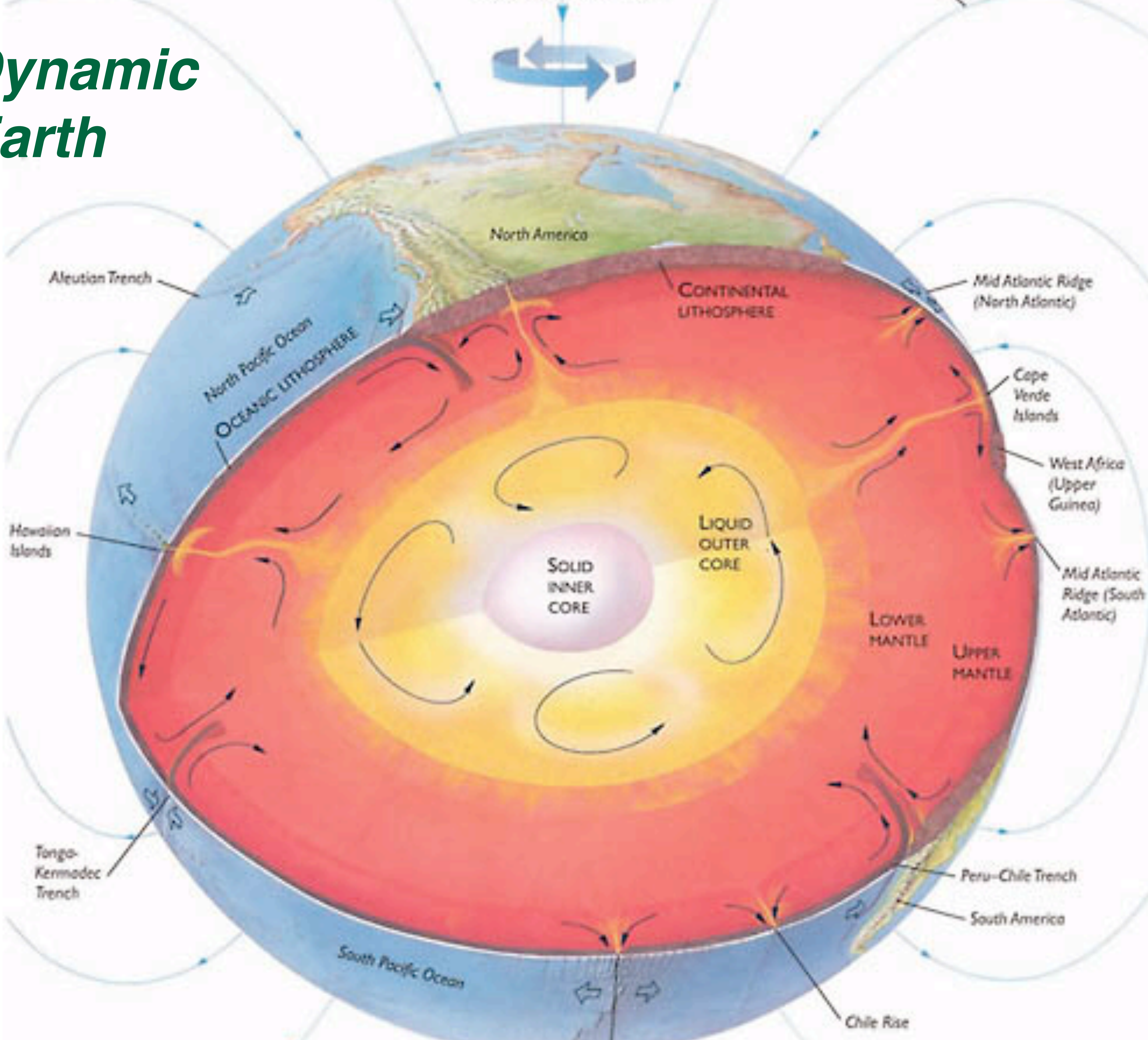
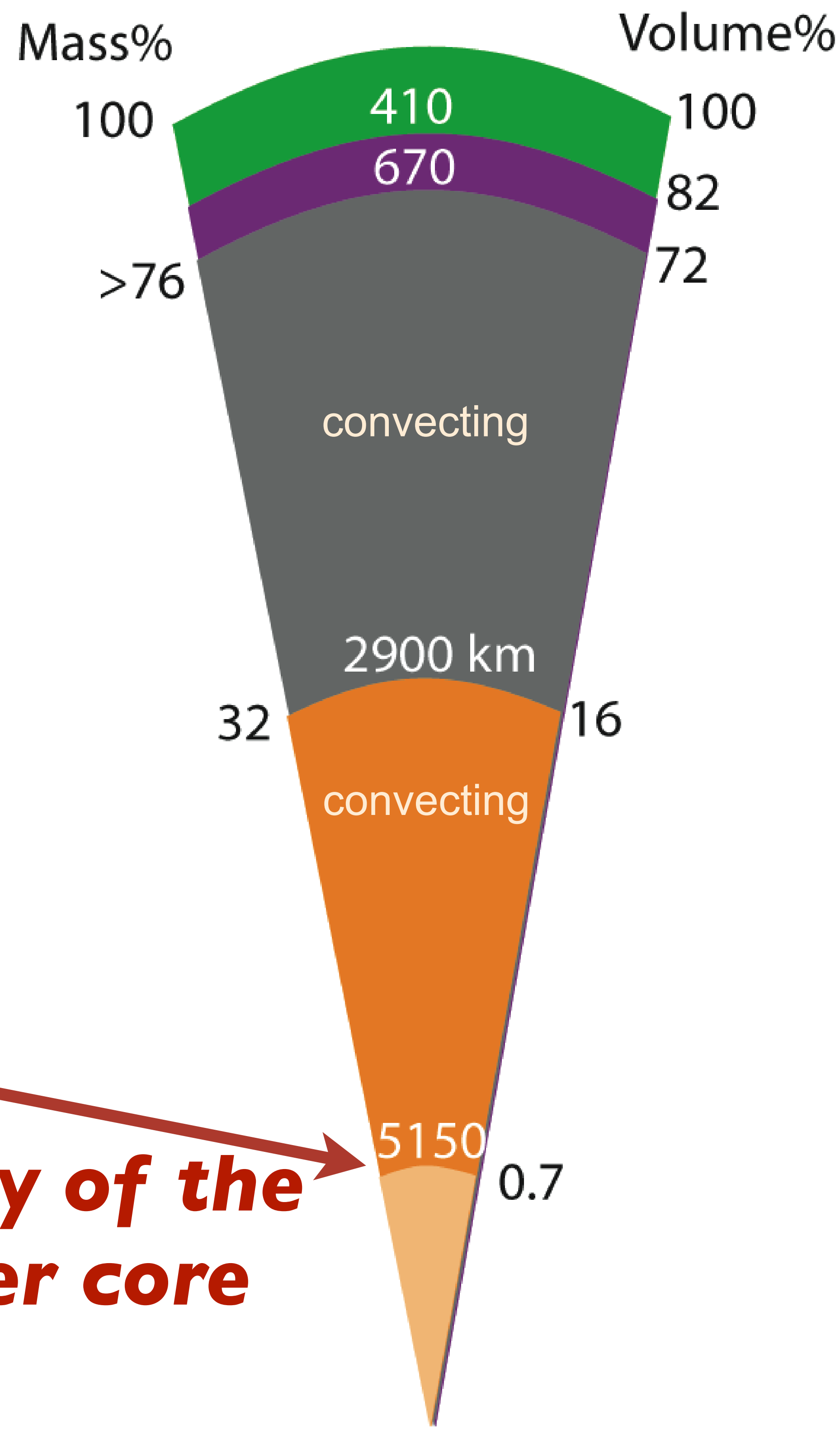
Dynamic Earth



Thermal State of the Earth
Part 1: Fixed Temperatures

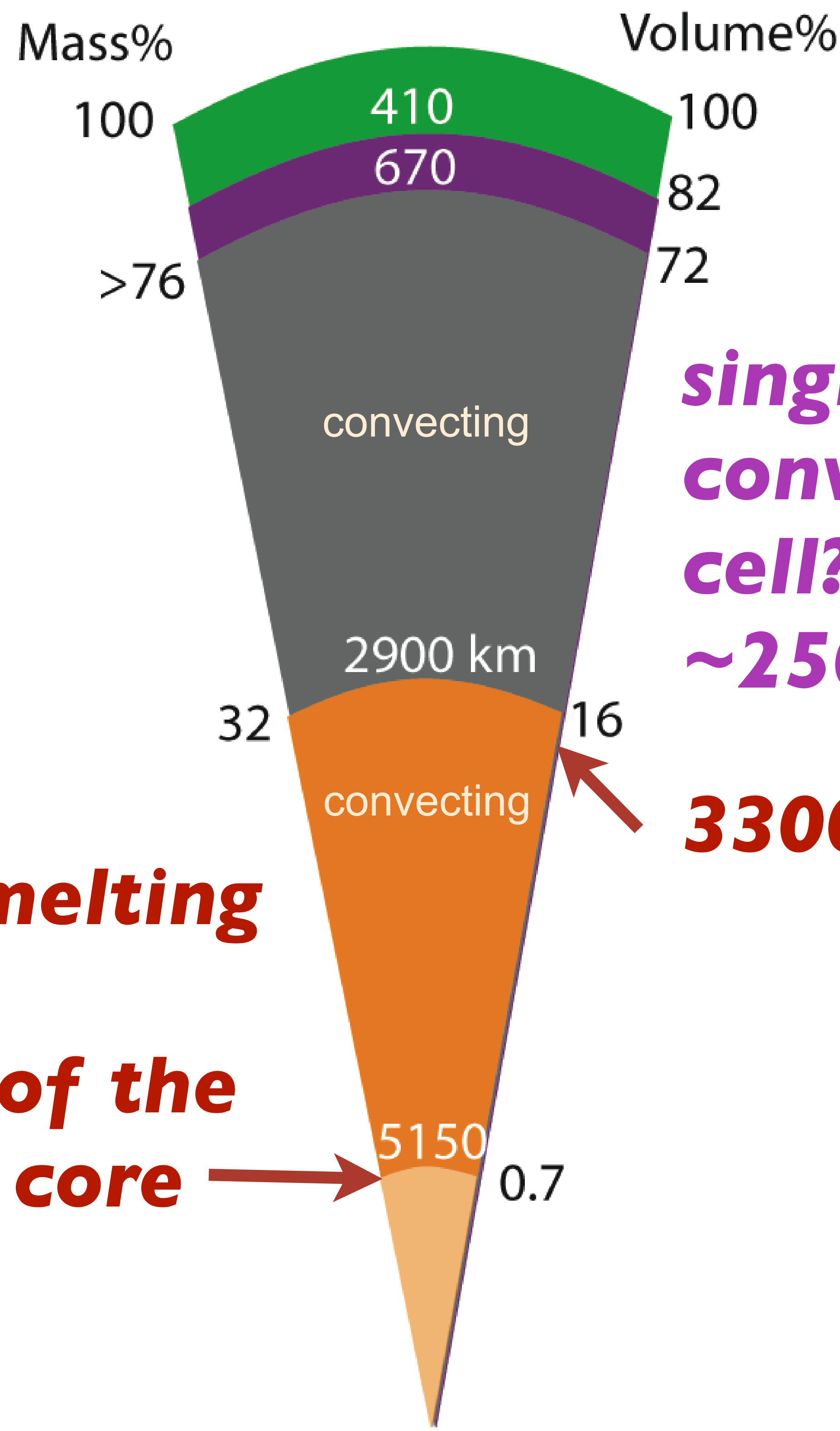
300 K

dT/dr



Iron melting temperature at the boundary of the inner core/outer core

Thermal State of the Earth
Temperature inferences



300 K

dT/dr

single convection cell?
~2500 K

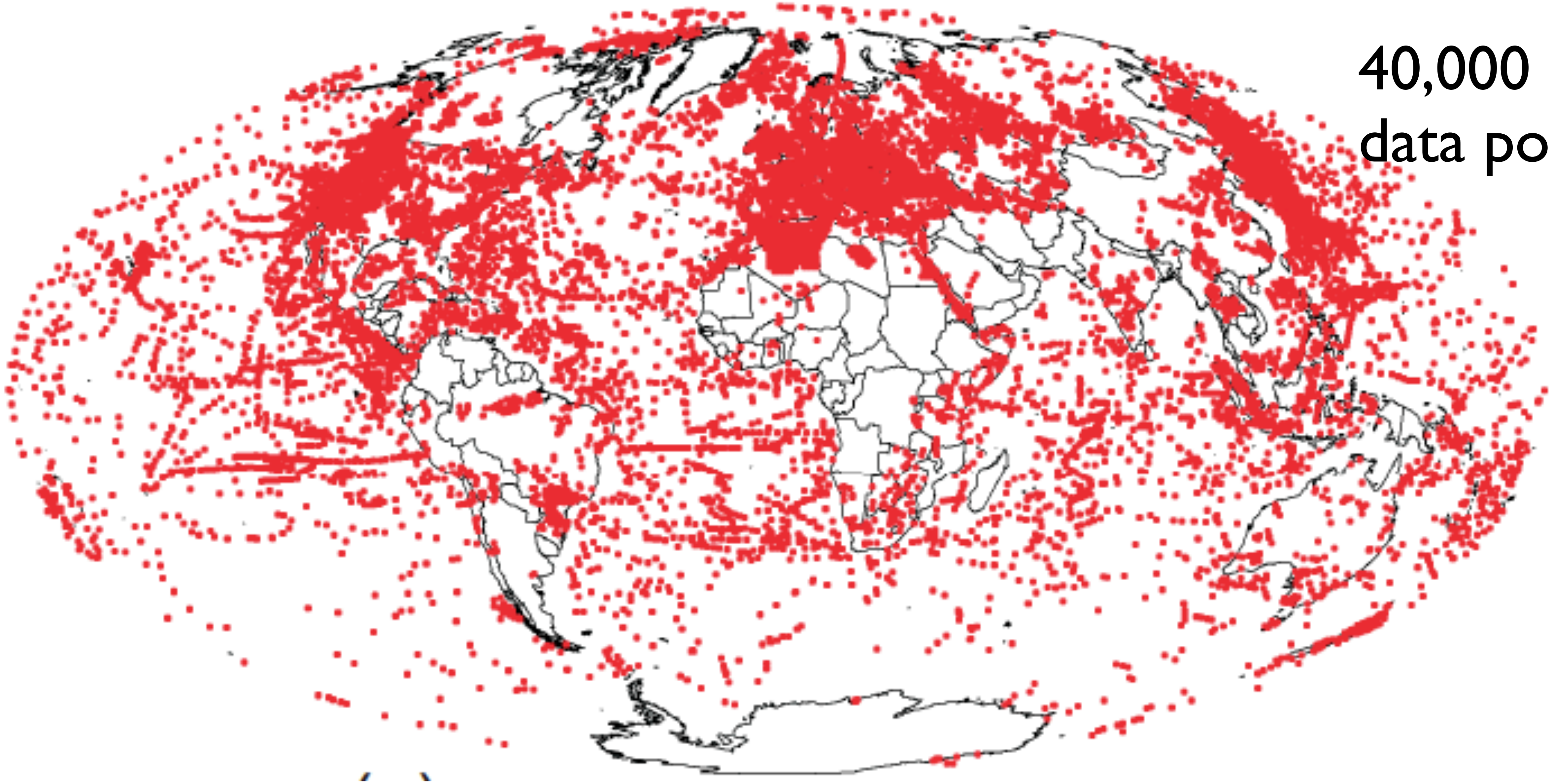
additional boundary layer?
~3100 K

3300 K

4300 K

Uncertain: iron melting temperature at the boundary of the inner core/outer core

Thermal State of the Earth
Part 2: Total heat flux constraints



40,000
data points

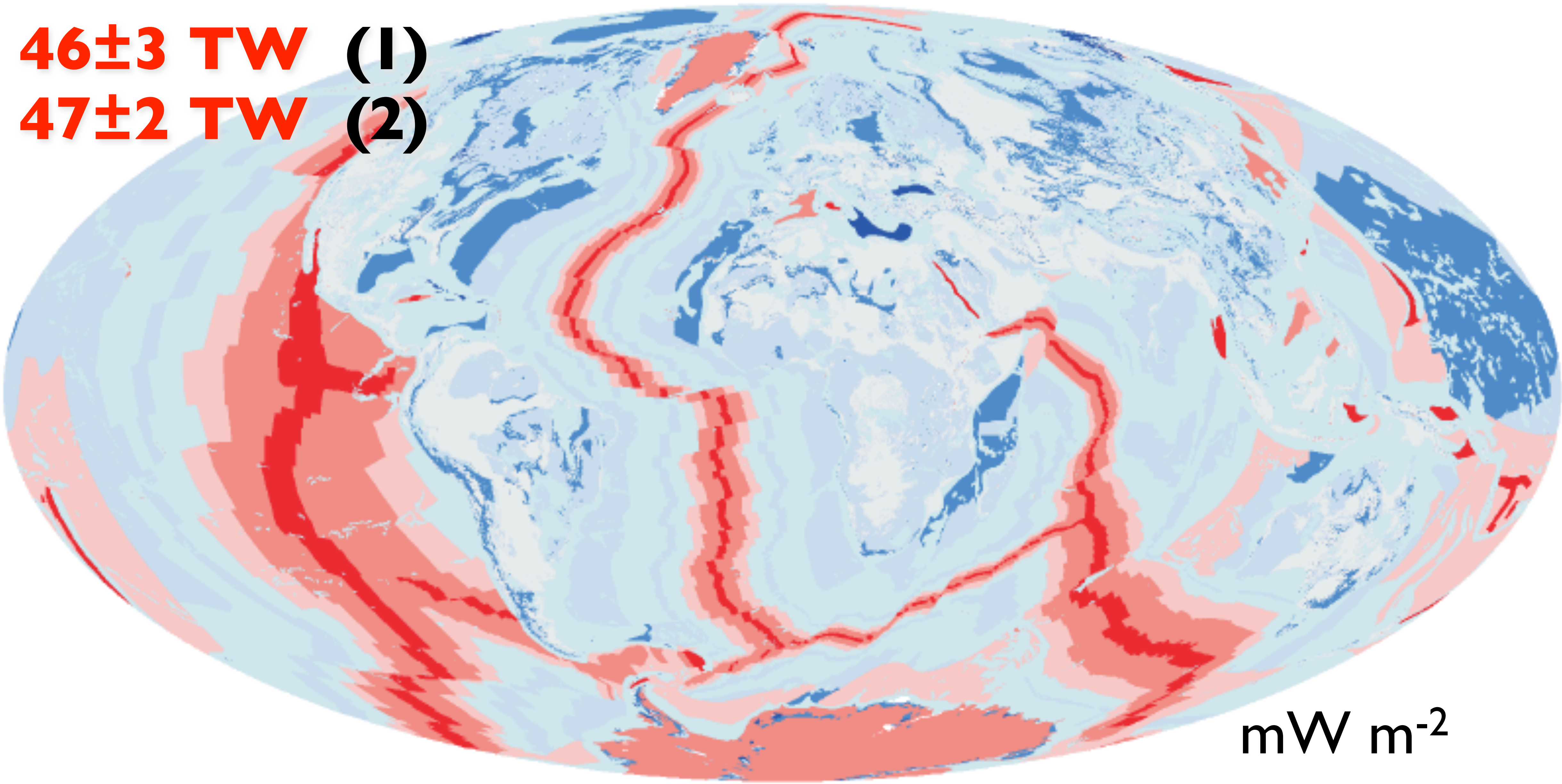
Conductive heat flow measured from bore-hole temperature gradient and conductivity

Earth's Total Surface Heat Flow

Surface heat flow

46±3 TW (1)

47±2 TW (2)



