}}$ (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 $\mathrm{Wm^{-1}K^{-1}}$ (Brown and McQueen (1986), Osako and Ito (1991), Hofmeister (1999), Goncharov et al. (2009), Manthilake et al. (2011), and Ohta et al. (2012)).

Chapter 4

Modelling the thermal conductivity of lower mantle minerals

4.1 Main Section 1

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Chapter 5

Modelling the lower mantle with variable thermal conductivity

5.1 Main Section 1

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Chapter 6

Summary/Discussion/Conclusion

6.1 Main Section 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}`.

Bibliography

Brown, J. M. and R. G. McQueen (1986). "Phase Transitions, Grüneisen Parameter, and Elasticity for Shocked Iron Between 77 GPa and 400 GPa". In: *Journal of Geophysical Research* 91.B7, pp. 7485–7494.

Goncharov, Alexander F. et al. (2009). "Thermal conductivity of lower-mantle minerals". In: *Physics of the Earth and Planetary Interiors* 174.1-4, pp. 24–32. ISSN: 00319201. DOI: 10.1016/j.pepi.2008.07.033. URL: http://linkinghub.elsevier.com/retrieve/pii/S0031920108001945.

Hofmeister, A. M. (1999). "Mantle Values of Thermal Conductivity and the Geotherm from Phonon Lifetimes". In: *Science* 283, pp. 1699–1706. ISSN: 00368075. DOI: 10.1126/science.283.5408.1699. URL: http://www.sciencemag.org/cgi/doi/10.1126/science.283.5408.1699.

Lay, T., J. Hernlund, and B. A. Buffett (2008). "Core–mantle boundary heat flow". In: *Nature Geoscience* 1, pp. 25–32. ISSN: 1752-0894. DOI: 10.1038/ngeo.2007.44. URL: http://www.nature.com/doifinder/10.1038/ngeo.2007.44.

Manthilake, G. M. et al. (2011). "Lattice thermal conductivity of lower mantle minerals and heat flux from Earth's core." In: *Proceedings of the National Academy of Sciences of the United States of America* 108, pp. 1–4. ISSN: 1091-6490. DOI: 10.1073/pnas.1110594108. URL: http://www.pubmedcentral.nih.gov/articlerender.fcgi?artid=3207700{\&}tool=pmcentrez{\&}rendertype=abstract.

Ohta, K. et al. (2012). "Lattice thermal conductivity of MgSiO3 perovskite and post-perovskite at the core–mantle boundary". In: *Earth and Planetary Science Letters* 349-350, pp. 109–115. ISSN: 0012821X. DOI: 10.1016/j.epsl.2012.06.043. URL: http://linkinghub.elsevier.com/retrieve/pii/S0012821X12003354.

Osako, M. and E. Ito (1991). "Thermal diffusivity of MgSiO3 perovskite". In: *Geophysical Research Letters* 18, pp. 239–242. URL: http://onlinelibrary.wiley.com/doi/10.1029/91GL00212/full.

Snyder, G Jeffrey and Eric S Toberer (2008). "Complex thermoelectric materials". In: *Nature materials* 7.2, pp. 105–114. ISSN: 1476-1122. DOI: 10.1038/nmat2090. arXiv: 1512.00567.

Tosi, Nicola et al. (2013). "Mantle dynamics with pressure- and temperature-dependent thermal expansivity and conductivity". In: *Physics of the Earth and Planetary Interiors* 217, pp. 48–58. ISSN: 00319201. DOI: 10.1016/j.pepi.2013.02.004. URL: http://dx.doi.org/10.1016/j.pepi.2013.02.004.