Influences of Thermal Conductivity and Depth-Dependent Thermal Expansivity

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Depth-dependent thermal expansivity were first studied
in 1987 with Wuling Zhao in looking at the influences
of adiabatic cooling on rising plumes. Later we focussed
on the global mantle circulation (Hansen et al., PEPI, 1993,
Zhang and Yuen (1995, 1996) in spherical-shell convection.

Depth-dependent thermal expansivity, which decreases with increasing
pressure, allows for larger convection cell (longer wavelength). It
also permits plumes to rise faster and retains more heat, without
excessive adiabatic cooling.

Variable thermal conductivity:

This consists of phonon, photon and electron transport.

Phonon part has temperature- and pressure dependence.
The temperature-part decreases with increasing T , similar to viscosity
The pressure part increases with depth in a linear fashion.

The photon part is strictly temperature-dependent and increases with temperature in a nonlinear fashion, T**3 . Important in the lower mantle and D” layer.

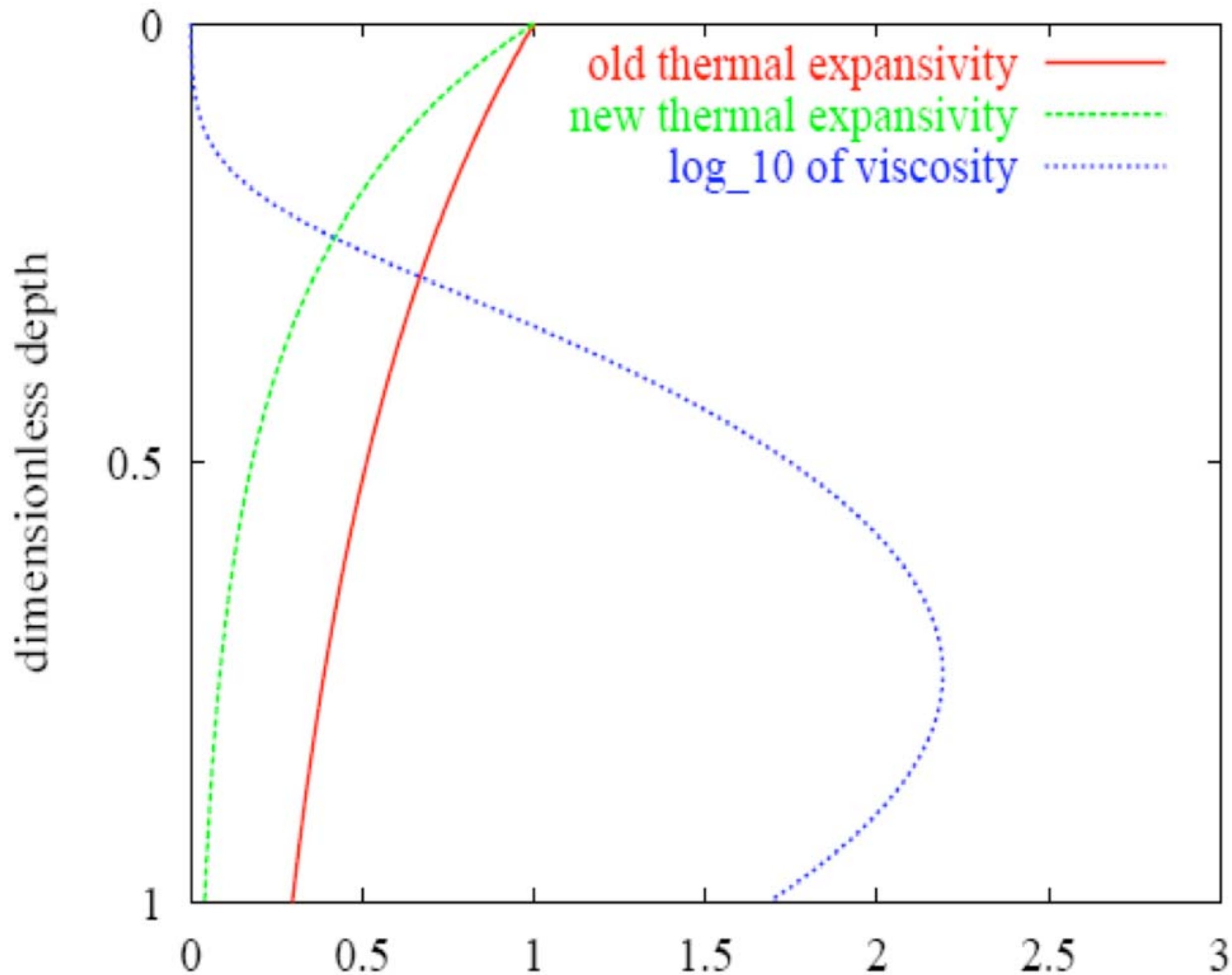
Electron part is important in exosolar planet, depends exponentially on T like the viscosity and high t , like above 8000 K, , Post perovskite decomposition , (see Science, February, 17, 2006 , Umemoto et al.)