(1) Jaupart et al (2008) *Treatise of Geophys.*

(2) Davies and Davies (2010) *Solid Earth*

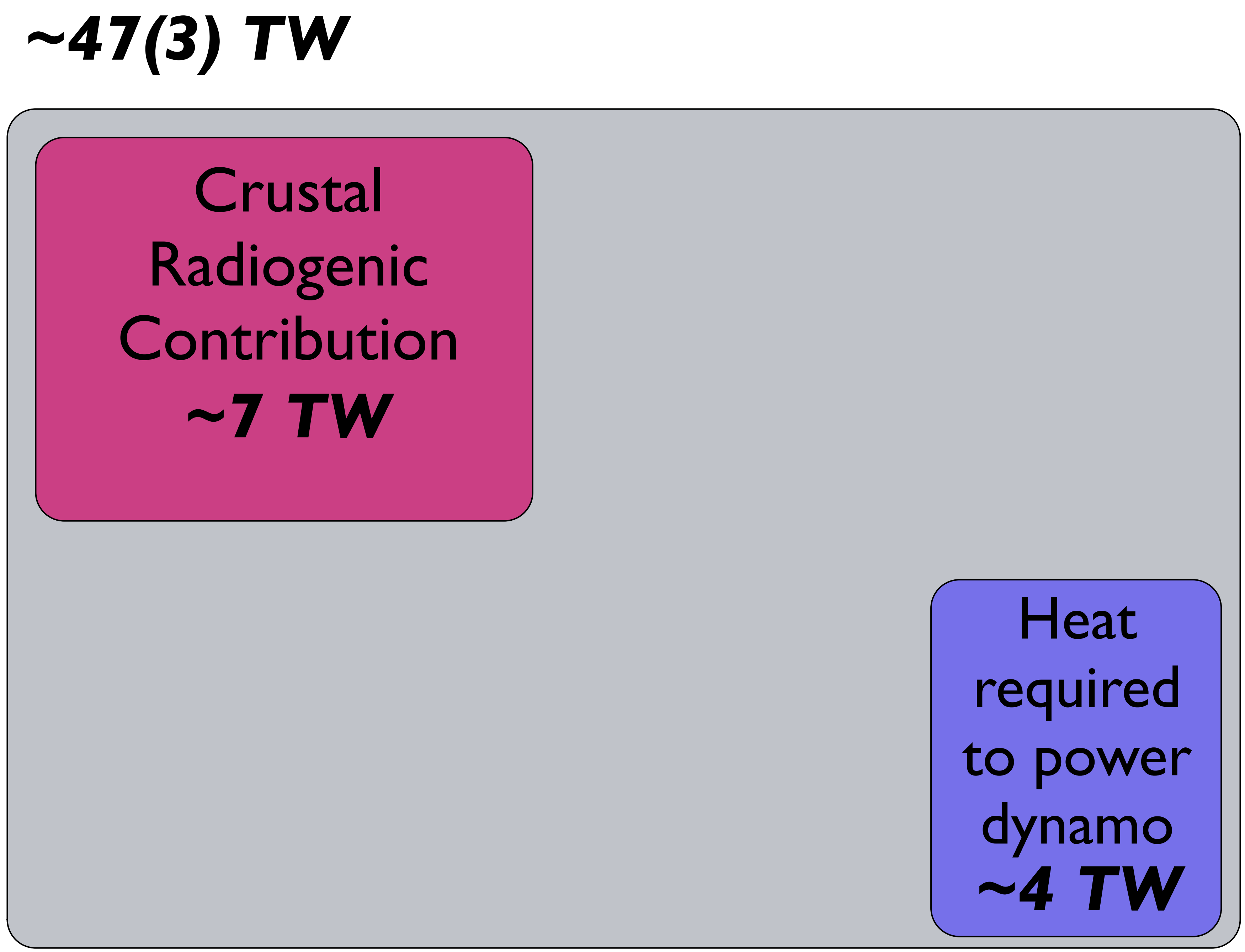
Thermal State of the Earth

~47(3) TW

Radiogenic
Contribution
(U, Th, K)

Earth
Interior
Cooling

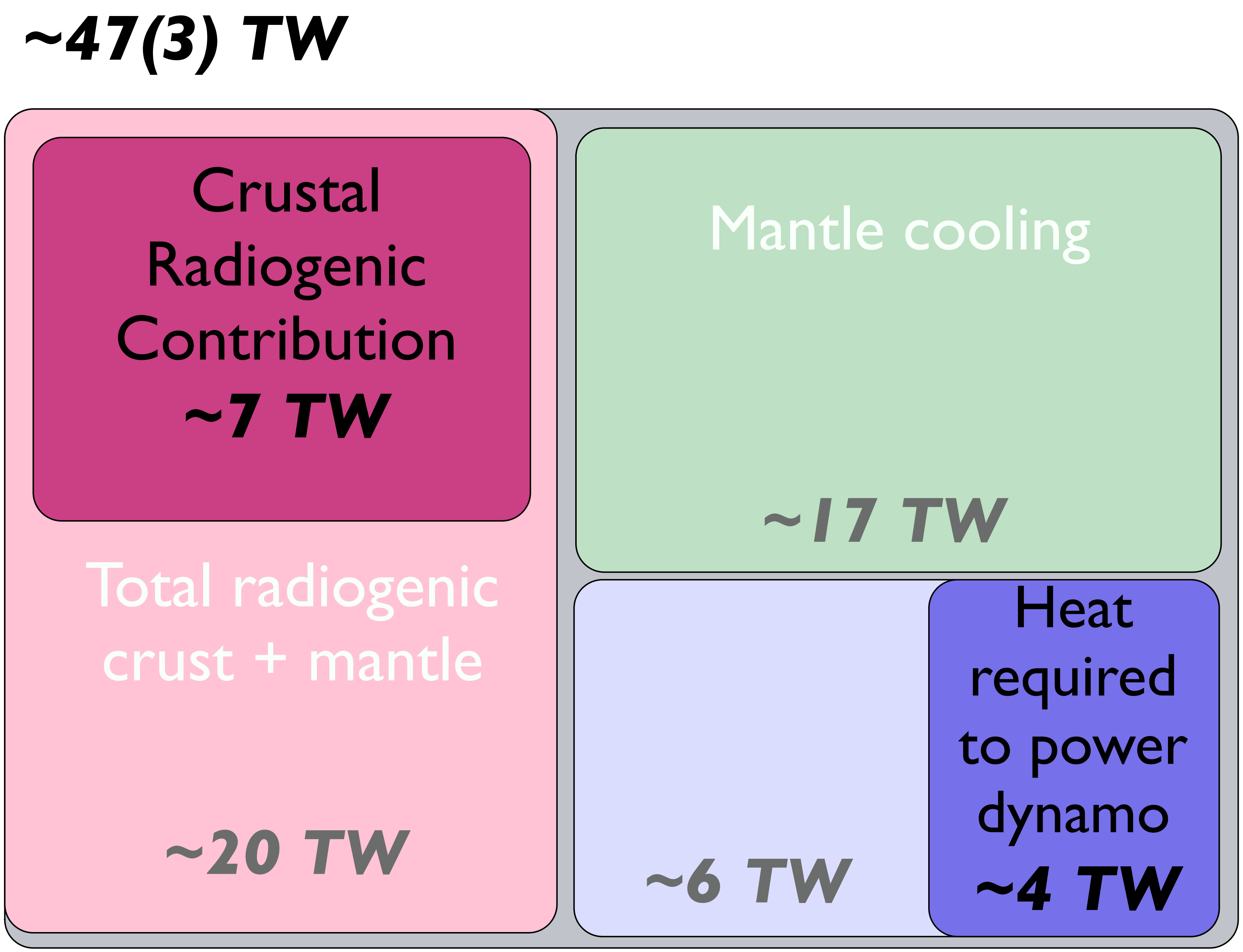
Constraints on the thermal state of the Earth



values from McDonough & Sun, Chem. Geol., 120, 223-253, 1995

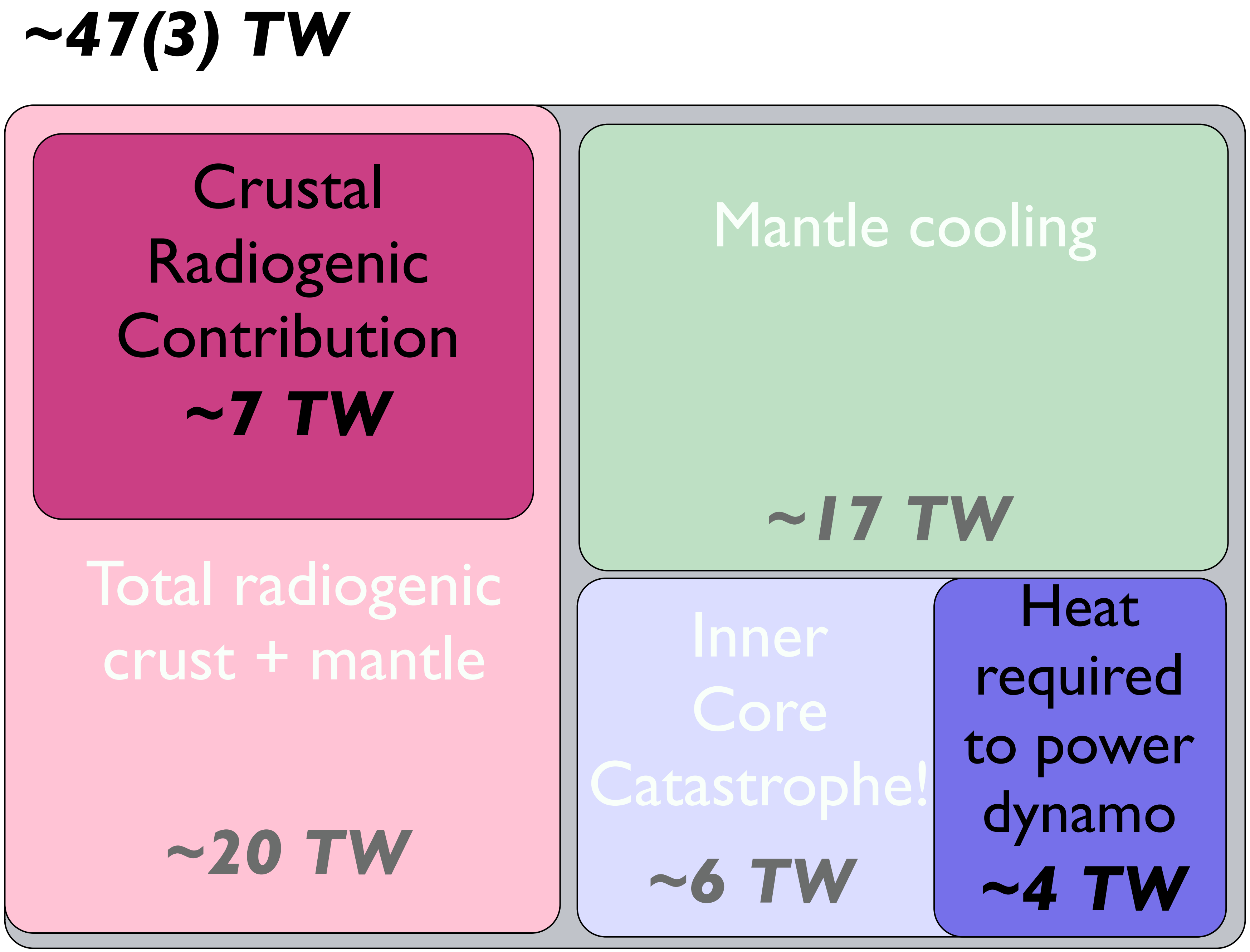
Buffett 2002

Constraints on the thermal state of the Earth



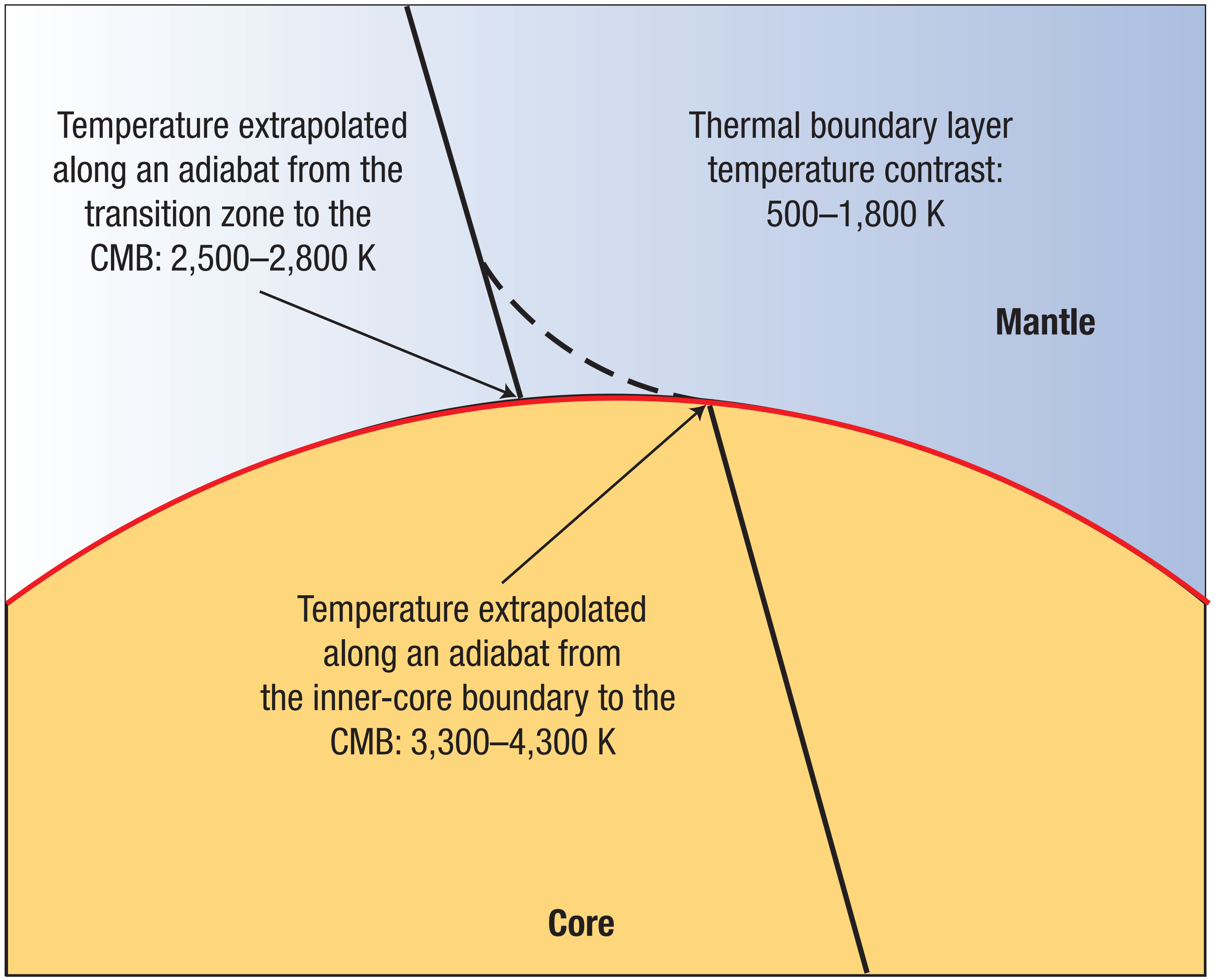
Buffett 2002

Constraints on the thermal state of the Earth



Buffett 2002--Inner core formed very recently/ Early Temps were very hot!

Thermal Conductivity Definition



Lay, Hernlund, Buffett, 2008

Heat Flux = $\kappa_{cond} \nabla T$

At core/mantle thermal boundary:

Length scale~150(±50) km

∇T ~ 500-2000 K

κ_{cond} very uncertain ~10±5 W/m/K

Core/mantle heat flux uncertain ~4-20 TW

Approaches to thermal conductivity of insulators

1. Determine phonon behavior
2. Measure heat flow via Q=dT/dx

THERMAL DIFFUSIVITY OF $MgSiO_3$ PEROVSKITE

Masahiro Osako

Section of Astronomy and Geophysics, National Science Museum, Tokyo

Eiji Ito

Institute for Study of the Earth's Interior, Okayama University

Abstract. Thermal diffusivity of $MgSiO_3$ perovskite has been measured in the temperature range of 160 K to 340 K using a sample synthesized in a uniaxial split-sphere high-

perovskite increases by a factor of 4 with depth throughout the lower mantle and reaches to 12 $Wm^{-1}K^{-1}$ in the vicinity of the mantle-core boundary. The D" layer might not be a thermal boundary layer insulating the high core-temperature, if this layer mainly consists of the perovskite.

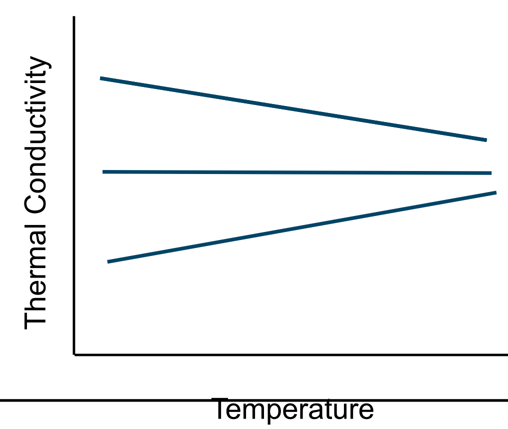
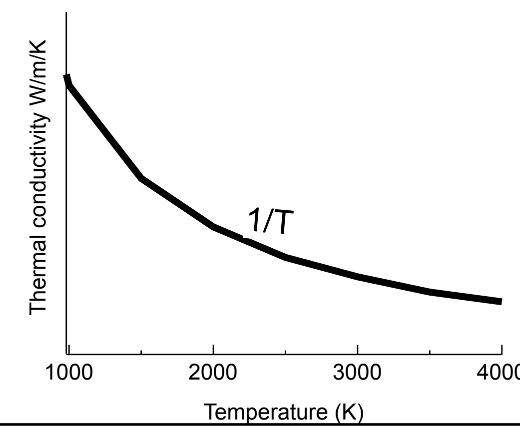
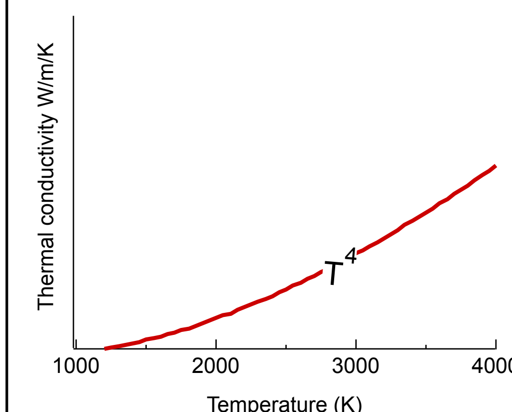
and reaches to 12 $Wm^{-1}K^{-1}$ in the v

measurements and discuss the thermal conductivity under the lower mantle conditions.

mental

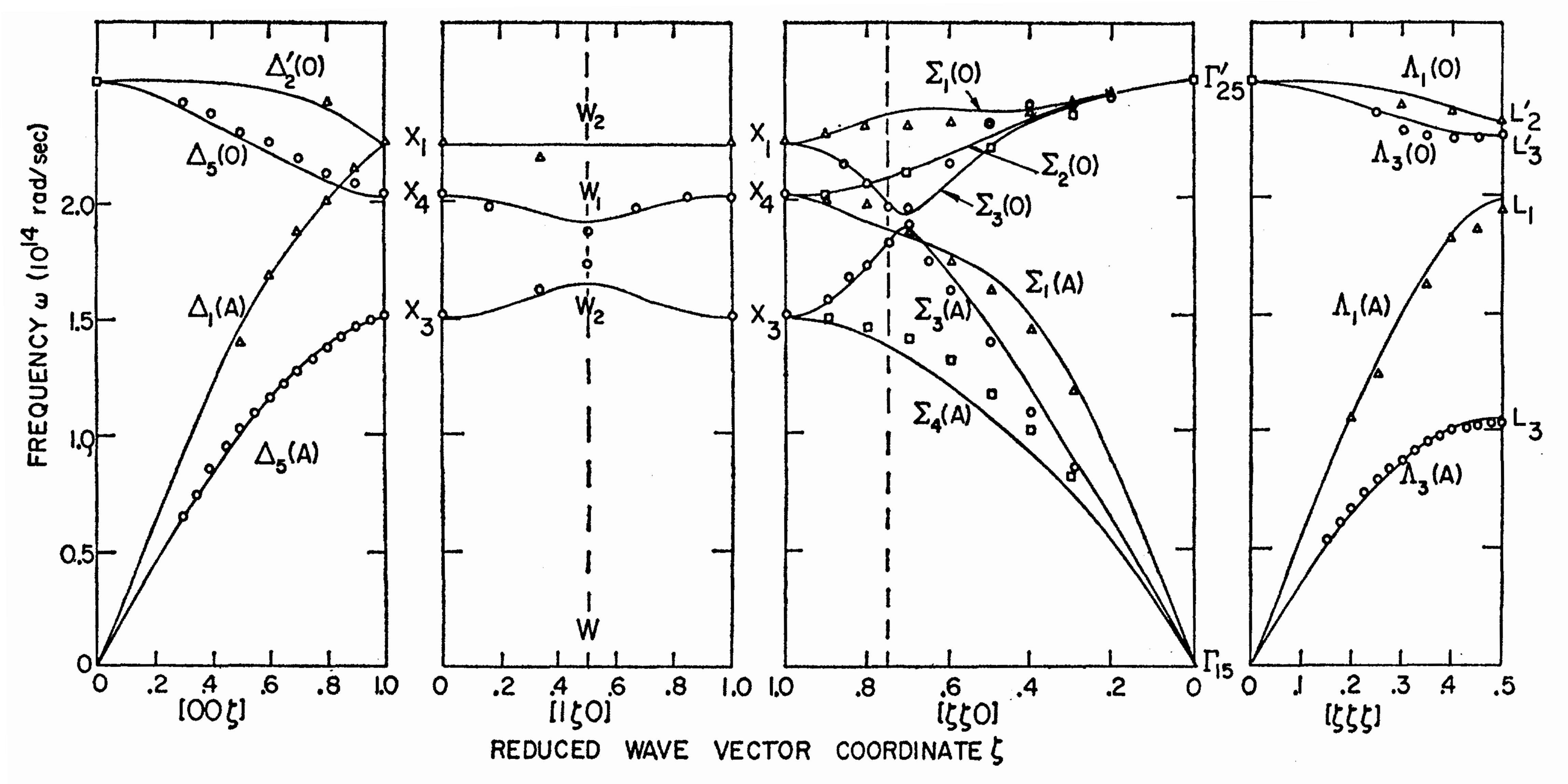
was converted to $MgSiO_3$ 570 °C for one hour, using a uniaxial split-sphere high-pressure apparatus (USSA 5000) [Ito and Yamada, 1982]. The quenched perovskite sample, weighing 9.4 mg, had a slightly-distorted cylindrical shape and was of harf transparency (Figure 1). The sample was confirmed to be a polycrystalline aggregate of $MgSiO_3$ perovskite by a micro-focused X-ray diffractometer. For the

