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

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# 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 ($\mathrm{J\,s^{-1}}$) |
| $\omega$ | 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?

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# 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 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 $Wm^{-1}K^{-1}$ (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 $Wm^{-1}K^{-1}$ (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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### 4.1.1 Subsection 1

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## 4.2 Adding iron

## 4.3 Making the model

Due to uncertainty in the lower mantle's compositional distrubution, properties like thermal conductivity are averaged considering the relative abundance of each mineral component. There are also endmember relations to consider within each mineral, the concentration of impurities, and mineral phase transitions. A simple weighted average can be taken to combine the contributions of individual minerals, whereas mixing of endmembers is not as linear. Ohta et al., 2017 provide an equation for interpolating conductivity between compositional endmembers, specifically (Mg,Fe)O (ferro)periclase. I apply it to (Mg,Fe)$SiO_3$ perovskite [[[PRESUMABLY ALSO WORKS FOR bdg<->p-Pv?]]]. Okuda et al., 2017 present a temperature scaling relation for bridgmanite, which I additionally apply to the Fe-endmember. By having temperature-dependent values I am able to obtain an equation that gives thermal conductivity as a function of both temperature and composition, for a given (studied/fit?) endmember pair.

### 4.3.1 Fitting the data

Determine lattice thermal conductivity as a function of temperature and composition, using calculated and fit constants.

Equations from Ohta et al. 2017 (eq. 7,8,9), and Okuda et al. 2017 (eq. 5).

default parameters refer to [Mg,Fe]$SiO_3$ perovskite, bridgmanite, at 136 GPa, CMB pressure.

xN is a wildcard, N = 0 or 1 x0 in variable names refers to x=0 endmember (default = [Mg]SiO3) x1 in variable names refers to x=1 endmember (default = [Fe]SiO3)

#### Compositional dependence

Ohta et al., 2017

Ohta eq. 7 - k = k_linear * omega_ratio * np.arctan(1.0/omega_ratio)

k - output conductivity as function of t & x (W/m.K), considering mineral specific parameters k_linear - the composition-dependent conducitivity, if it were linearly interpolated between endmembers (W/m.K) omega_ratio - temperature-dependent parameter to perturb k_linear, to create the "trough" trend in composition-dependent conductivity

Ohta eq. 8 - omega_ratio = np.sqrt(chi_t / (x*(1-x)))

omega_ratio - temperature-dependent parameter to perturb k_linear, to create the "trough" trend in composition-dependent conductivity chi_t - temperature-dependent parameter to ... ??? x - composition mix of interest (dimensionless, values between 0 and 1)

chi_t scaling - chi_t = a * np.exp(b*t)

chi_t - temperature-dependent parameter to ... ??? a - coefficient in chi_t variation with temperature b - exponent in chi_t variation with temperature t - temperature of interest (K, default data fit between 1000 - 5000 K, but extrapolation should be reasonable)

Ohta eq. 9 - k_linear = ((1 - x) * k_x0) + x*k_x1

k_linear - the composition-dependent conducitivity, if it were linearly interpolated between endmembers (W/m.K) x - composition mix of interest (dimensionless, values between 0 and 1) k_x0 - temperature and volume-dependent conductivity for x=0 endmember (W/m.K) k_x1 - temperature and volume-dependent conductivity for x=1 endmember (W/m.K)

#### Temperature dependence

Okuda et al., 2017

Okuda eq. 5 - k_x0 = ref_k_x0 * (ref_t/t)**a_x0 * (ref_v_x0 / v_x0)**g_x0 k_x1 = ref_k_x1 * (ref_t/t)**a_x1 * (ref_v_x1 / v_x1)**g_x1

k_xN - temperature and volume-dependent conductivity of an endmember (W/m.K) ref_k_xN - reference conducitivty of an endmember (W/m.K) ref_t - reference temperature at which above conductivities are calculated (K) t - temperature of interest (K, default data fit between 1000 - 5000 K, but extrapolation should be reasonable) a_xN - exponent controlling temperature-dependent conducitvity of an endmember ref_v_xN - reference volume of an endmember (E-30 $m^3$) v_xN - temperature-dependent volume of an endmember (E-30 $m^3$) g_xN - exponent controlling volume | density-dependent conducitvity of an endmember

Volume scaling - v_xN = m_xN * t + c_xN

v_xN - temperature-dependent volume for x=0 endmember (E-30 $m^3$) m_xN - fit gradient for x=0 endmember (E-30 $m^3$/K) t - temperature of interest (K, default data fit between 1000 - 5000 K, but extrapolation should be reasonable) c_xN - intercept volume for x=0 endmember (E-30 $m^3$)

# 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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