Numerical Simulations Versus Laboratory Experiments of Convection

1. Numerical simulations can mimic a lot of the physics, not possible with laboratory experiments, such as phase transition in particular multiple phase transitions, variable viscosity with complicated depth-dependent rheology, variable thermal conductivity, equation of state, compressibility.

2. Laboratory experiments may be good in obtaining some 3-D effects, but this is becoming no longer true, as high-resolution calculations become available especially in spherical geometry.

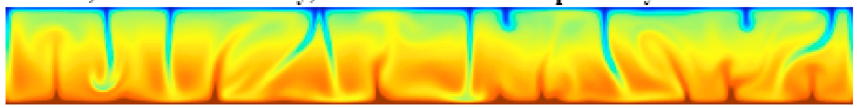
Depth Dependent Properties



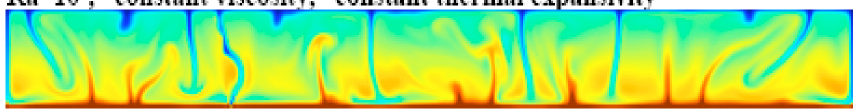
Simple Physics

No phase changes, k=1, Di=0.5, R=3

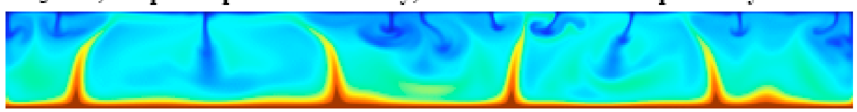
$Ra=10^6$, constant viscosity, constant thermal expansivity



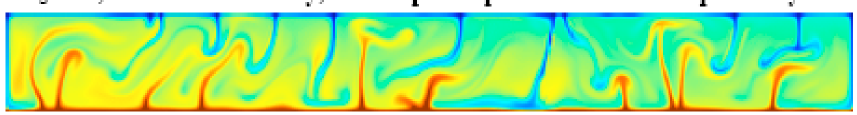
$Ra=10^7$, constant viscosity, constant thermal expansivity



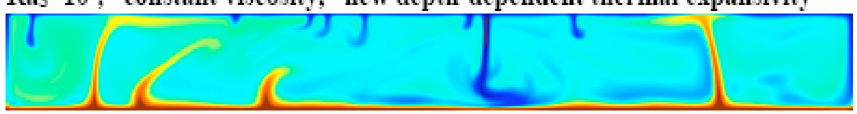
$Ra_S=10^7$, depth-dependent viscosity, constant thermal expansivity