Thermal Conductivity of Materials

<table>
<tr><th>mechanisms:</th><th>electrons</th><th>atoms/ molecules</th><th>photons</th></tr>
<tr><td>Governing Equations</td><td>$\kappa\rho = LT$</td><td>$\kappa \sim C\, v^2\, T_{eff}$</td><td>(solutions for radiative heat flow)</td></tr>
<tr><td>Temperature dependence</td><td>
</td><td>
</td><td>
</td></tr>
<tr><td>Examples (W/m/K)</td><td>lead 35
iron 80
gold 310</td><td>asbestos 0.2-0.8
granite 2-4
Al_2O_3 30
diamond >1000</td><td></td></tr>
<tr><td>Trivia</td><td>$\kappa_{melt} < \kappa_{solid}$</td><td>$SiO_2$ qtz 9.5/6.1
SiO_2 glass 1.46</td><td>goes in & out of fashion</td></tr>
</table>

Thermal Conductivity in Crystalline Insulators:

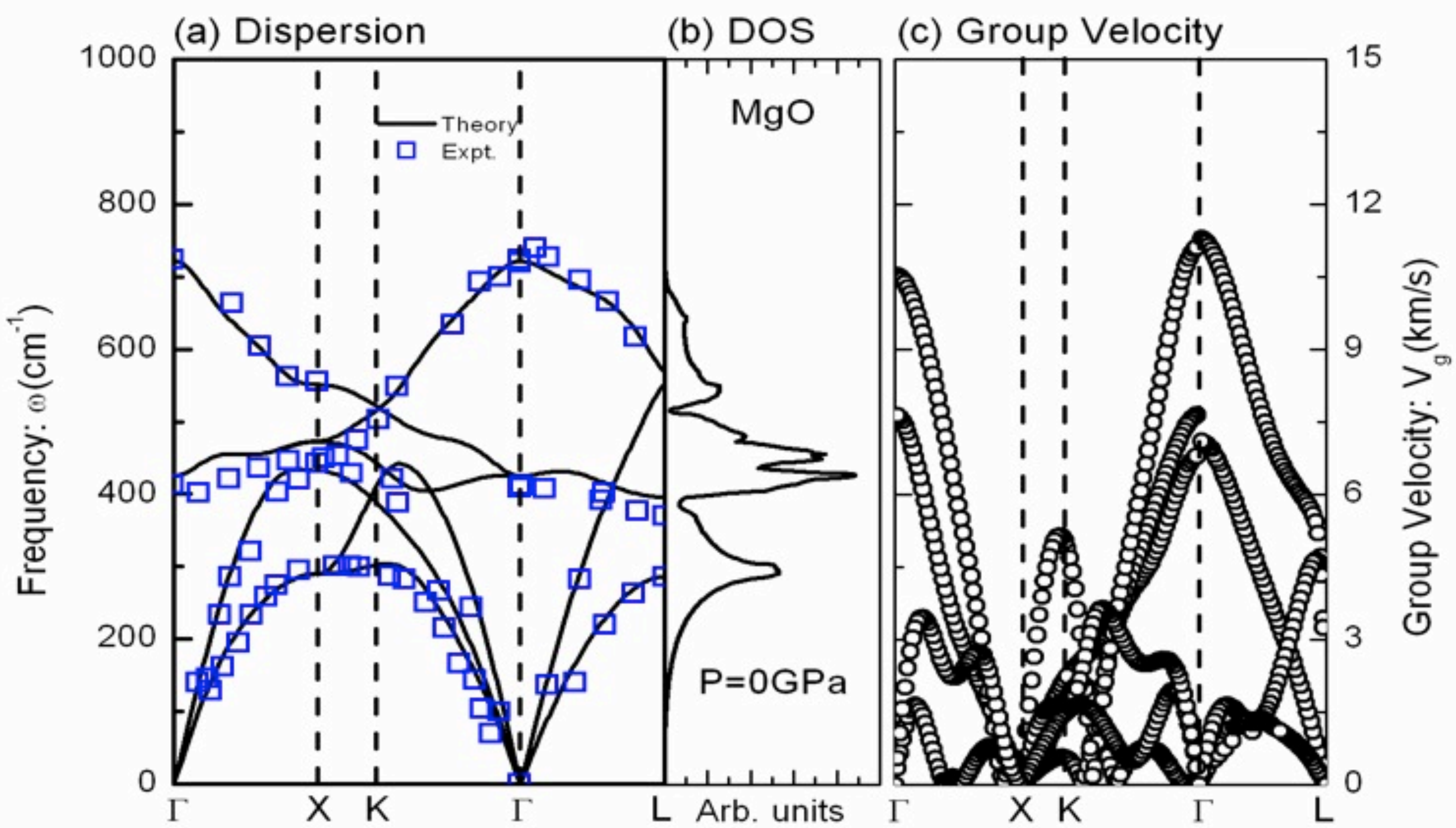
Momentum transfer due to phonon interactions



Phonon dispersion curve of diamond
Warren et al., 1967

Approaches to thermal conductivity of insulators

1. Determine phonon behavior-experiment/theory
2. Measure heat flow directly via Q=dT/dx



MgO

Tang & Dong, 2010

Approaches to thermal conductivity of insulators

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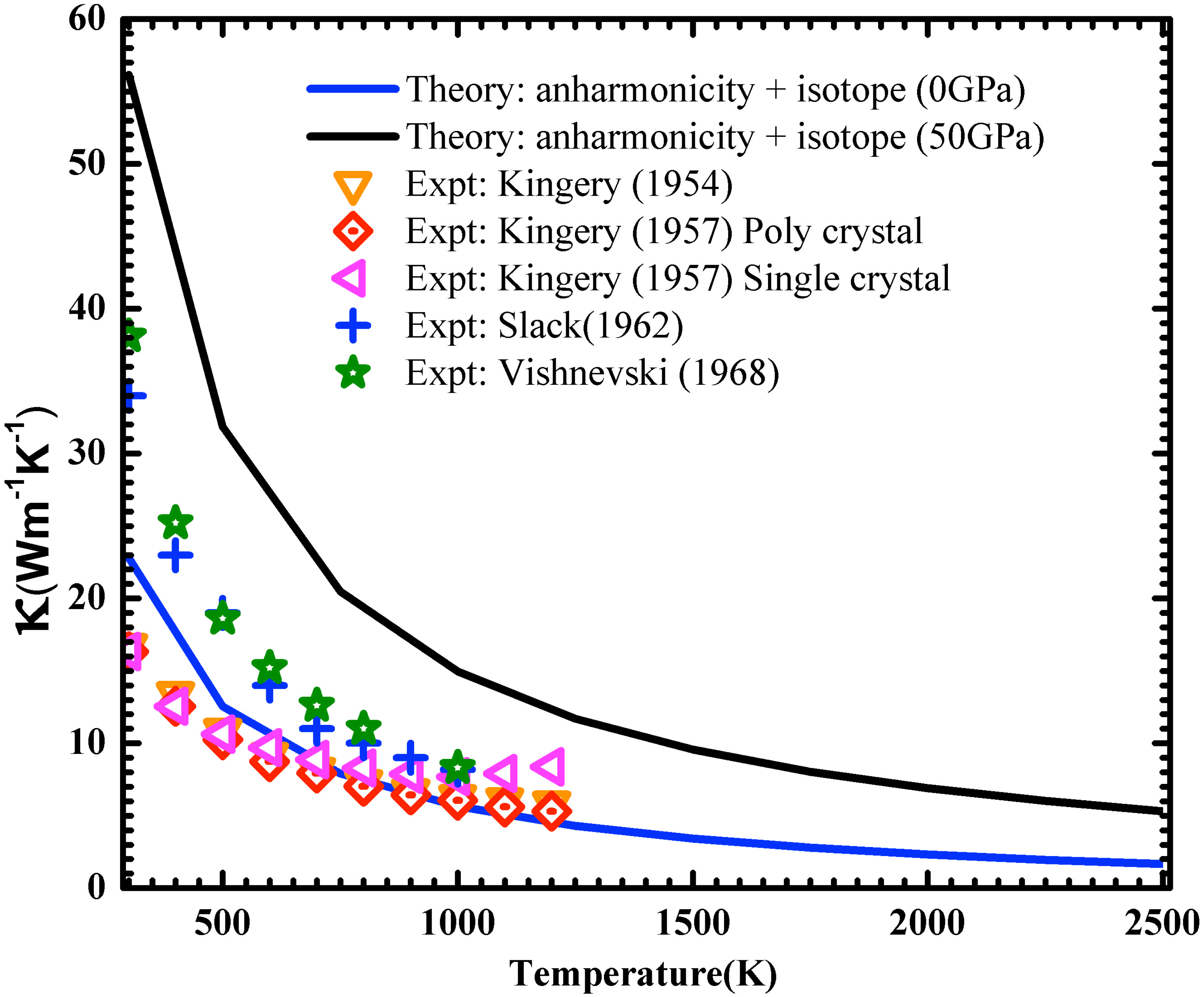
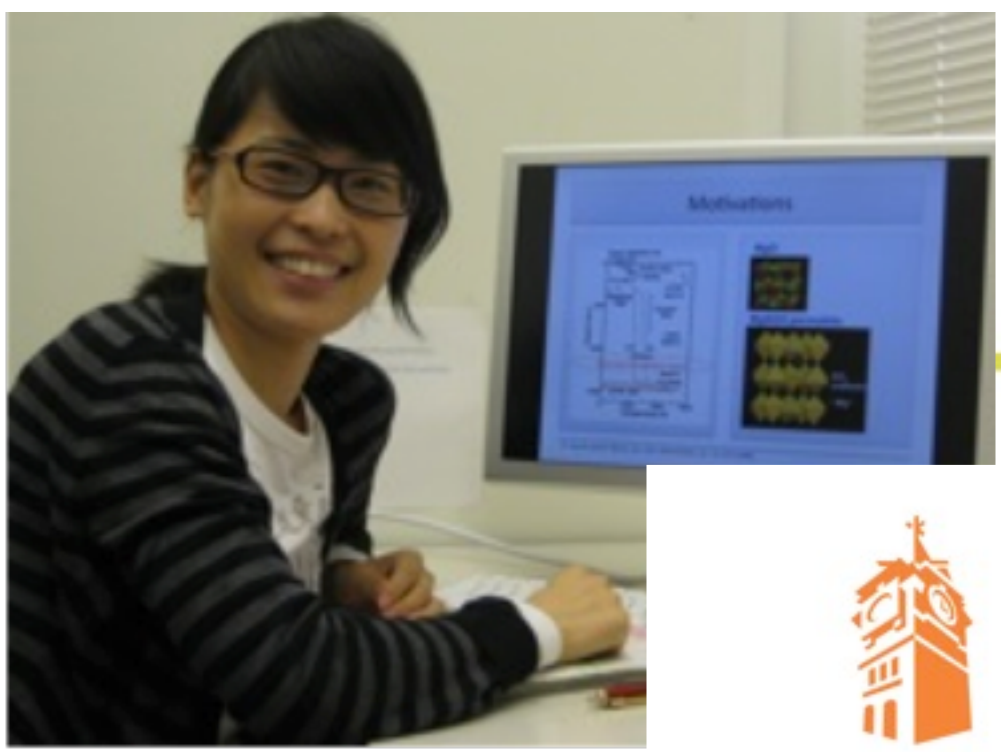


Thermal conductivity of MgO shows good agreement between theory and experiment

Tang & Dong 2010
de Koker 2009

Thermal Conductivity of $MgSiO_3$-pv and Heat Transport in the Earth's Mantle

Xiaoli Tang (Now at: CalTech, Applied Physics)
Abby Kavner (Earth & Space Science, UCLA)
Jianjun Dong (Physics, Auburn University)
Laurent Pilon (Mech E., UCLA)
Emma Rainey (Earth & Space Science, UCLA)



AUBURN UNIVERSITY

NSF

UCLA

Approach: Solve the Peierls-Boltzmann kinetic transport equation for phonons

$$\kappa = \frac{1}{3}\sum_{i,\vec{q}} c_V(i,\vec{q})\, v_g{}^2(i,\vec{q})\, \tau(i,\vec{q})$$

Lattice thermal conductivity (W/m/K)

Heat capacity J/K/m³

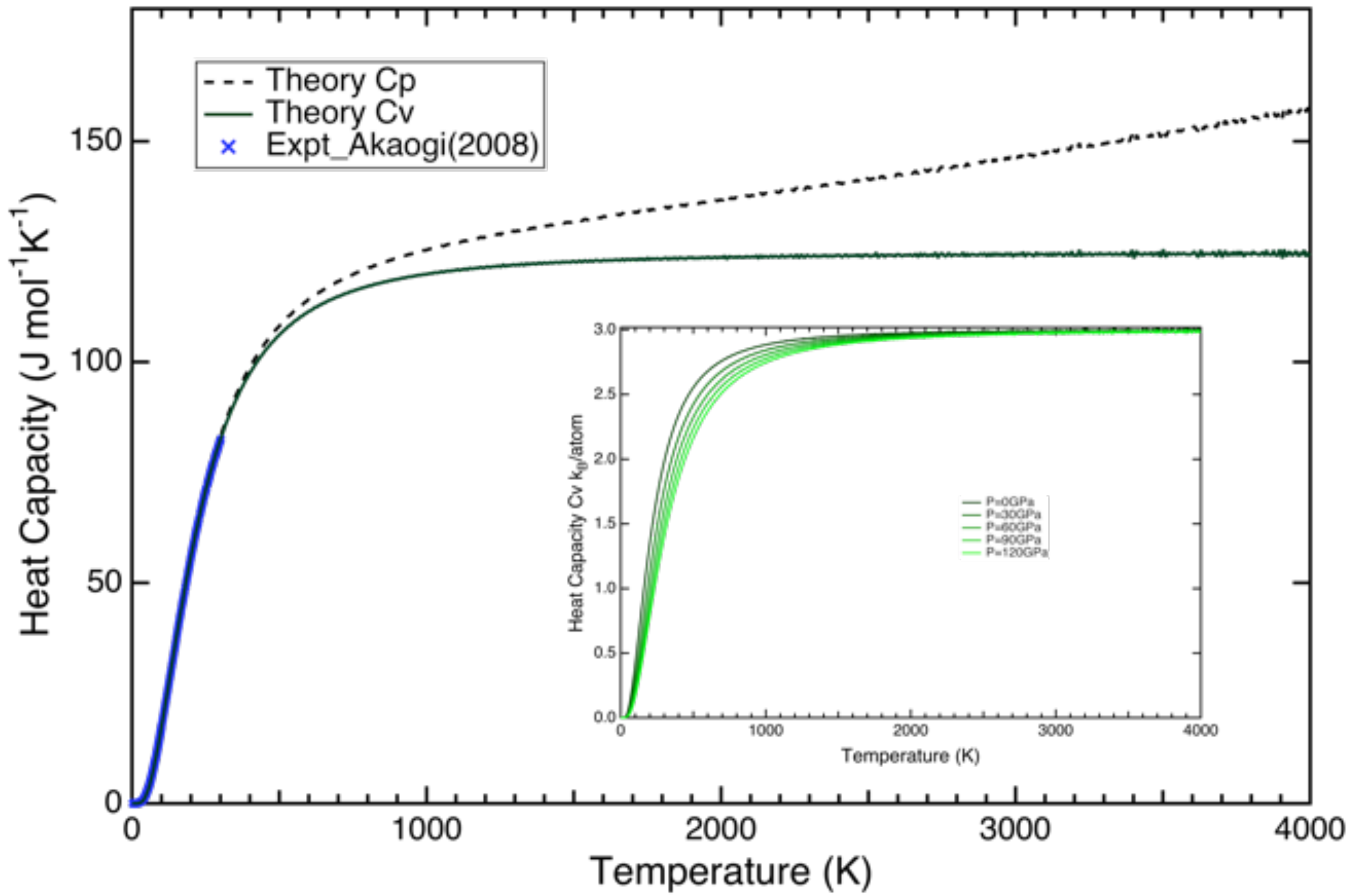
Phonon group velocity (m/s)²

Phonon lifetime s

Integrate over all phonon modes in three dimensions

Heat Capacity C_V

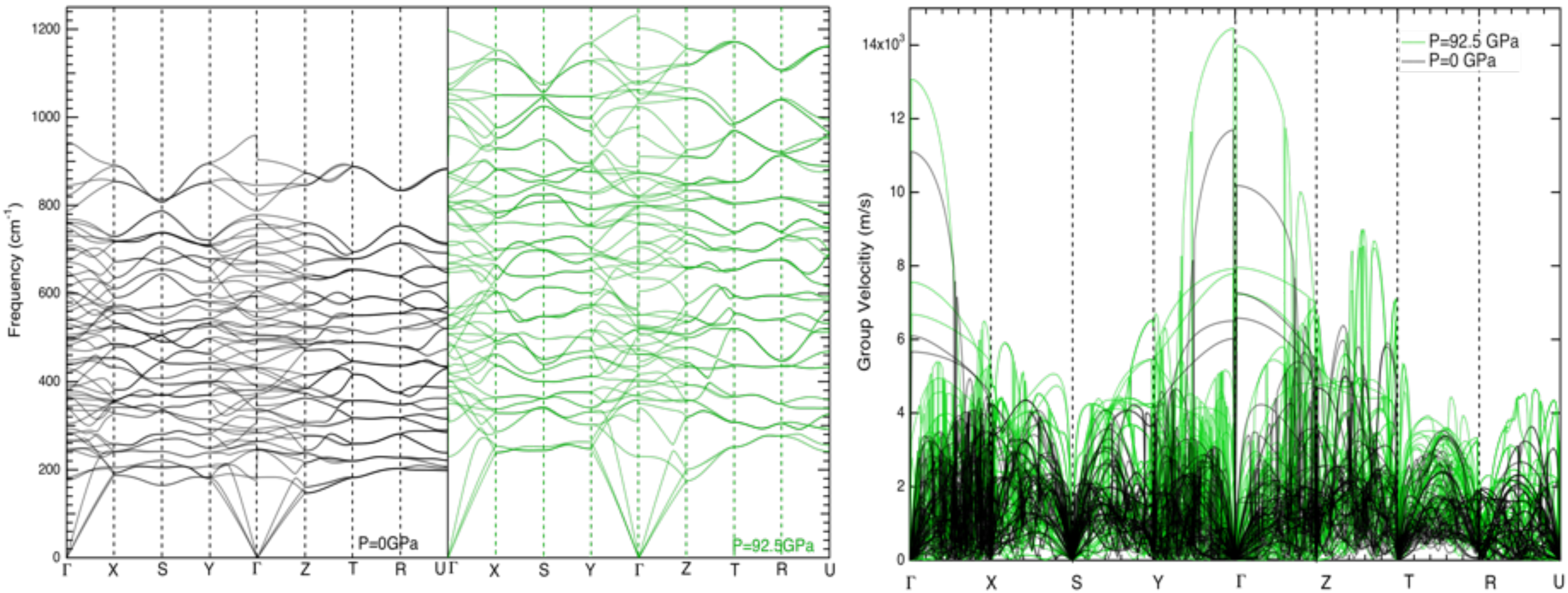
$k = C_v v_g^2 \tau$



- Heat capacity only varies in low-temperature range ($T<\theta_D$).
- Heat capacity changes insignificantly with pressure.

