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:

Do it!
Just do it!

Don't let your dreams be dreams.
Yesterday you said tomorrow, so just do it!
Make your dreams come true!
Just do it!

Some people dream of success,
while you're gonna wake up,
and work hard at it!
Nothing is impossible!

You should get to the point,
where anyone else would quit,
and you're not going to stop there.
No, what are you waiting for?

Do it!
Just do it!
Yes you can!
Just do it!

If you're tired of starting over,
stop giving up.

Shia LeBeouf

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…

Everyone is smart, set yourself apart by being kind.

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

Introduction

1.1 Why is thermal conductivity important?

1.1.1 Man-made applications

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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 between 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

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

I want to determine lattice thermal conductivity as a function of temperature and composition, using calculated and fit constants. For the method I will use I need to know how the conductivity of endmember minerals changes with physical conditions. In order to keep temperature the only dependent variable, I will scale volume linerarly with temperature [FIGURE]. At this point I can scale the conductivity of an endmember with temperature within the fitted range (Okuda et al., 2017).

Considering Ohta et al., 2017 the linear interpolation between the conductivities two endmembers can be perturbed, forming the trough characteristic of varying composition. While $FeSiO_3$ generally has a lower thermal conductivity than $MgSiO_3$, the minimum is located at an intermediate composition. The effect of impurity scattering is larger than inherent changes due to chemistry.

Compositional dependence

Ohta et al., 2017
* = already cited somewhere above

Ohta eq. 7

$$\kappa_{latt} = \kappa_i \left(\frac{\omega_0}{\omega_M} \right) arctan \left(\frac{\omega_M}{\omega_0} \right)$$

κ_{latt} - output conductivity as function of t & x ($Wm^{-1}K^{-1}$), considering mineral specific parameters
κ_i - the composition-dependent conducitivity, if it were linearly interpolated between endmembers ($Wm^{-1}K^{-1}$)
ω_0/ω_M - temperature-dependent parameter to perturb κ_i, to create the "trough" trend in composition-dependent conductivity
ω_0 - *"the phonon frequency where the intrinsic mean free path is equal to that due to solute atoms"*
ω_M - *"the phonon frequency corresponding to the maximum of the acoustic branch of the phonon spectrum"*

Ultimately this is the equation we are trying to solve. The two components κ_i and ω_0/ω_M, are both temperature and composition-dependent. κ_i gives the compositionally-weighted average conductivity, a linear interpolation between endmembers at a certain temperature. ω_0/ω_M controls the conductivity decrease due to the impurity effect, the magnitude of which depends on the temperature and composition of interest.

Ohta eq. 8

$$\left(\frac{\omega_0}{\omega_M} \right)^2 = \frac{\chi^T}{C\,(1-C)}$$

*ω_0/ω_M - temperature-dependent parameter to perturb κ_i, to create the "trough" trend in composition-dependent conductivity
*ω_0 - *"the phonon frequency where the intrinsic mean free path is equal to that due to solute atoms"*
*ω_M - *"the phonon frequency corresponding to the maximum of the acoustic branch of the phonon spectrum"*

χ^T -temperature-dependent parameter to …???
χ - *"a constant"*…
T - temperature of interest (K, default data fit between 1000 - 5000 K, but extrapolation should be reasonable)
C - composition mix of interest (dimensionless, values between 0 and 1)

The equation that splits ω_0/ω_M into its temperature and composition-dependent components. χ is a temperature-dependent constant unique to an endmember pair. $C(1-C)$ is largest when $C = 0.5$ *or* 50%, relating to the shape of the trough formed by this fit.

χ^T scaling

$$\chi^T = A\, e^{BT}$$

*χ^T -temperature-dependent parameter to …???
*χ - *"a constant"*…
*T - temperature of interest (K, default data fit between 1000 - 5000 K, but extrapolation should be reasonable)
A - coefficient in χ^T variation with temperature
B - exponent in χ^T variation with temperature

Ohta eq. 9

$$\kappa_i = (1-C)\,\kappa_{MgSiO_3} + C\,\kappa_{FeSiO_3}$$

*κ_i - the composition-dependent conducitivity, if it were linearly interpolated between endmembers ($Wm^{-1}K^{-1}$)
*C - composition mix of interest (dimensionless, values between 0 and 1)
κ_{MgSiO_3} - temperature and volume-dependent conductivity for Mg endmember ($Wm^{-1}K^{-1}$)
κ_{FeSiO_3} - temperature and volume-dependent conductivity for Fe endmember ($Wm^{-1}K^{-1}$)

Temperature dependence

Okuda et al., 2017

Okuda eq. 5

$$\kappa_{adj} = \kappa_{ref} \left(\frac{T_{ref}}{T}\right)^a \left(\frac{V_{ref}}{V}\right)^g$$

κ_{adj} - temperature and volume-dependent conductivity of an endmember ($Wm^{-1}K^{-1}$)
κ_{ref} - reference conducitivty of an endmember ($Wm^{-1}K^{-1}$)
T_{ref} - 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 - exponent controlling temperature-dependent conducitvity of an endmember
V_{ref} - reference volume of an endmember (E-30 m^3)
V - temperature-dependent volume of an endmember (E-30 m^3)
g - exponent controlling volume | density-dependent conducitvity of an endmember

Volume scaling

$$y = mx + c$$

$$V = \frac{\partial V}{\partial T} T + V_{T_0}$$

*V - temperature-dependent volume of an endmember (E-30 m^3)
$\partial V / \partial T$ - fit gradient, change of volume with temperature (E-30 m^3/K)
*T - temperature of interest (K, default data fit between 1000 - 5000 K, but extrapolation should be reasonable)
V_{T_0} - intercept volume for T=0 K (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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