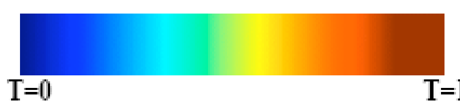


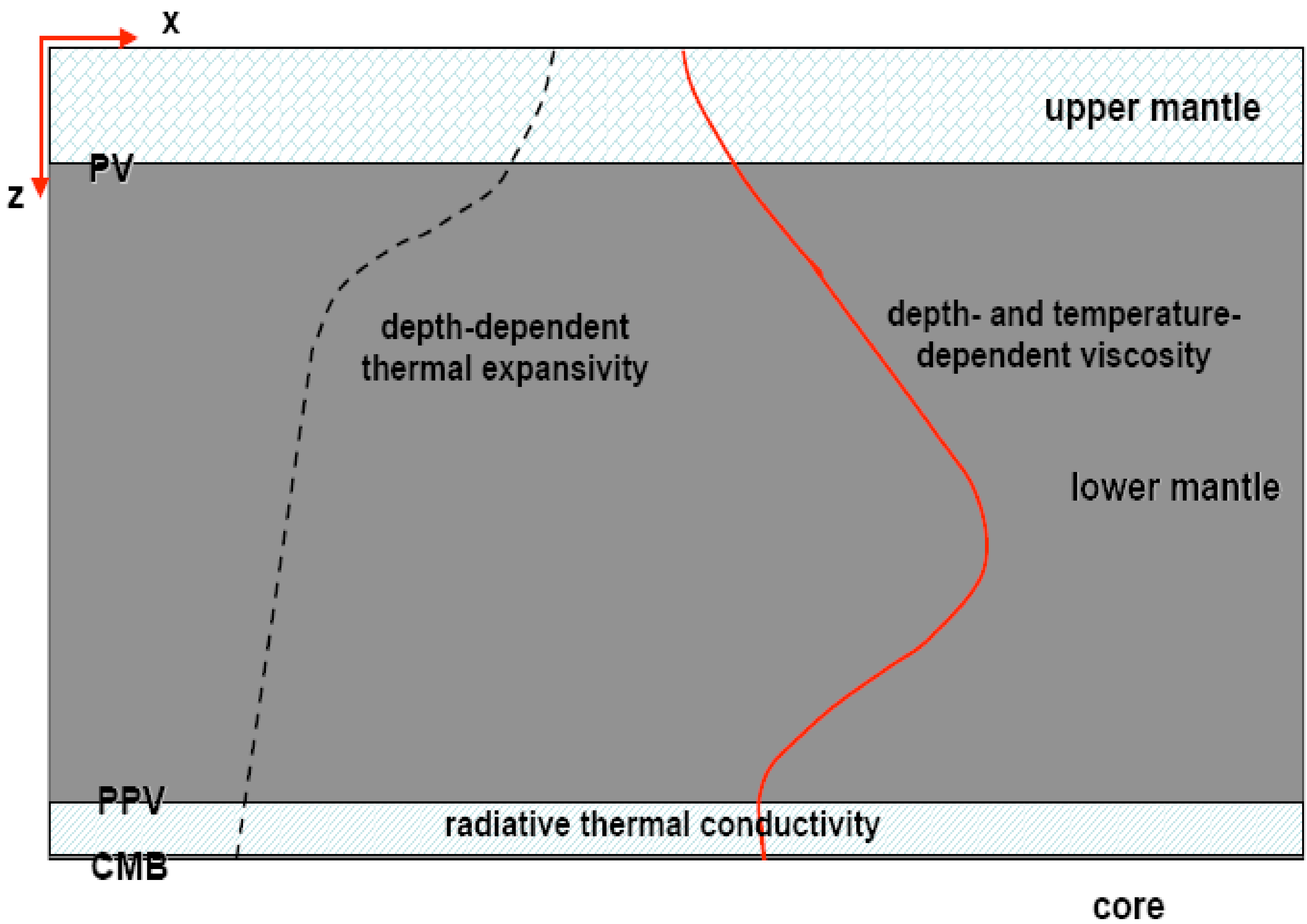
$Ra_S=10^7$, constant viscosity, old depth-dependent thermal expansivity