Phonon Group Velocity Vg

$k = C_v v_g^2 \tau$



- Phonon frequencies increase as pressure goes up.
- Overall phonon group velocity also increases at higher pressure.
- Mode-by-mode group velocities have large variablility

Phonon Life Time τ_{eff}

$k = C_v v_g^2 \tau$

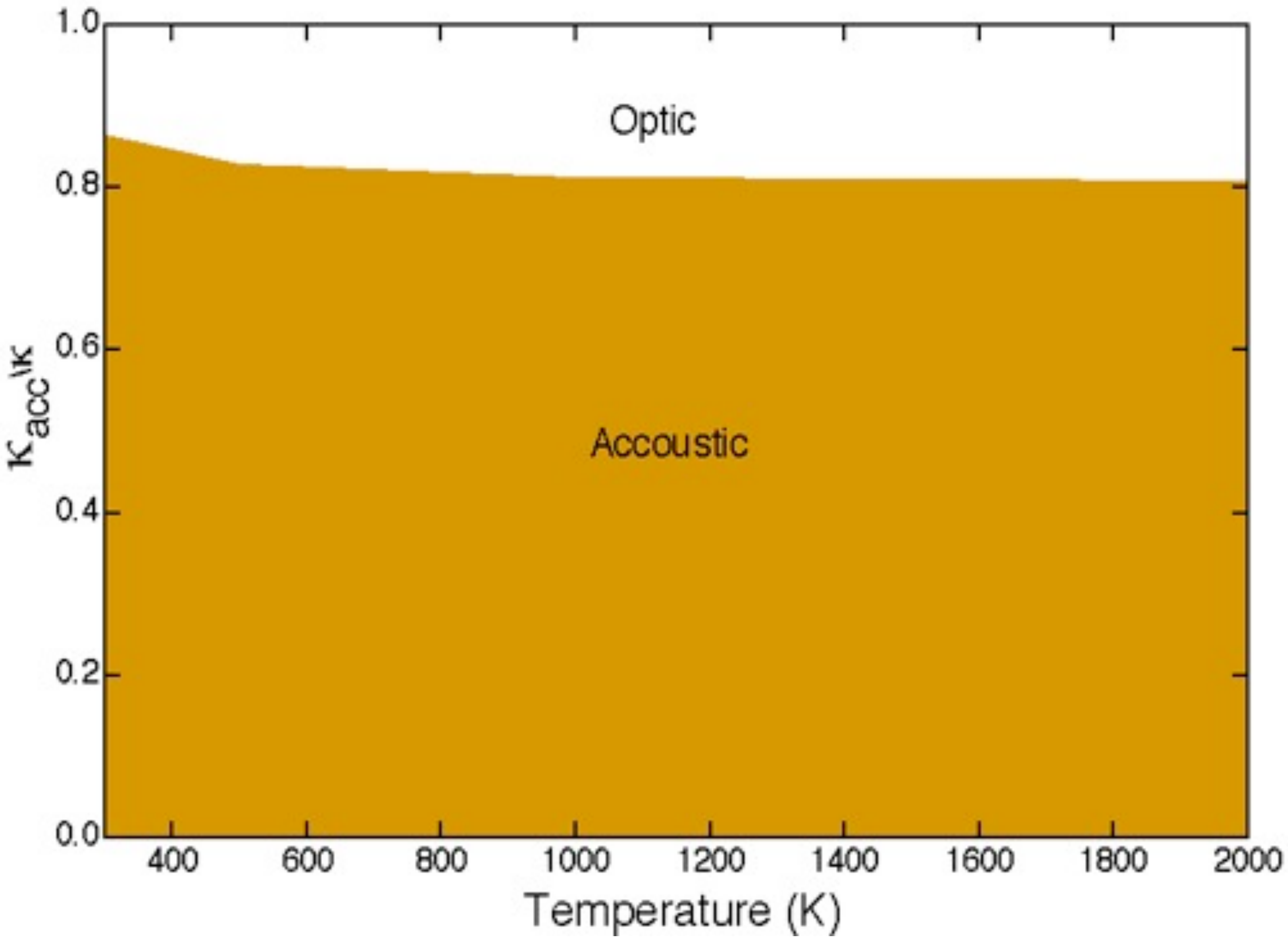
MgSiO₃: (3 acoustic + 57 optic) v.s MgO: (3 acoustic + 3 optic)

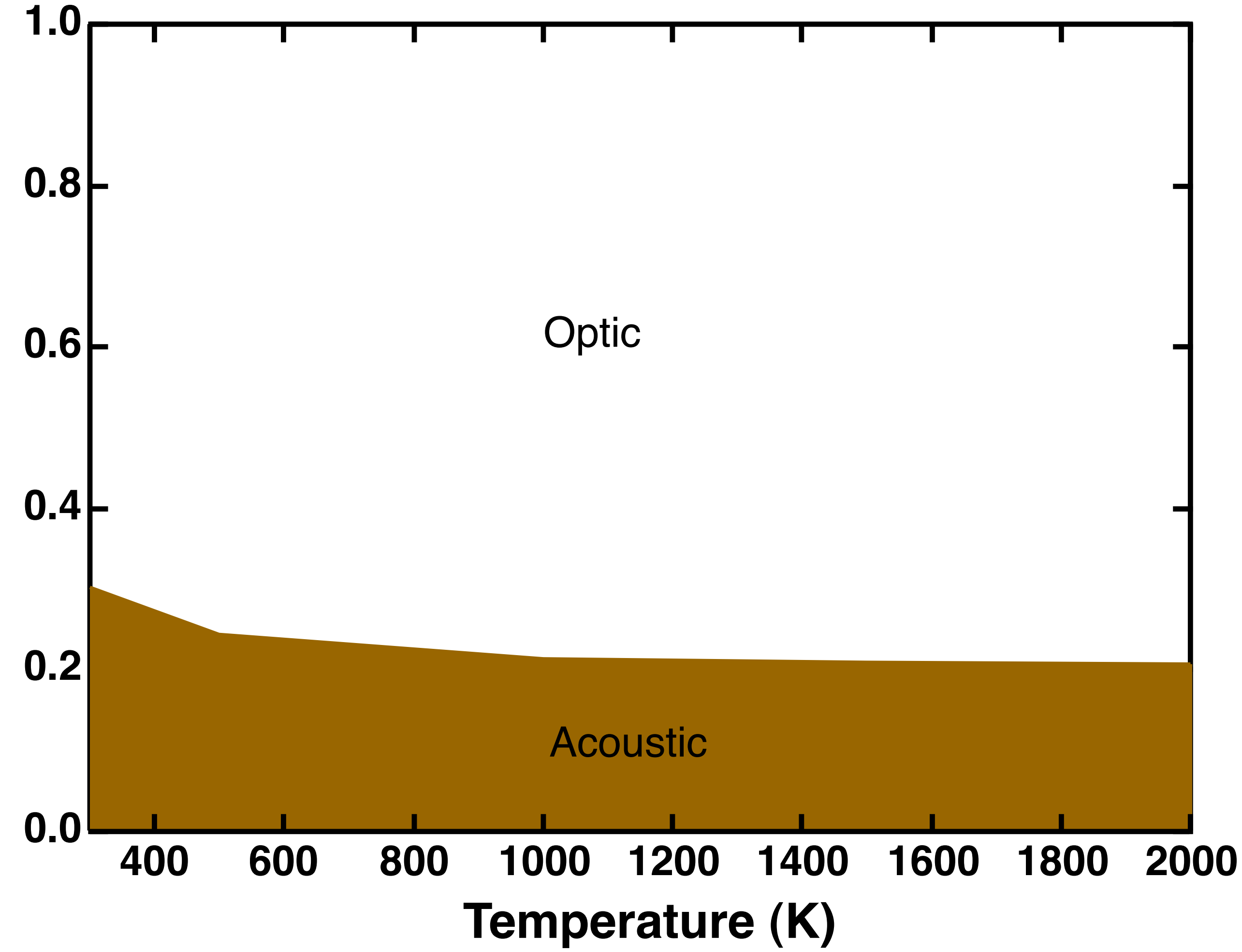
Typical ***τ_{eff}***	τ_{eff}(acoustic) T=300K (ps)	τ_{eff}(acoustic) T=3000K (ps)	τ_{eff}(optic) T=300K (ps)	τ_{eff}(optic) T=3000K (ps)
$MgSiO_3$	1.7	0.14	0.16	0.008
MgO	8.5	3.03	0.91	0.34

Phonon lifetimes are much smaller in MgSiO3 than in MgO

Mode contributions: optic vs. acoustic

$$\kappa = \kappa_{acoustic} + \kappa_{optic}$$

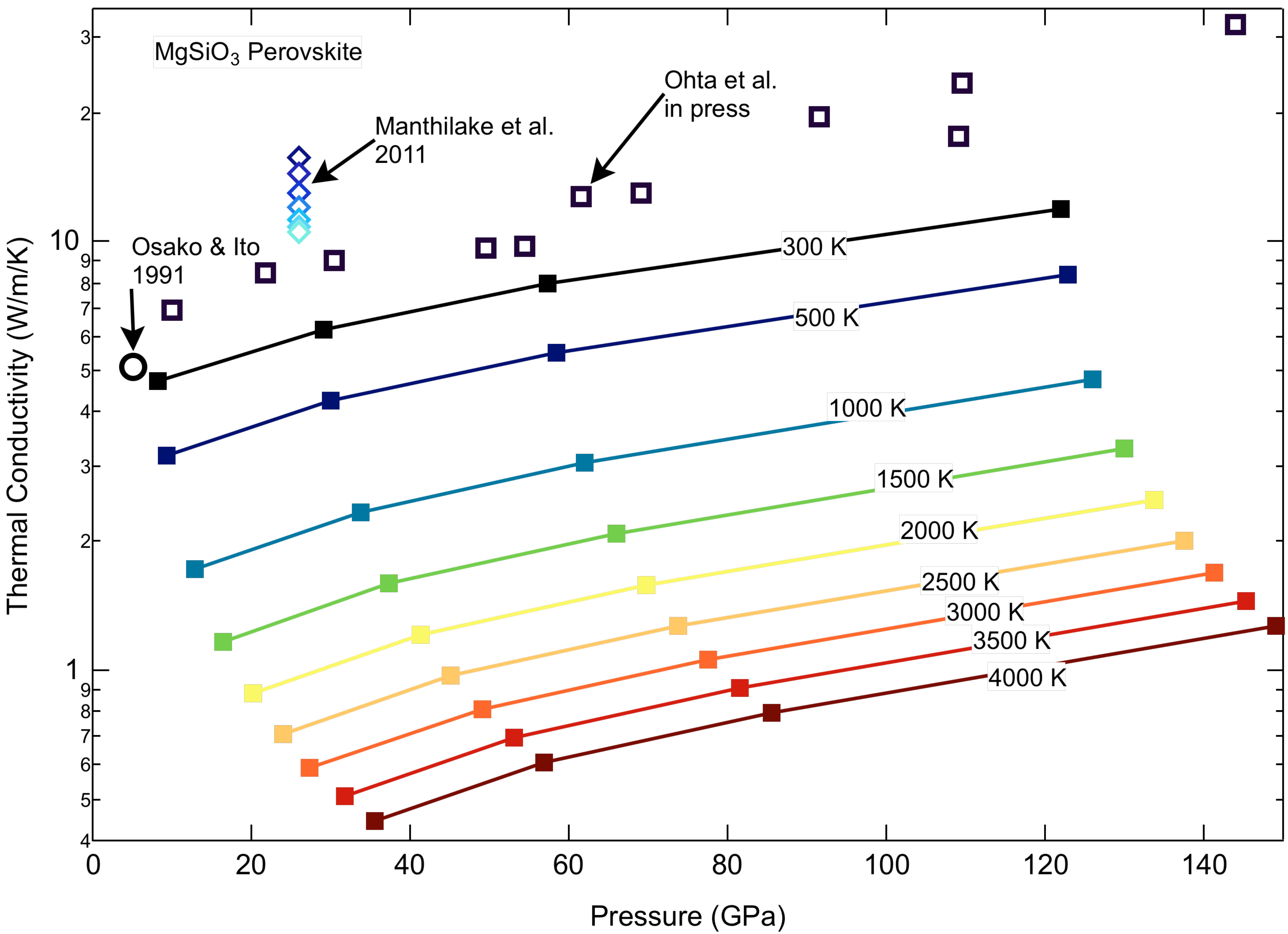




quick quiz: which is MgO?

which is $MgSiO_3$? why?

Results--Thermal conductivity $MgSiO_3$



Additional considerations for Earth's mantle

1. Effect of iron

2. Radiative contribution to heat flow

3. Composite material

✔1. Changes mass

✔2. Adds impurities

3. Chemical effects

for now:

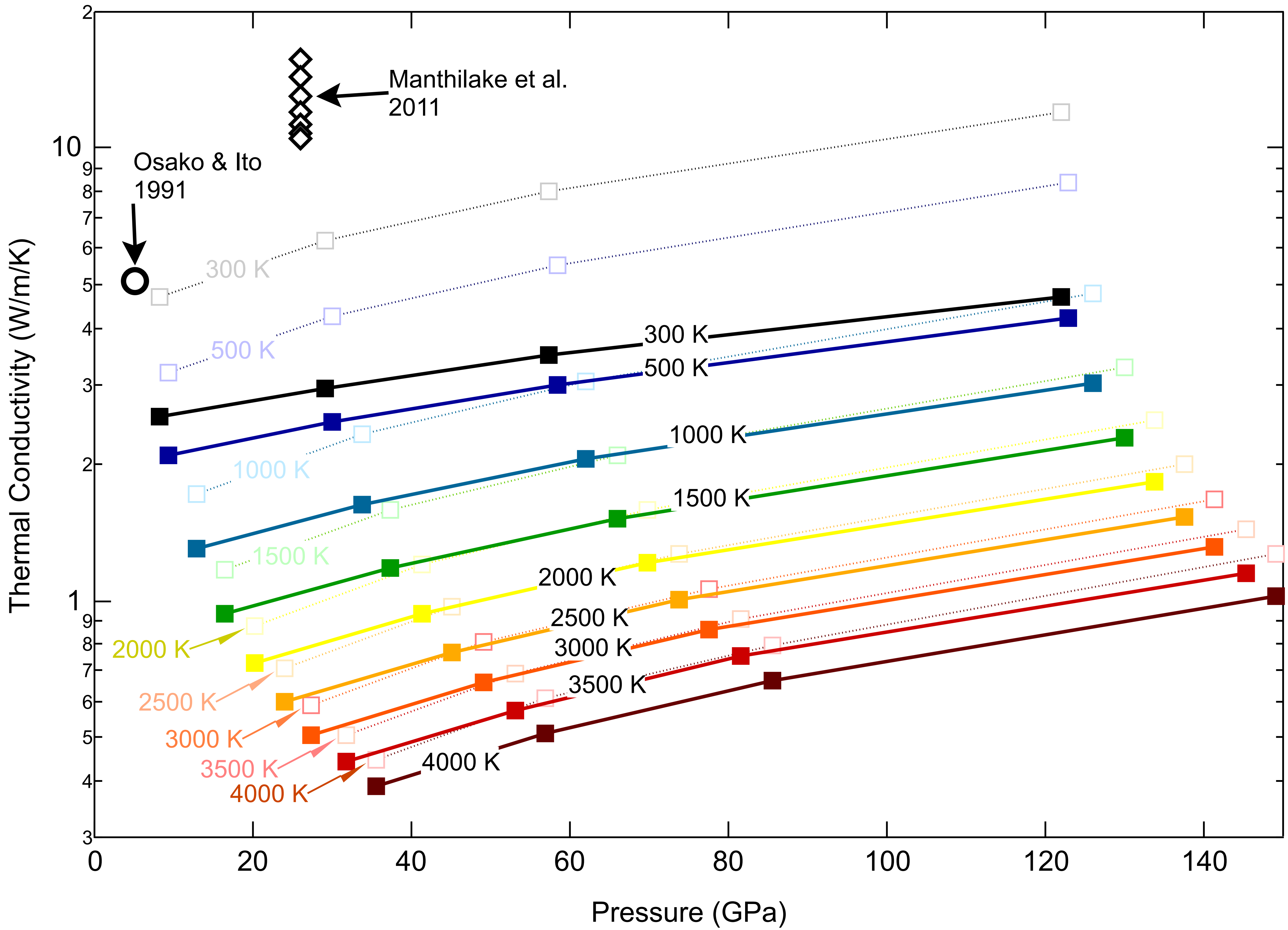
i. Fe+2 substitution for Mg+2

ii. high spin in Pv

iii. low spin in MgO

Reference : Moses C. Natm, Jianjun Dong, manuscript in preparation

Thermal conductivity $(Mg_{.85},Fe_{.15})SiO_3$



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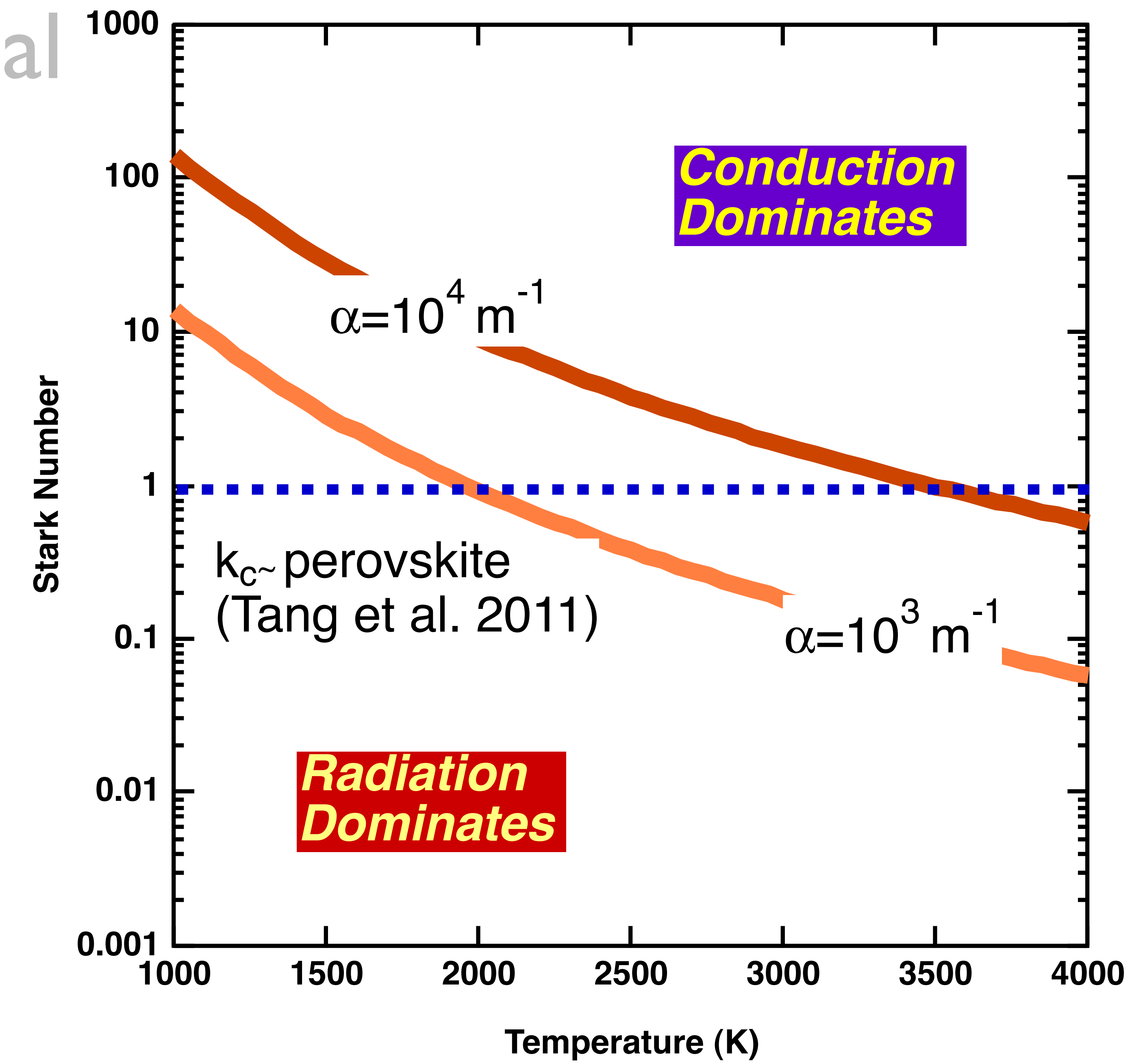


Stark Number:
Non dimensional parameter to determine relative importance of radiative transport
$N=\kappa_{cond}\alpha_{abs}/4\sigma T^3$

$1/\alpha_{abs}$ ~absorption length scale

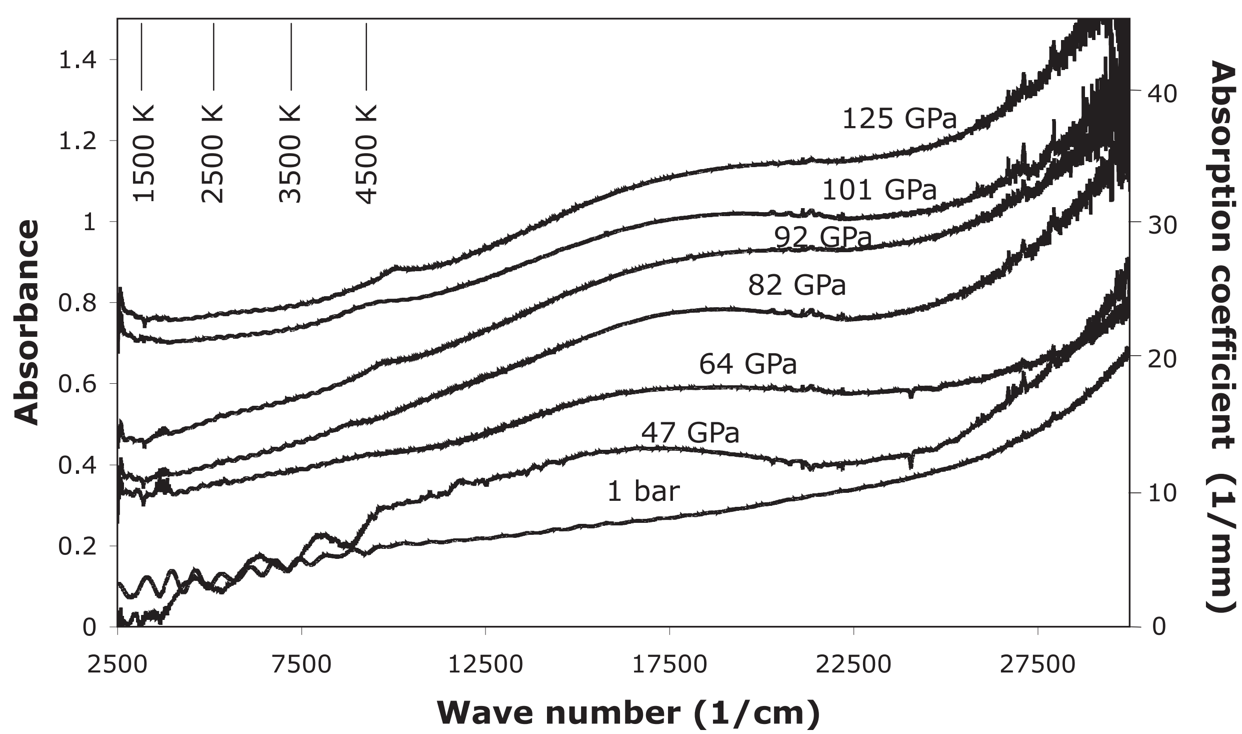
Competing Measurements of Absorption Coefficients

Science, 2008

Nature, 2008

Optical Absorption and Radiative Thermal Conductivity of Silicate Perovskite to 125 Gigapascals

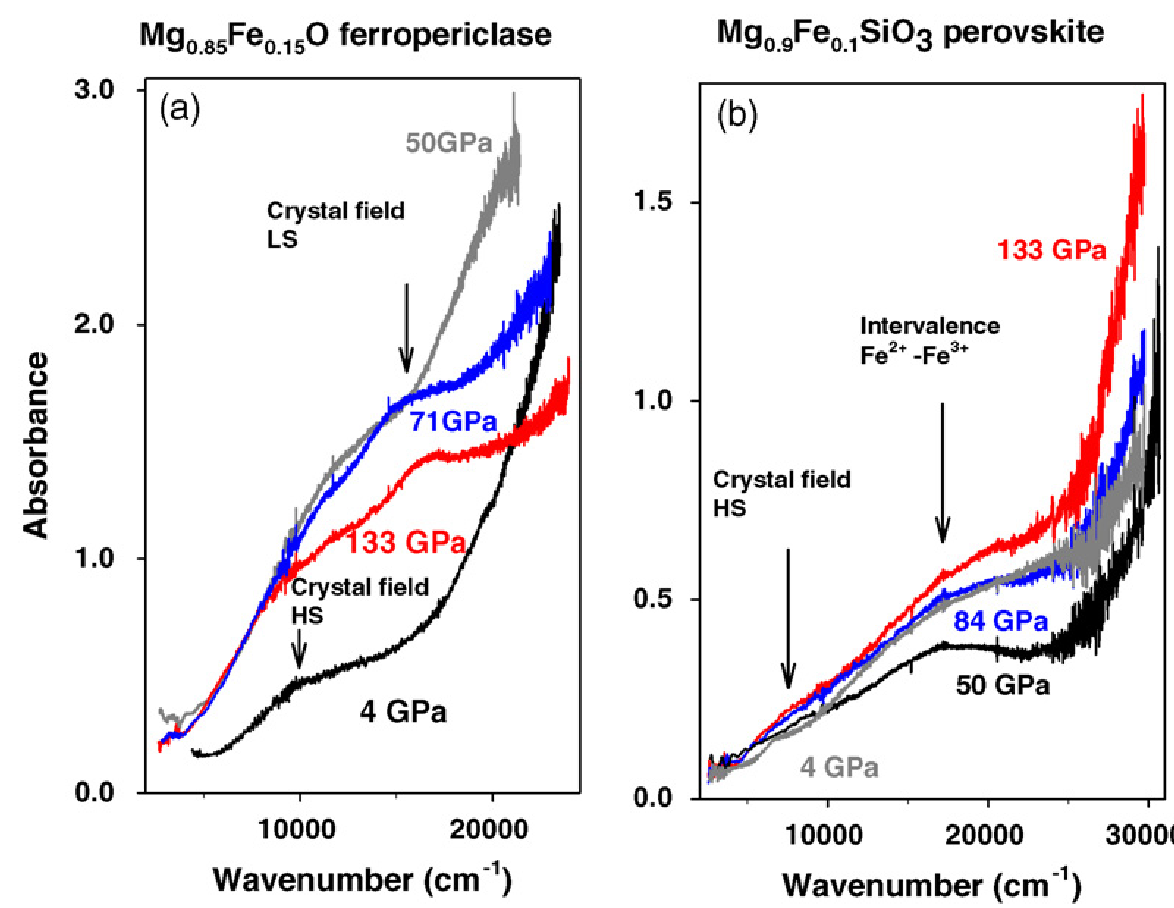
Hans Keppler,[1]* Leonid S. Dubrovinsky,[1] Olga Narygina,[1] Innokenty Kantor[1,2]



Thermal conductivity of lower-mantle minerals

Alexander F. Goncharov[a,*], Pierre Beck[a], Viktor V. Struzhkin[a], Benjamin D. Haugen[a,b], Steven D. Jacobsen[c]

[a] Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road N.W., Washington, DC 20015-1305, USA
[b] Department of Geological Sciences, University of Colorado, Boulder, CO 80309, USA
[c] Department of Earth and Planetary Sciences, Northwestern University, Evanston, IL 60208, USA



Competing Measurements of Absorption Coefficients

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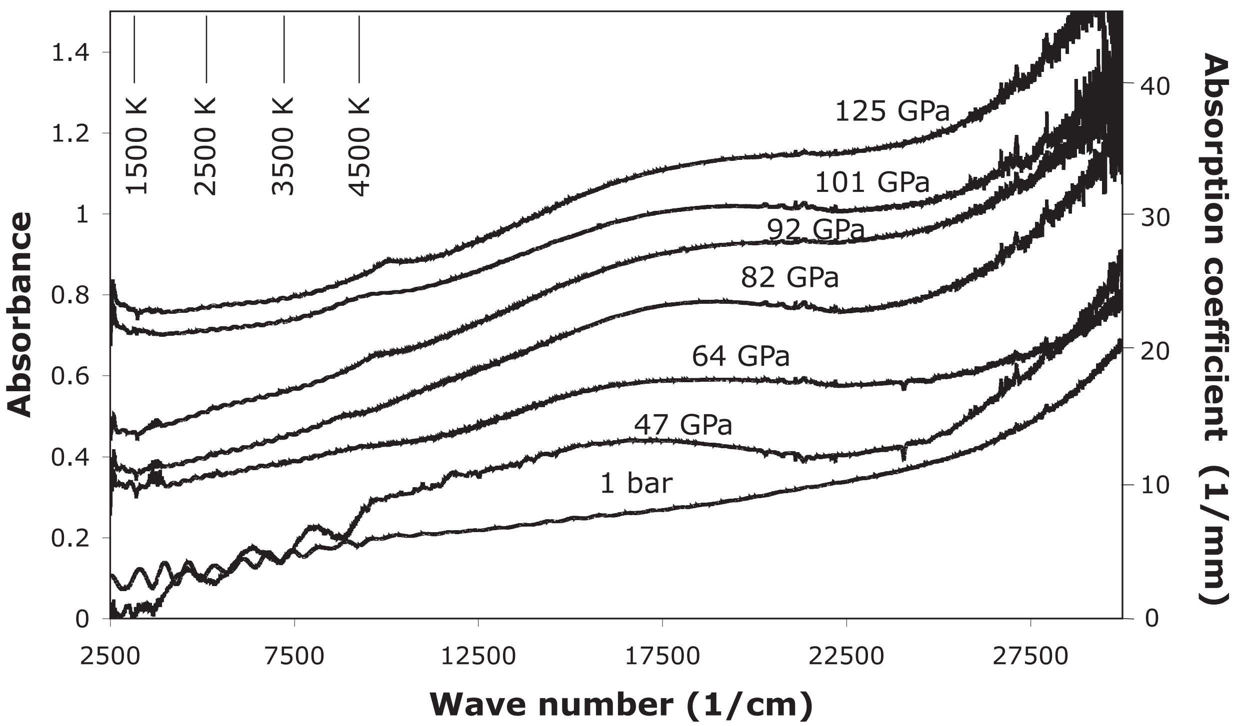
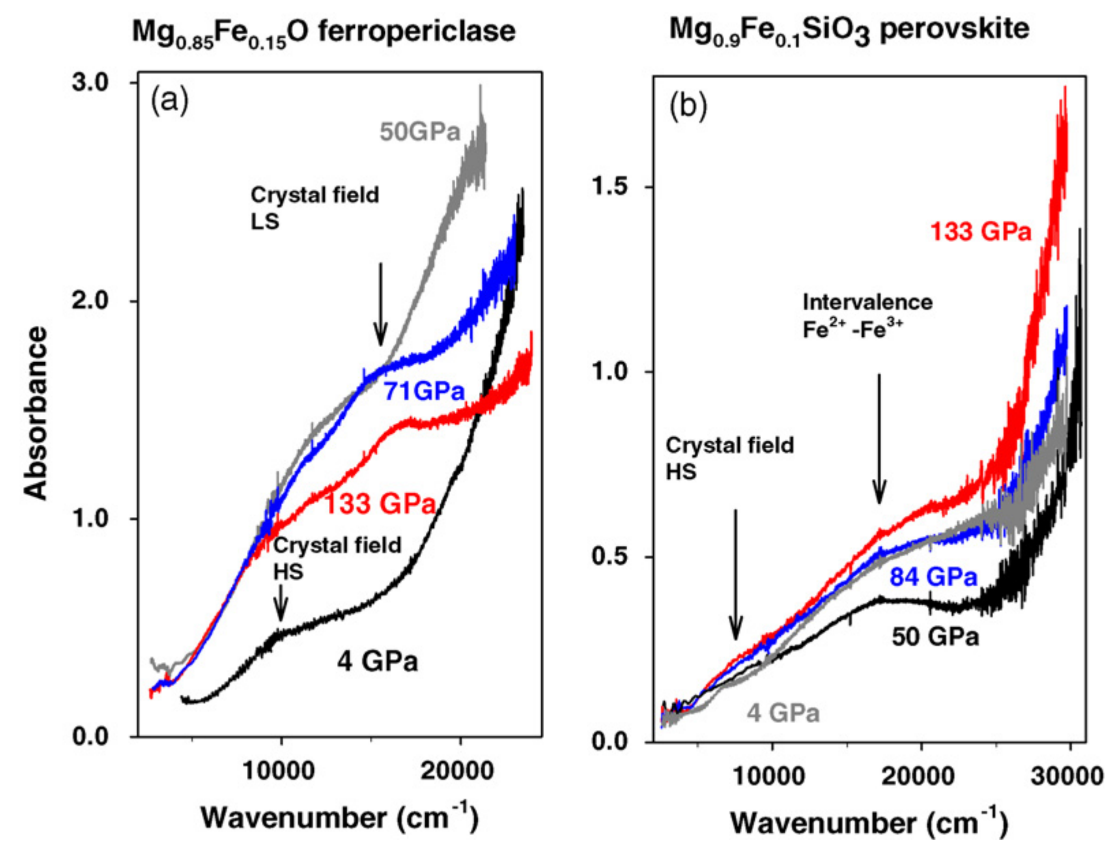
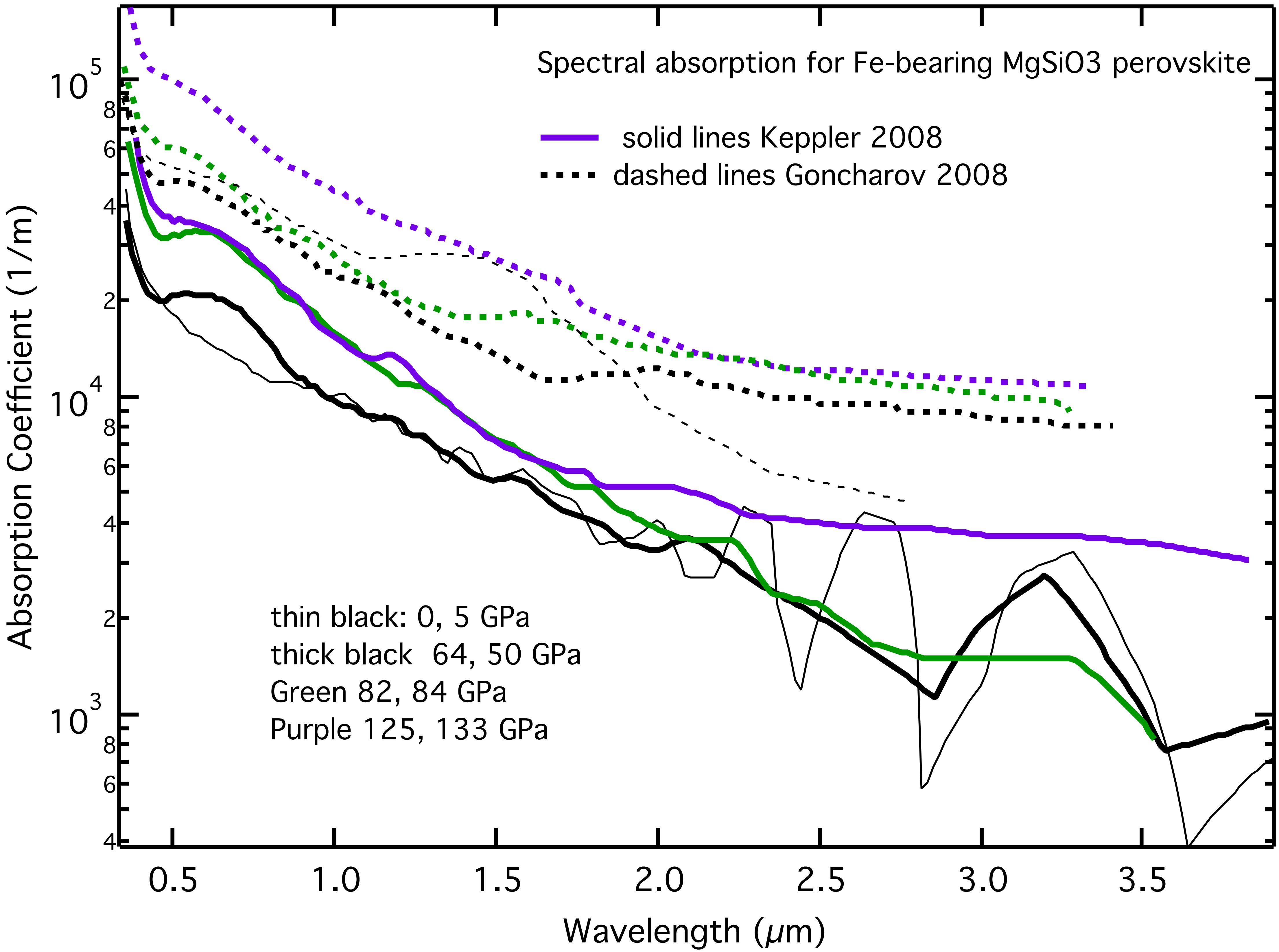