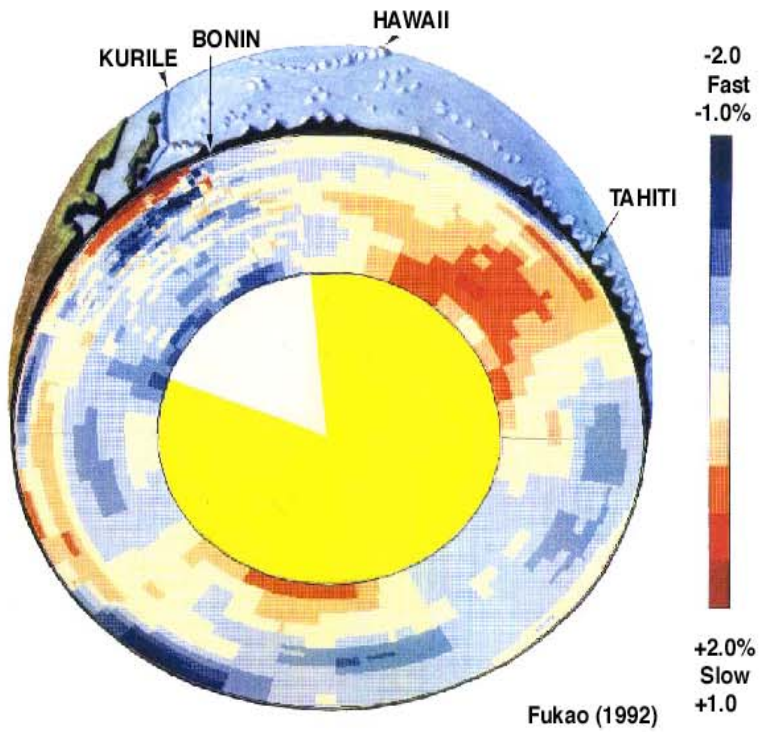


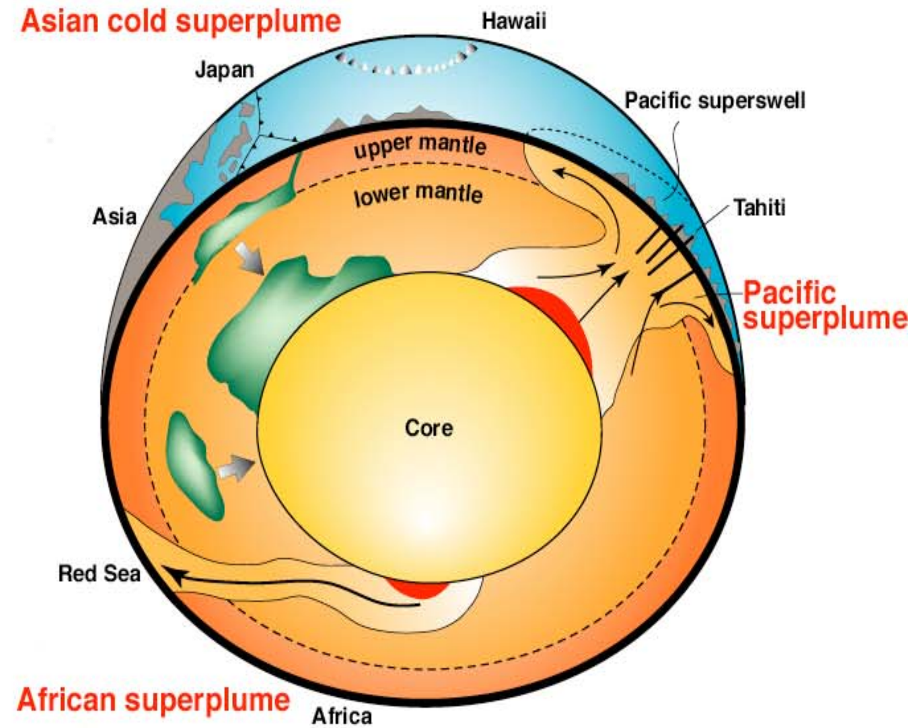
$Ra_S=10^7$, constant viscosity, new depth-dependent thermal expansivity






x
z
upper mantle
PV
depth-dependent
thermal expansivity
depth- and temperature-
dependent viscosity
lower mantle
PPV
radiative thermal conductivity
CMB
core



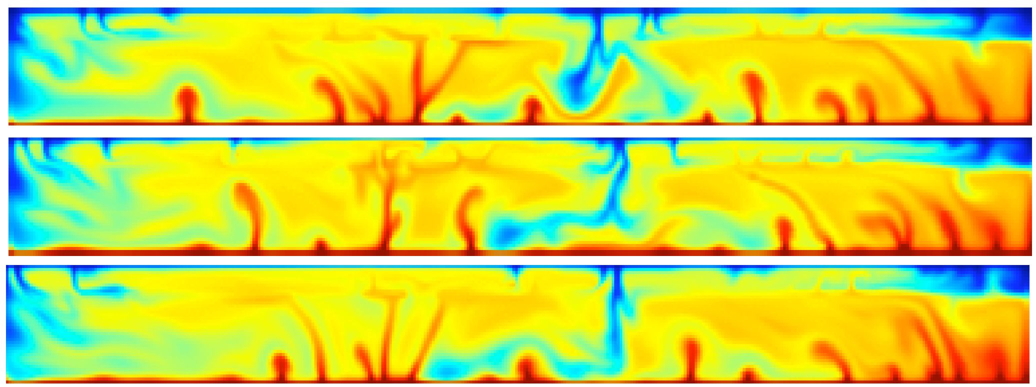


Maruyama (94,98)