"pristine mantle" radiative heat flow is important

"dirty mantle" radiative heat flow is not important

step 1: plot everything on same plot



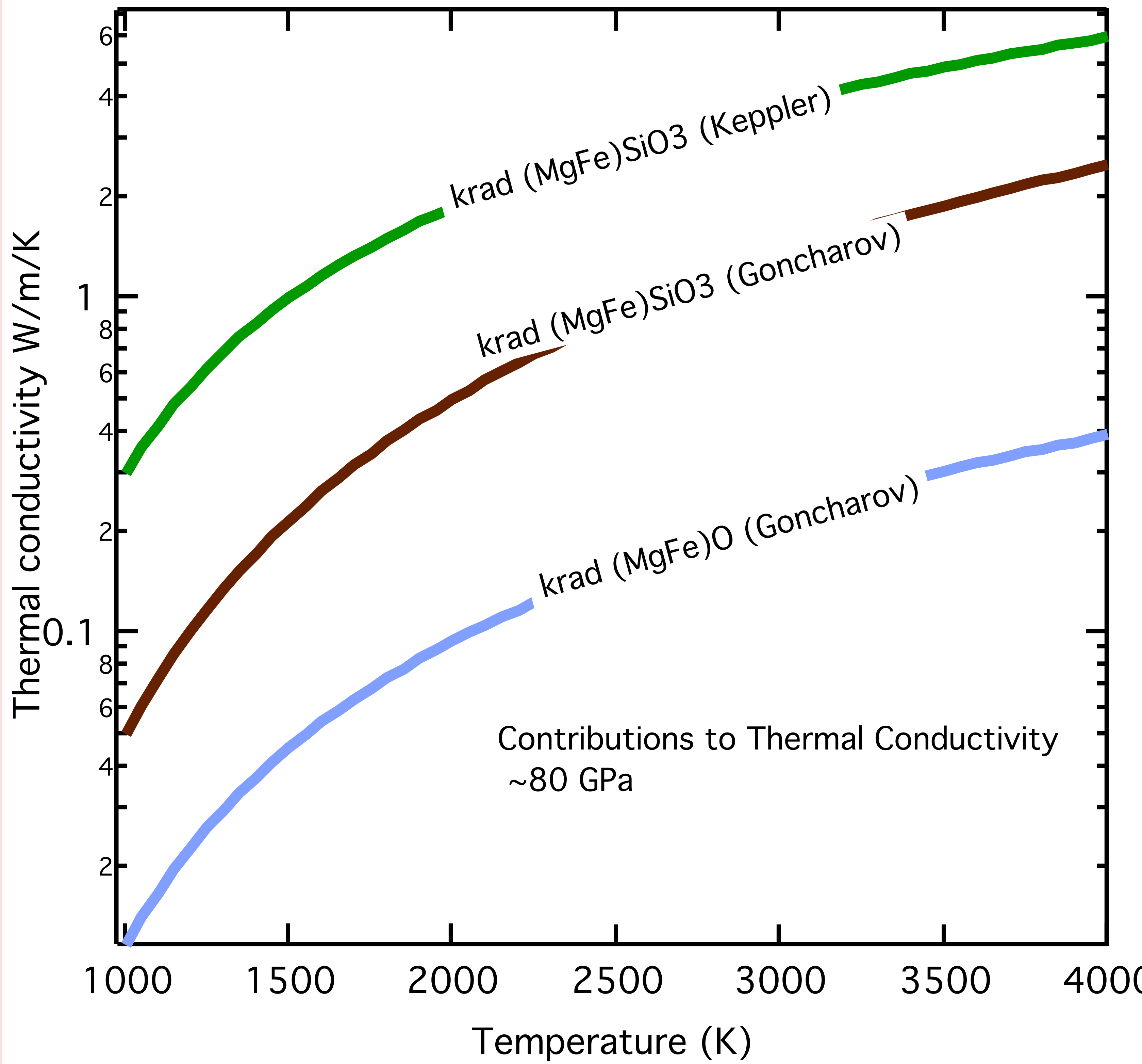
step 2: Re-analyze data

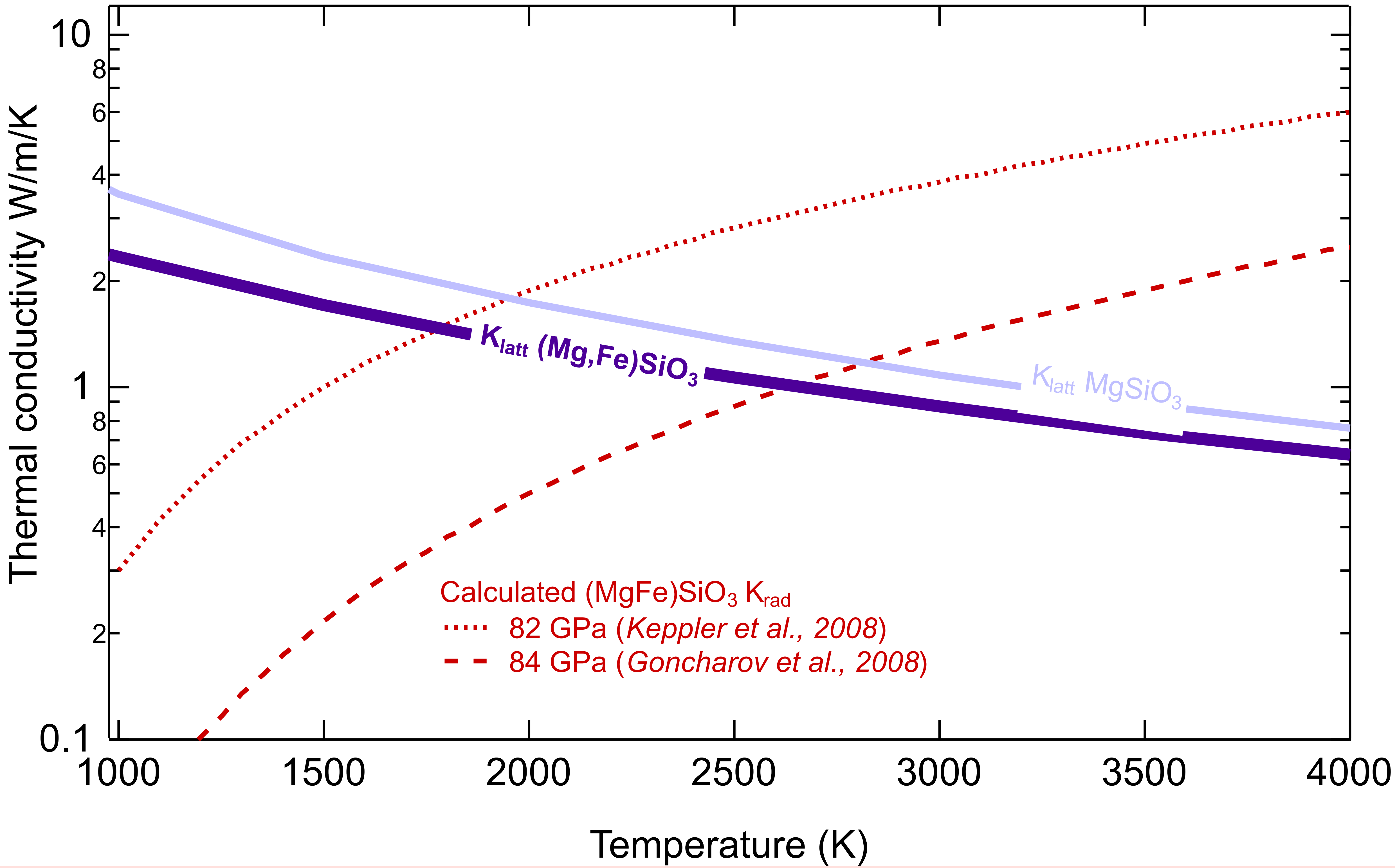
radiative contribution to thermal conductivity calculated via Rosseland approximation
(valid for optically thick)

$$k_{rad}(T) = \frac{16n^2\sigma T^3}{3\beta_R},$$

n: Index of refraction
T: Temperature
β: Rosseland mean extinction coefficient

$$\frac{n^2}{\beta_R} = \frac{\pi}{4\sigma T^3}\int_0^\infty \frac{n_\lambda^2}{\beta_\lambda}\frac{dI_{b,\lambda}}{dT}\,d\lambda.$$



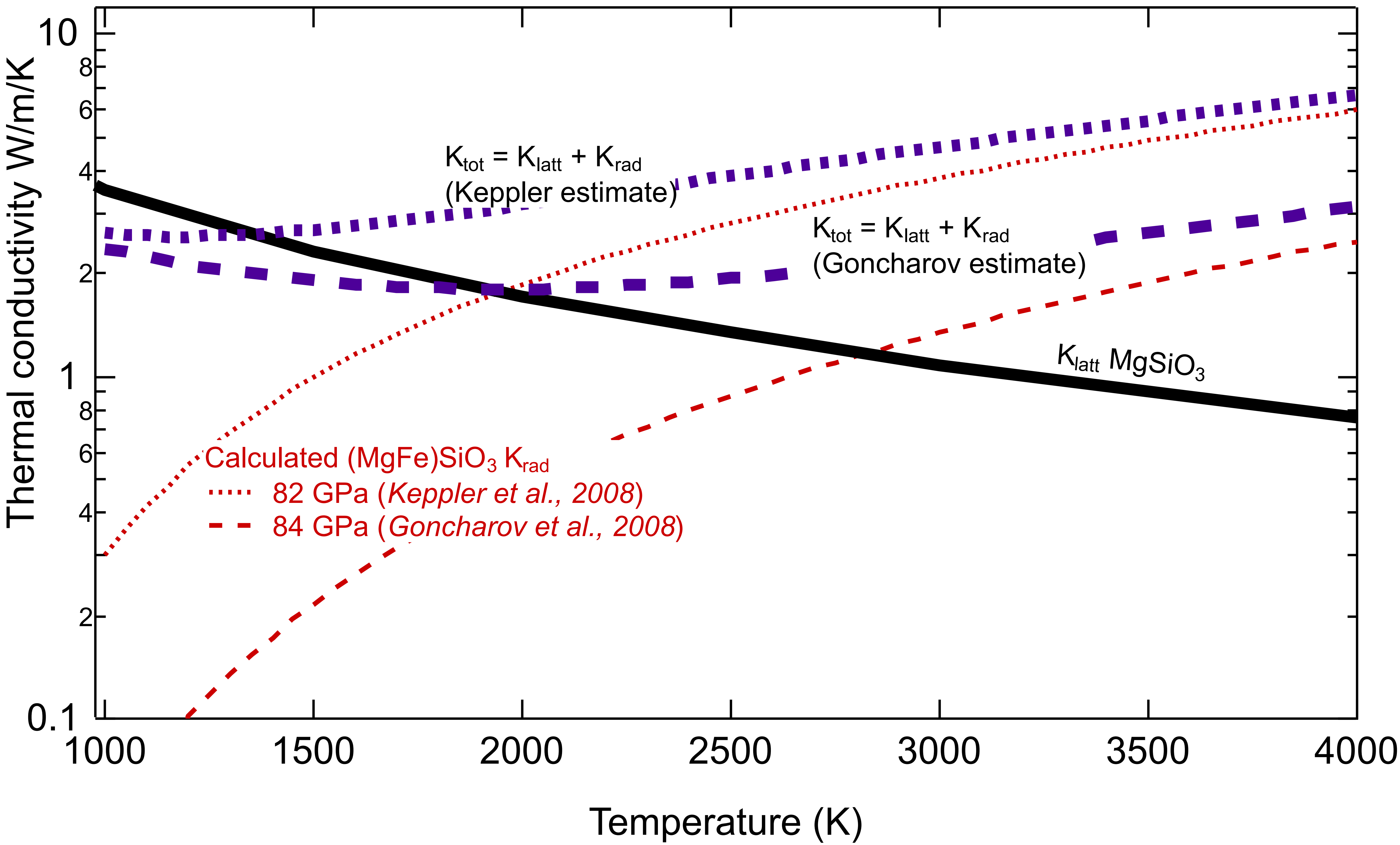


Lattice and radiative contributions to thermal conductivity have:

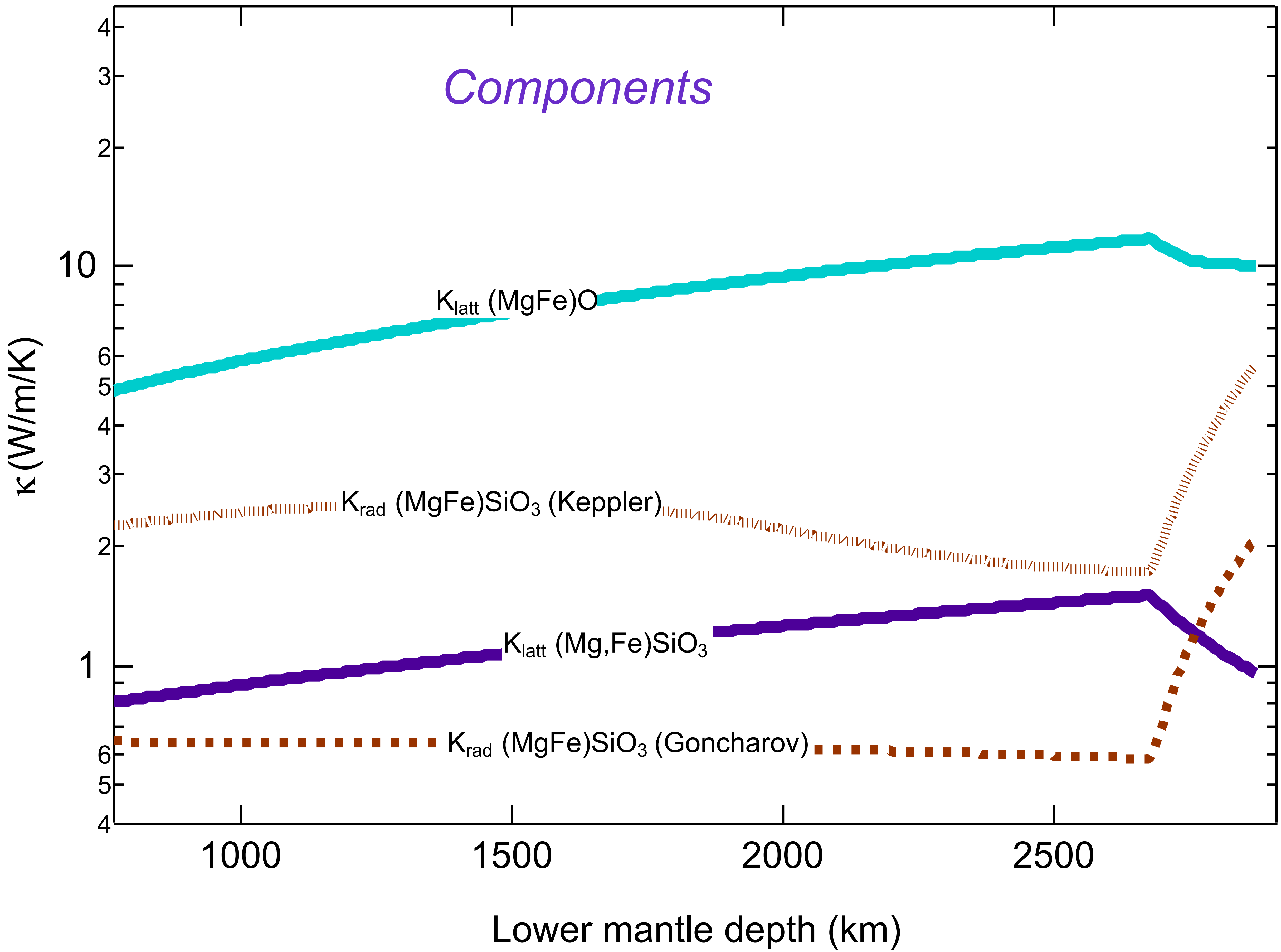
Similar magnitude

Opposite temperature dependence

Total thermal conductivity of perovskite



Depth-Dependent Contributions to Conductivity



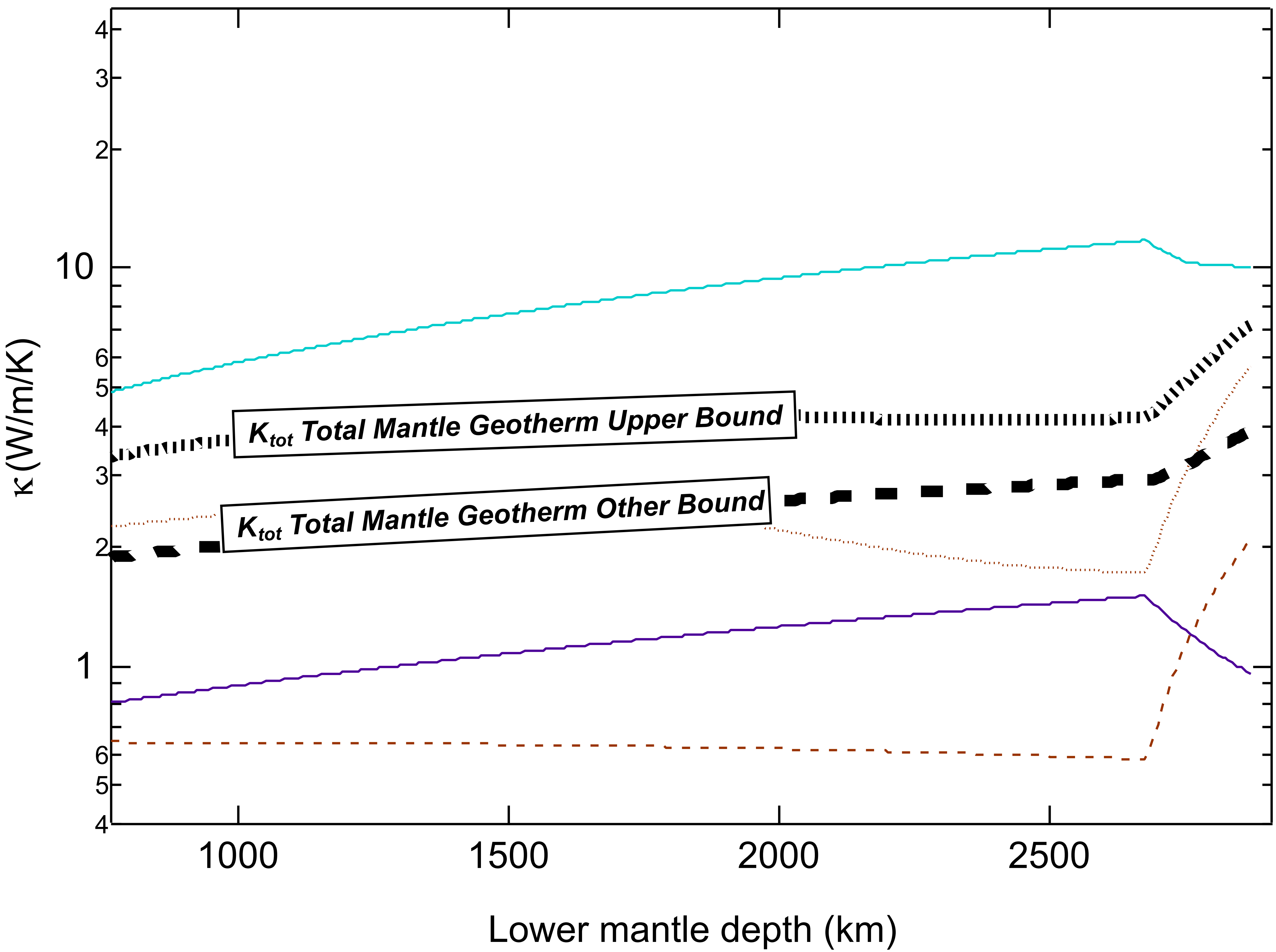
Additional considerations for Earth's mantle

1. Effect of iron
2. Radiative contribution to heat flow
3. ***Composite material***

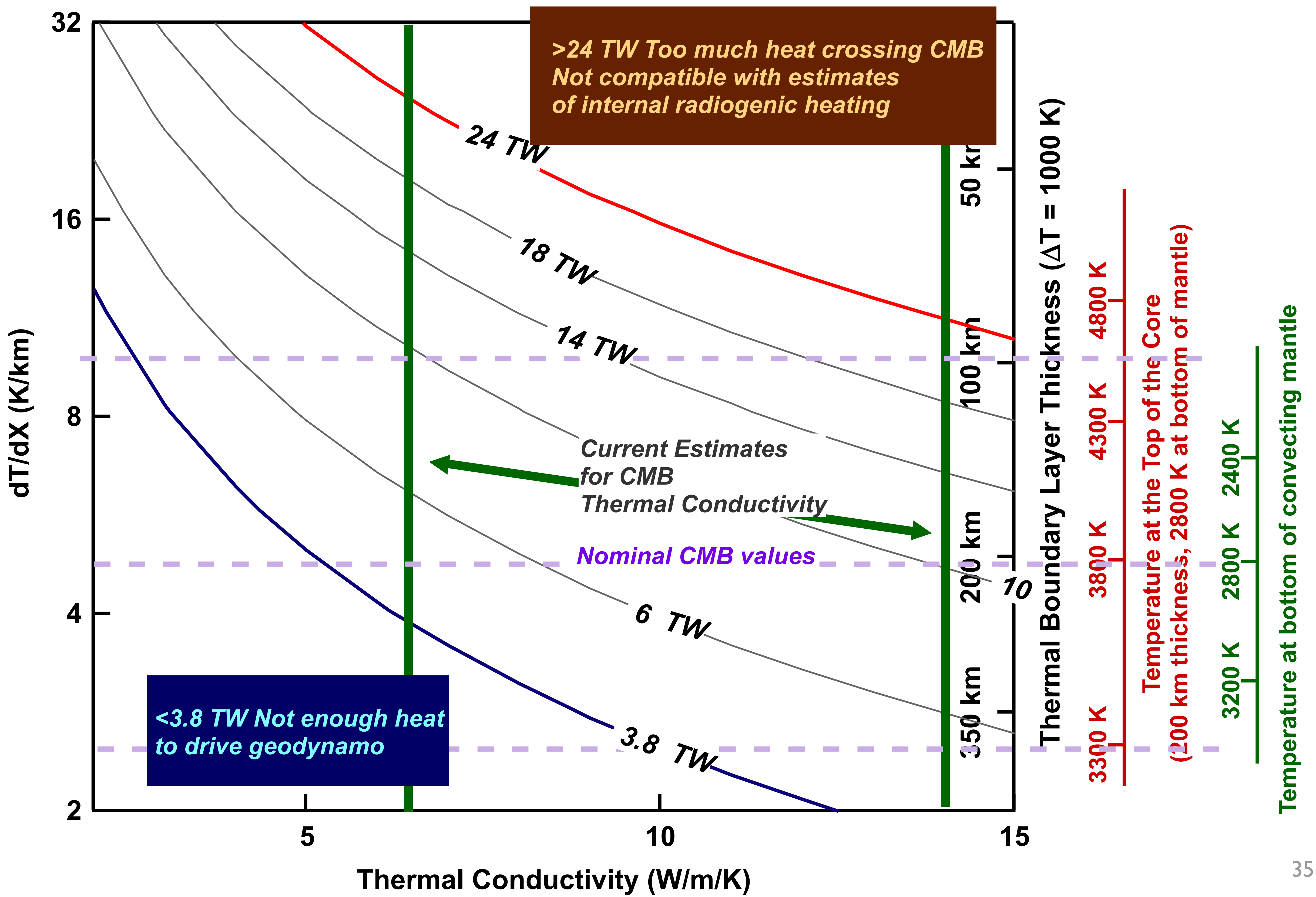
✪ Maxwell-Garnett Composite

	k_{latt}	k_{rad}	
$MgSiO_3$	P,T, Fe	P,T, Fe	$k_{latt}+k_{rad}$ $MgSiO_3$ ✪
MgO	P,T, Fe	P,T, Fe	$k_{latt}+k_{rad}$ MgO
	length scales: ***k_{latt} < 10 nm*** ***k_{rad} < 100μm*** ***grain size ~1mm***		

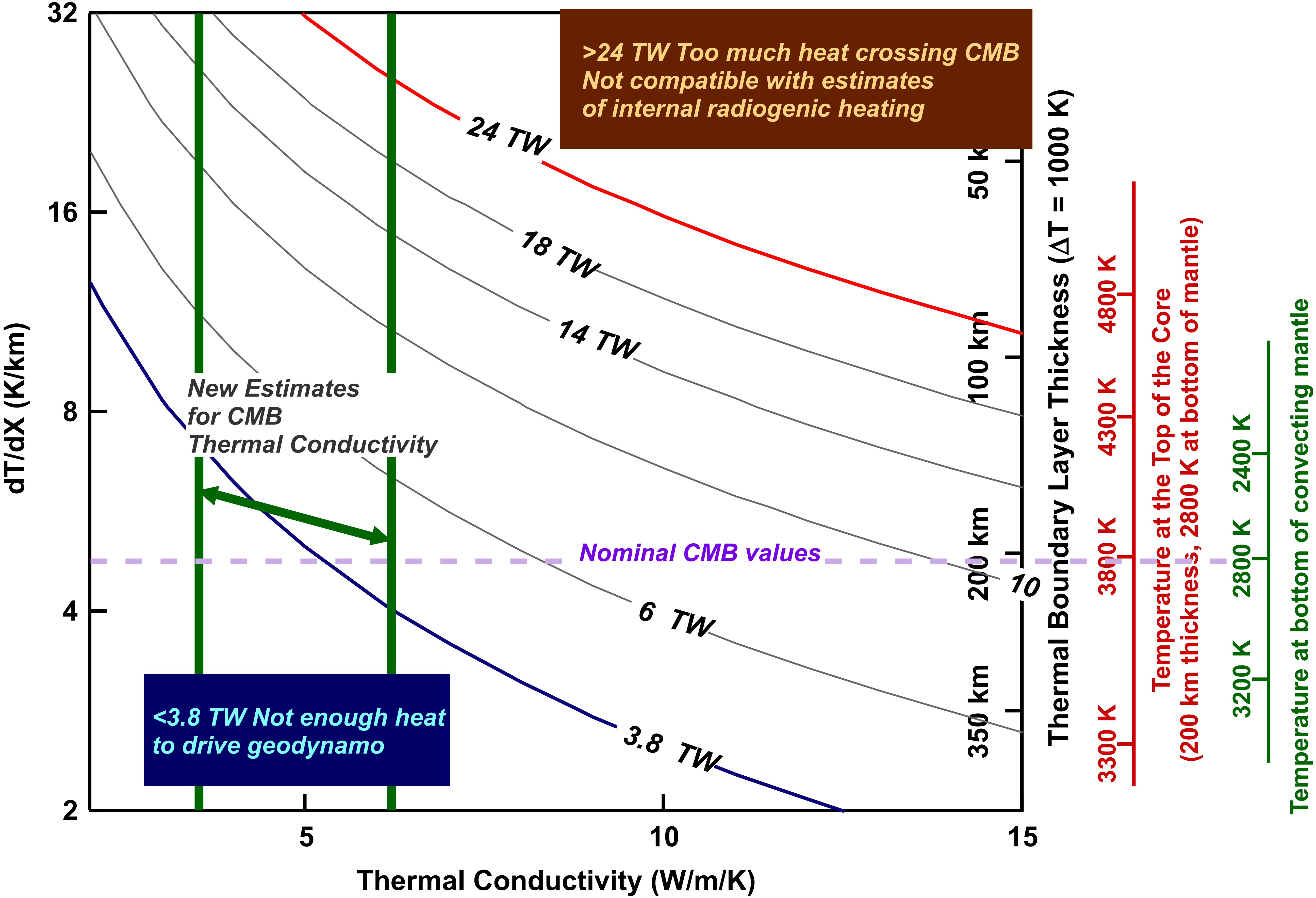
Best Estimates Earth Mantle Thermal Conductivity



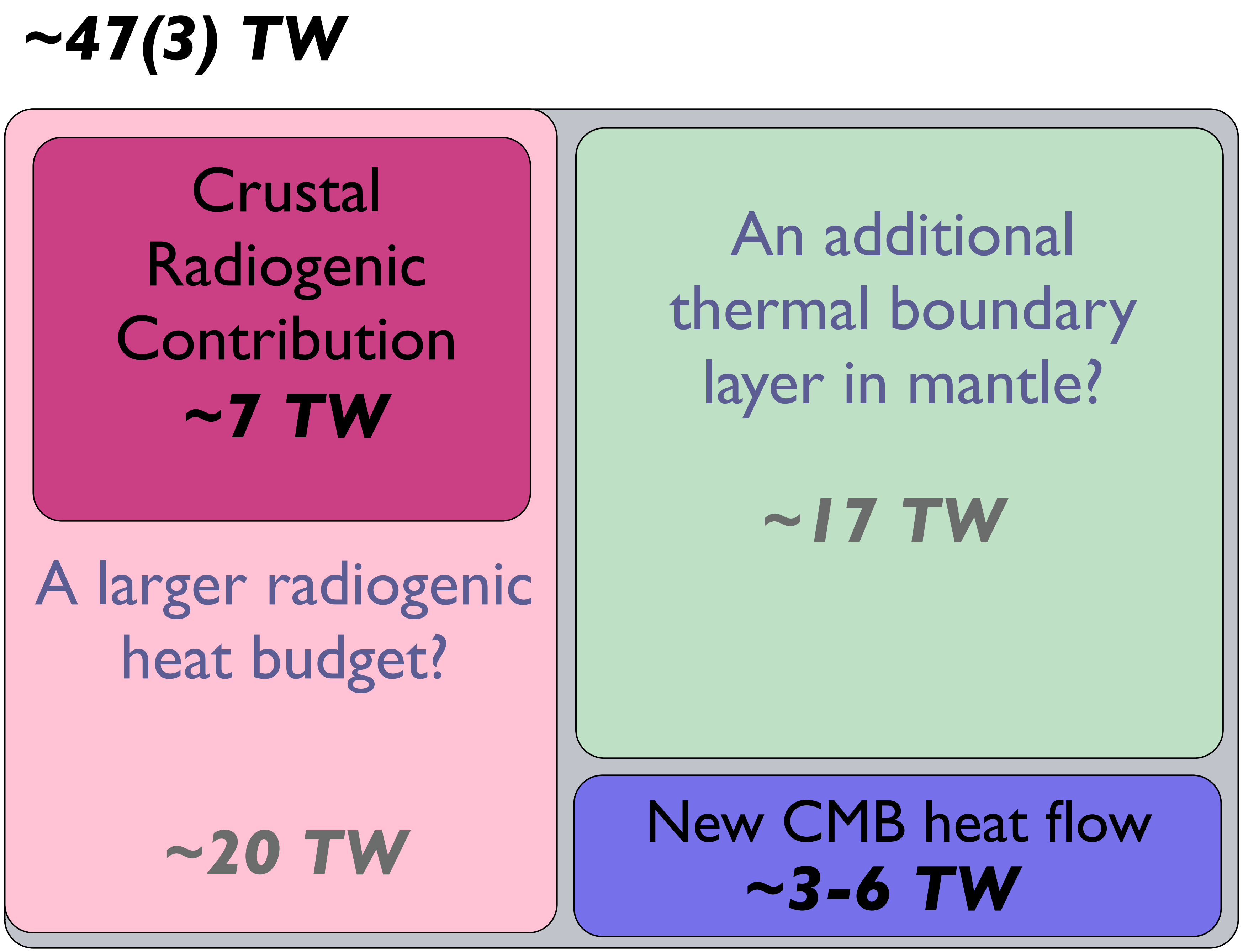
A reminder--before this study



Implications for Core/Mantle Boundary Heat flow

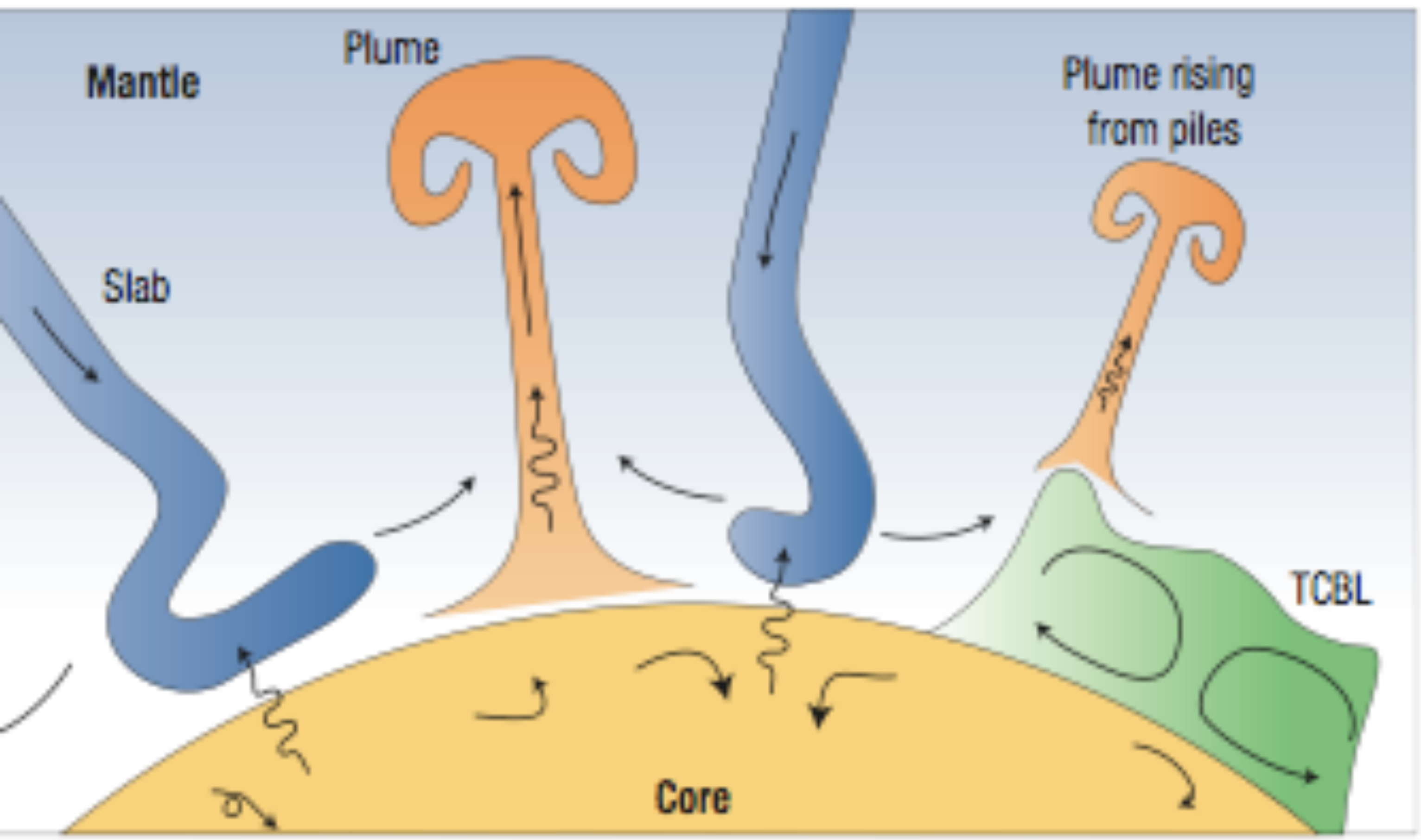


Constraints on the thermal state of the Earth



Tang et al., 2012, submitted

Resolution of the Goldilocks story: "Just Right" K



Lay, Hernlund, Buffett, 2008

Simple convecting mantle

Thermal conductivity has *weak* pressure and temperature dependencies

Core/Mantle boundary is an insulating area

1. Large temperature drop at core/mantle boundary
2. Partially molten lower mantle possible
3. Additional thermal boundary layer in the mantle or more radiogenic heating

Inner core timing

Relaxes constraints on timing of inner core formation (e.g. Buffett, 2009)

General Thermal Conductivity: General Boltzmann Transport Equation

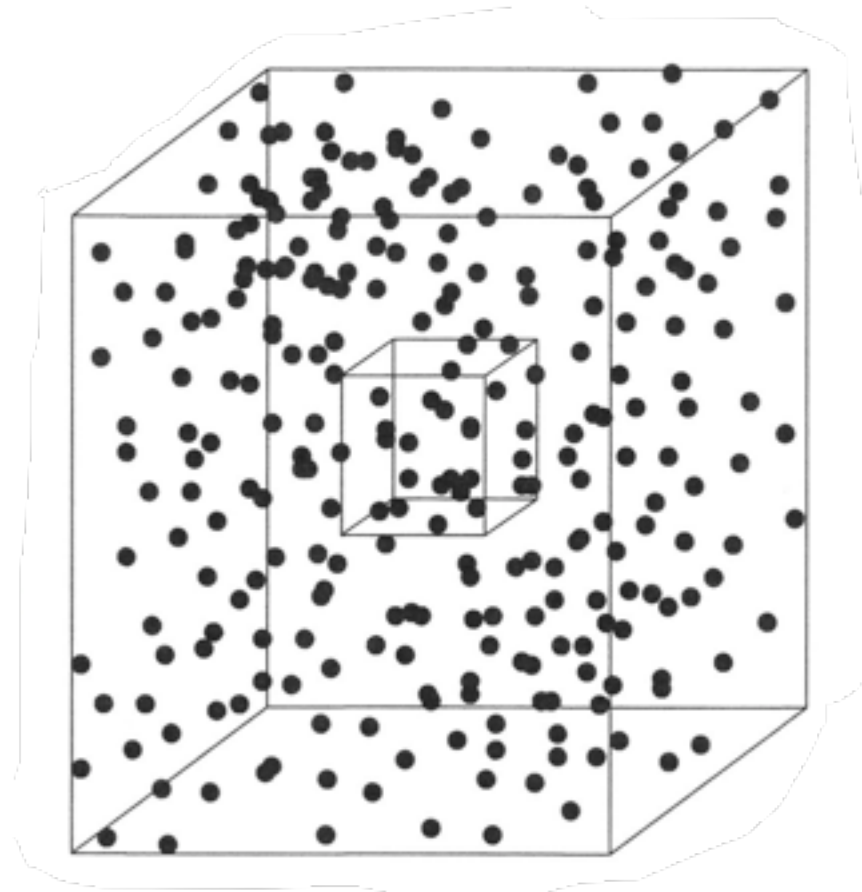
1. each particle defined by:
position ***x*** and momentum ***p***

2. define a probability density function
f(***x***,***p***,***t***) such that: $dN = f(\mathbf{x},\mathbf{p},t)\, d^3\mathbf{x}\, d^3\mathbf{p}$

3. $$\frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_{diffusion} + \left(\frac{\partial f}{\partial t}\right)_{force} + \left(\frac{\partial f}{\partial t}\right)_{collisions}$$

4a. for particles with classical statistics:
$f(t_0) \sim \exp(-\mathbf{E}/kT)$

4a. for particles with quantum statistics:
$f(t_0) \sim (\exp(\mathbf{E}/kT)-1)^{-1}$



N particles

Distribution functions are temperature-dependent

Kinetic Transport Equation

$$\kappa = \frac{1}{3}\sum_{i,\vec{q}} c_V(i,\vec{q}) v_g{}^2(i,\vec{q})\tau(i,\vec{q})$$

$k = C_v\, v_g^2\, \tau$

Quasi-Harmonic Approximation c_V, v_g

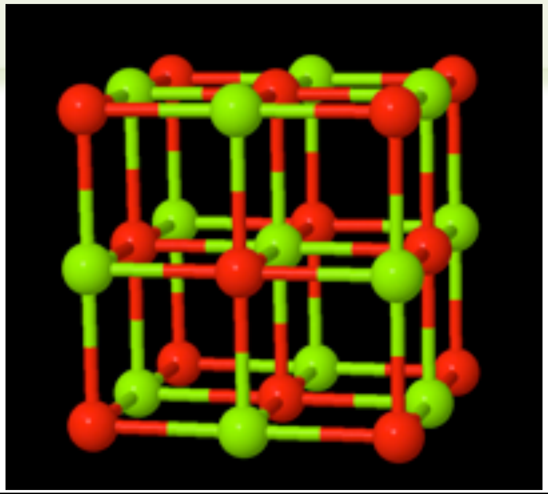
Quantum Scattering Theory τ

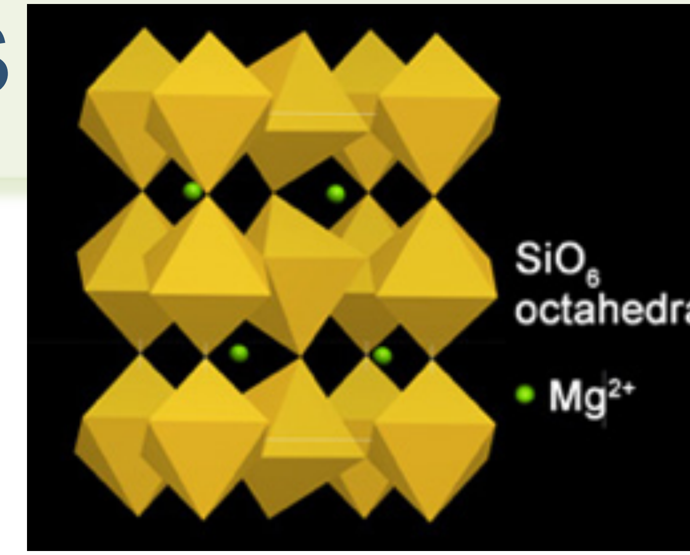
2nd-order force constant matrix: $\phi_{ij} = \frac{\partial^2 E}{\partial x_i \partial x_j}$

3rd-order lattice Anharmonicity: $A_{ijk} = \frac{\partial^3 E}{\partial x_i \partial x_j \partial x_k}$

First-Principles calculation of atomic forces: Finite-Displacement Super-Cell Method

Simulation Details



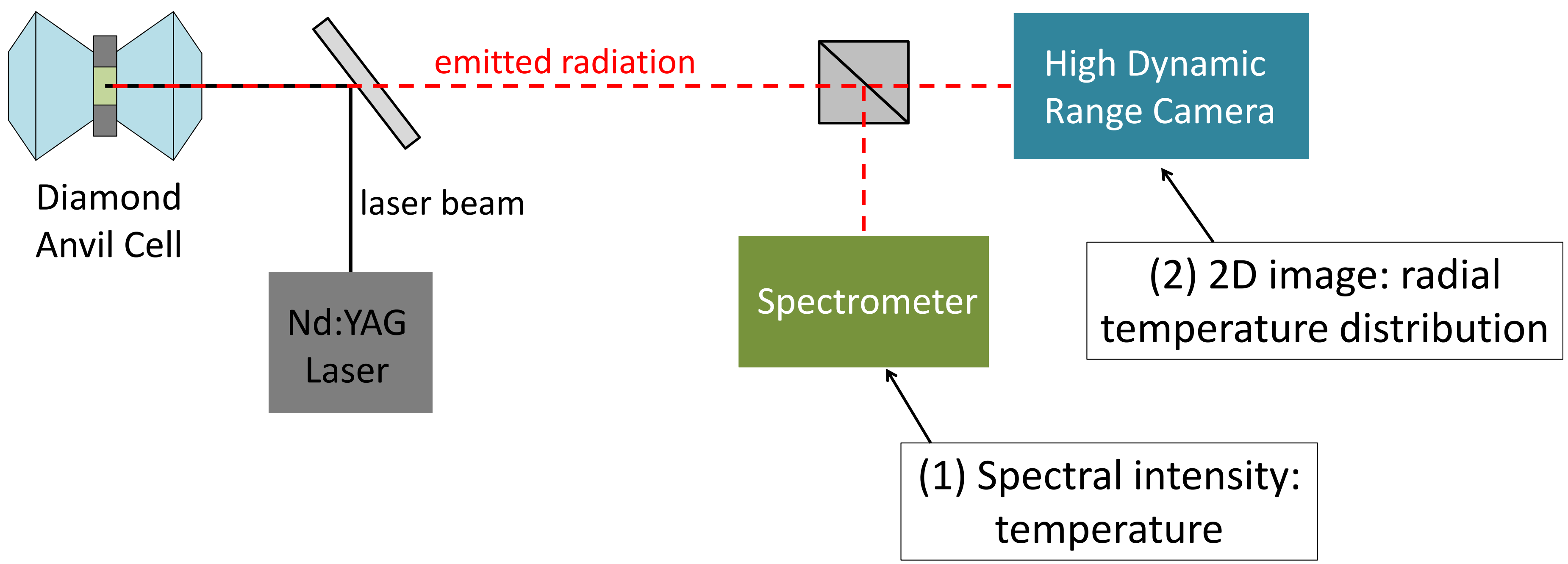


	MgO (Tang & Dong, 2009, 2010)	$MgSiO_3$
Static Energy	LDA, PAW, PW; 2-atom unit cell; 12x12x12 Monkhorst k-grid	LDA, PAW, PW; 20-atom unit cell; 8x8x6 Monkhorst k-grid
Forces	128-atom super cell; Gamma point sampling	160-atom super cell; Gamma point sampling;
Conductivity (C_v, V_g, τ)	16X16X16 q-point sampling; 5 X 9 grids in V-T domain	8X8X6 q-point sampling; 5 X 9 grids in V-T domain

Current research & ongoing questions

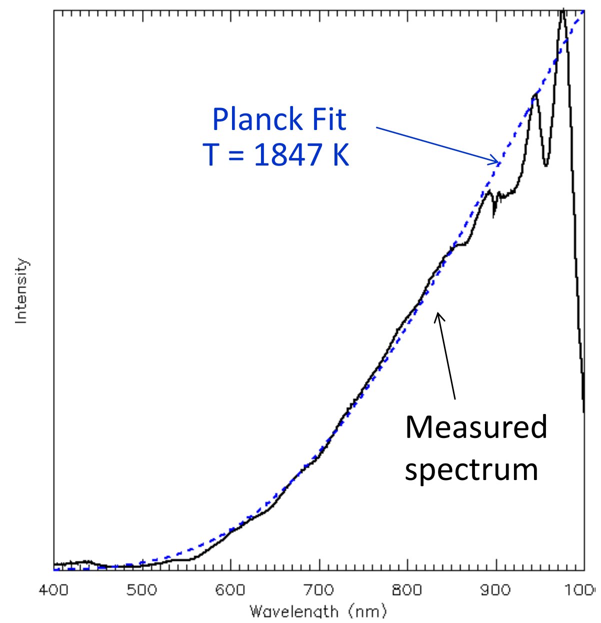
LASER HEATING EXPERIMENTS

UCLA Mineral Physics Lab Laser Heating System

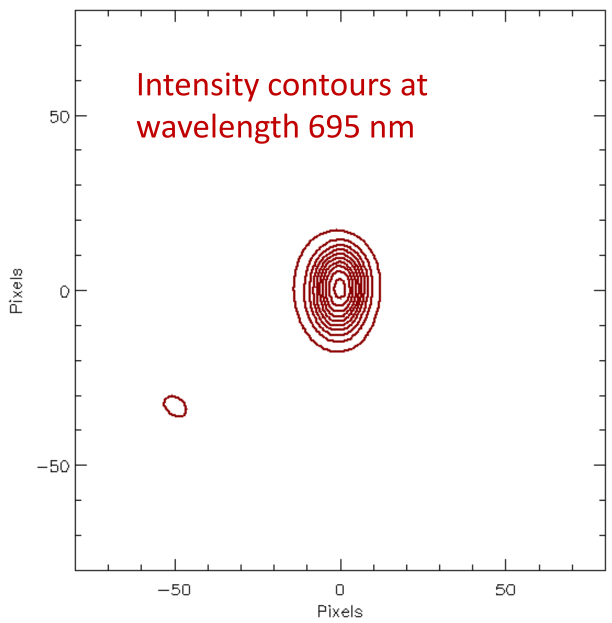


Laser Heating Measurements

(1) Hotspot Spectrum



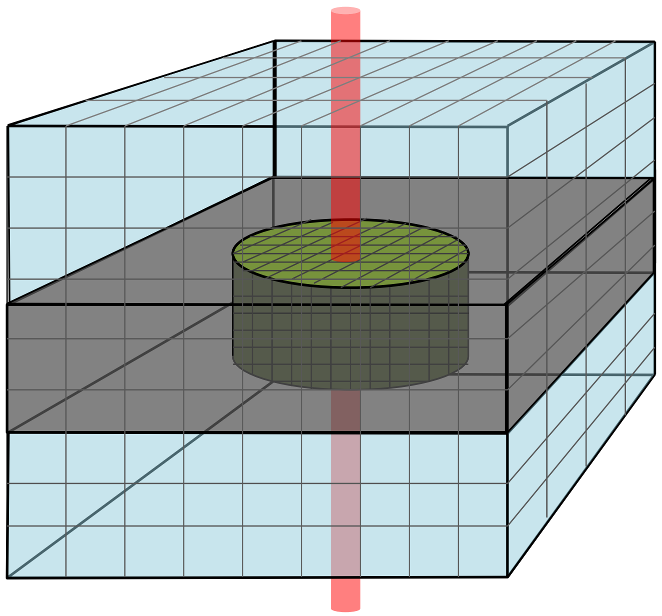
(2) 2D Hotspot Image



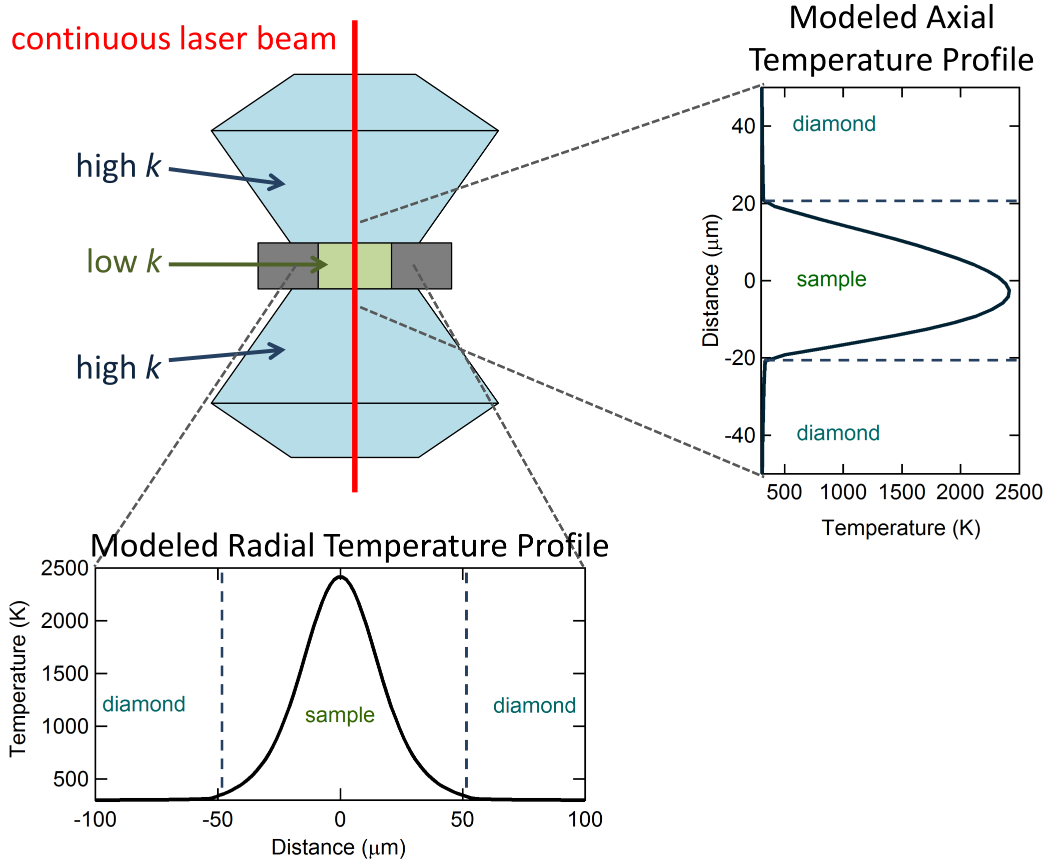
- Data taken during laser heating of AgI at pressure of 17 GPa in the LHDAC
- Planck fit for measured spectrum between 600 and 900 nm
- Entire hotspot spectrum was collected in order to minimize potential biases due to misalignment
- 2D hotspot intensity measured through bandpass filter with center wavelength 695 nm and width of 70 nm

Current research & ongoing questions

DIAMOND ANVIL CELL HEAT FLOW MODEL



- 3-D numerical model solves the steady-state heat equation using a full approximation storage multi-grid solver.
- Includes flexible laser and sample geometries and temperature-dependent material properties.
- Based on previous model for heat flow in multi-anvil press [1].

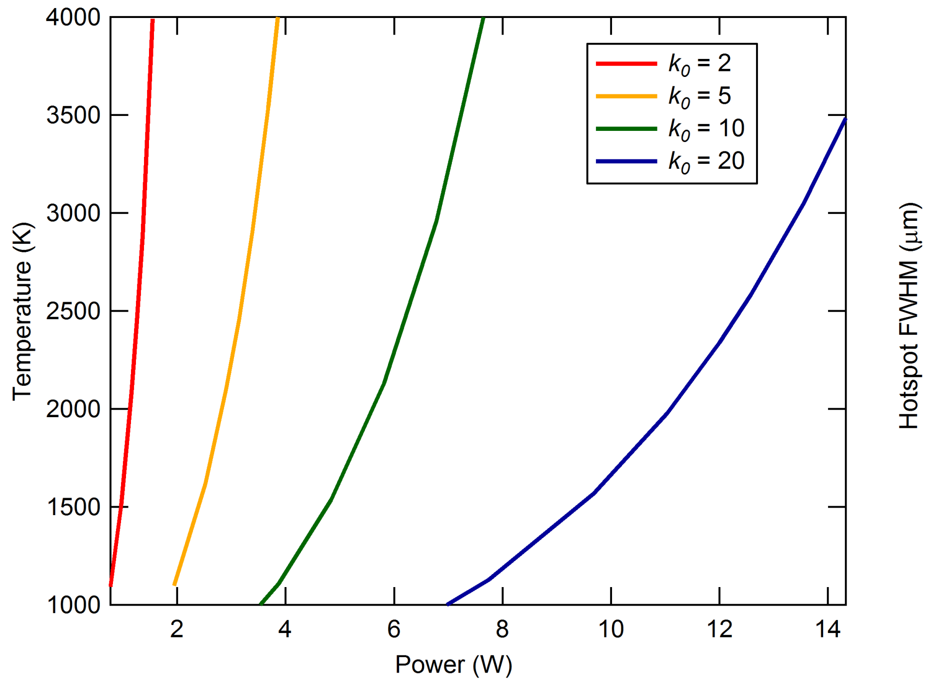


- Large 3-D temperature gradients form during continuous laser heating in the LHDAC.
- Temperature distribution depends on laser and sample geometry, and sample thermal conductivity and absorption properties.

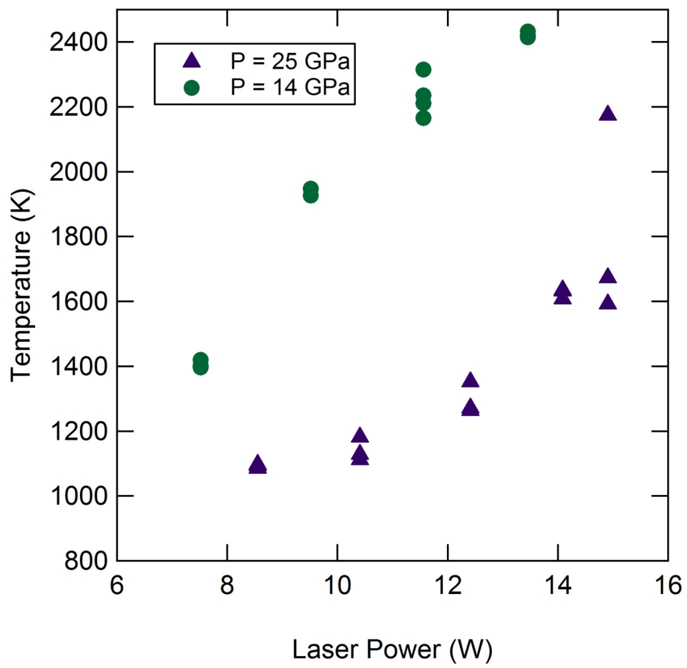
Current research & ongoing questions

PRELIMINARY EXPERIMENTAL DATA

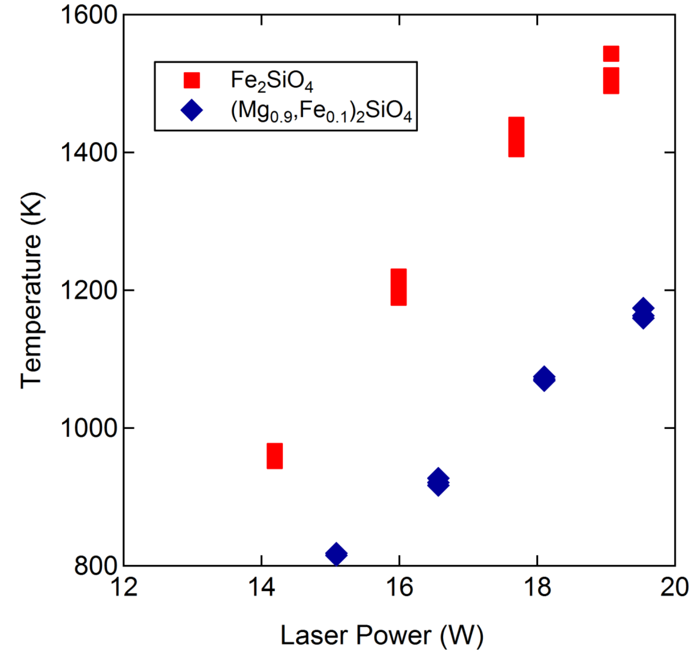
Modeled Temperature vs. Power



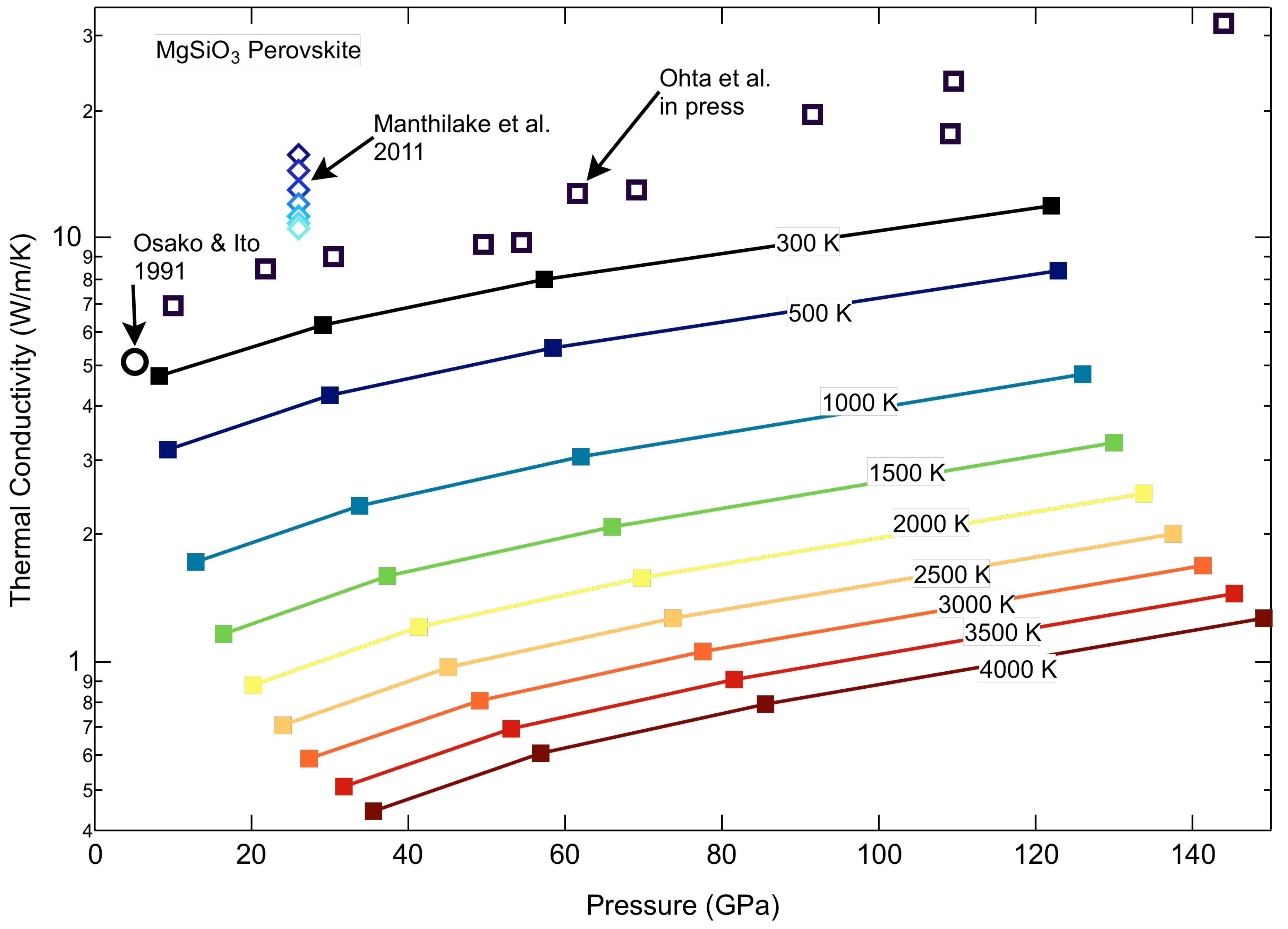
Temperature vs. Laser Power for $(Mg_{0.9},Fe_{0.1})_2SiO_4$ at 14 and 24 GPa



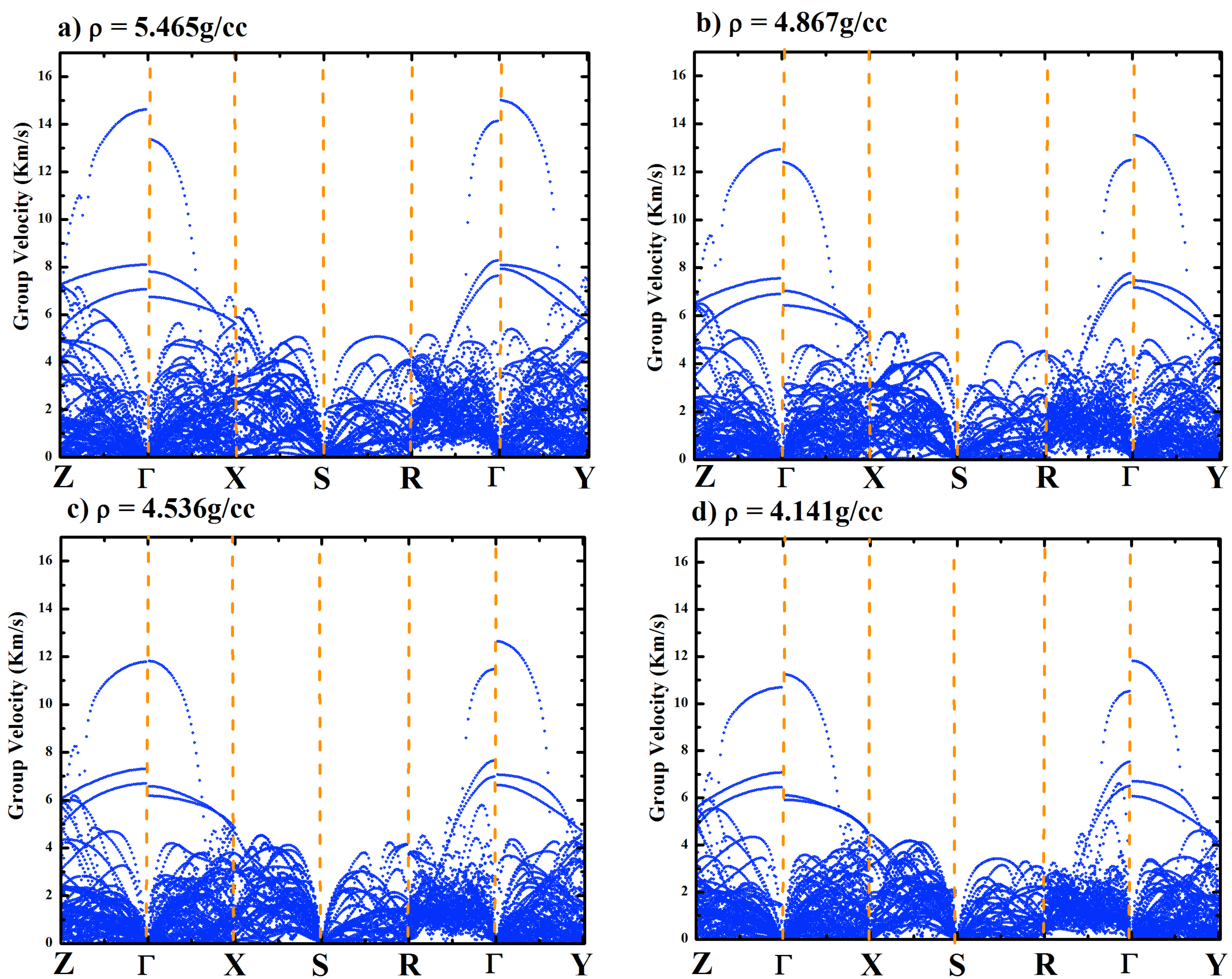
Temperature vs. Laser Power for $(Mg,Fe)_2SiO_4$ with variable Fe



Thermal Conductivity of Perovskite



pressure-dependent phonon calcs



Temperature-dependence