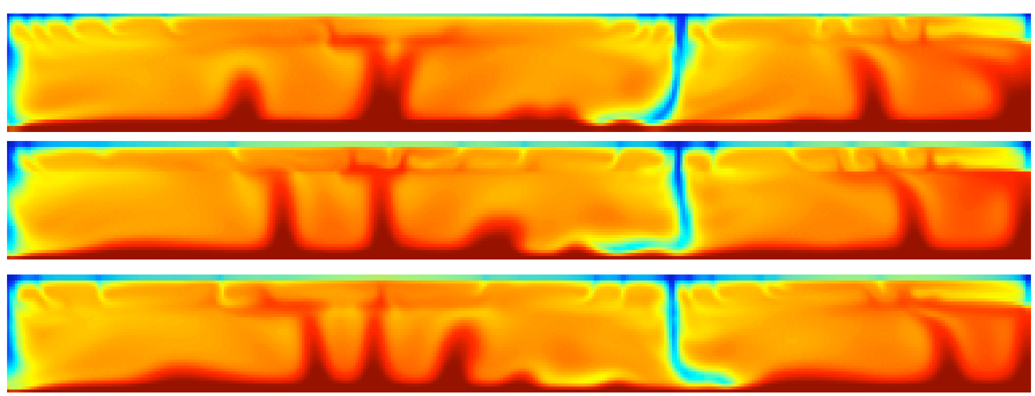
Superplumes Require Radiative Heat Transfer With Post-Perovskite Phase Transition

Temperatures with PPP
for weaker temperature dependence of viscosity
(two orders of magnitude)

k=1



k=k(T)



Extended Boussinesq Convection Equations

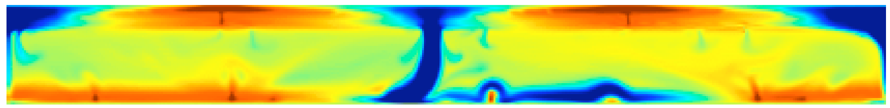
We include:

- Phase transitions, adiabatic and viscous heating, internal heating from radiogenic heat sources (1/4 the chondritic rate)
- Variable viscosity
- Radiative thermal conductivity
- Depth-dependent thermal expansivity (also with recent result from T. Katsura)

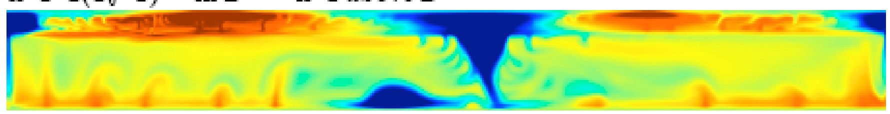
Thermal Anomalies

Old thermal expansivity $P_{670} = -0.15$ $P_{D''} = 0.10$

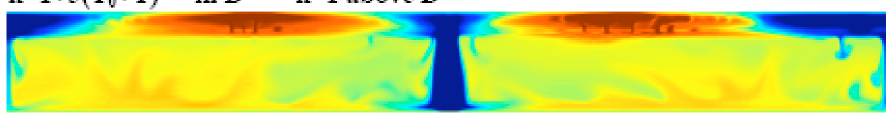
k=1



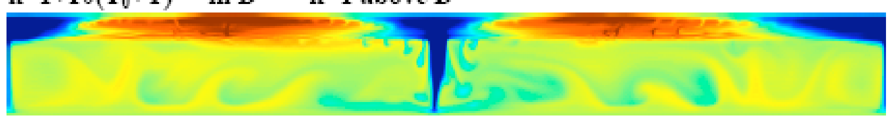
$k=1+2(T_0+T)^3$ in D'' k=1 above D''



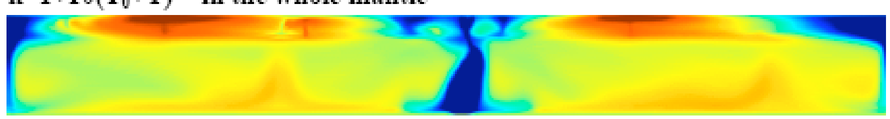
$k=1+5(T_0+T)^3$ in D'' k=1 above D''



$k=1+10(T_0+T)^3$ in D'' k=1 above D''



$k=1+10(T_0+T)^3$ in the whole mantle

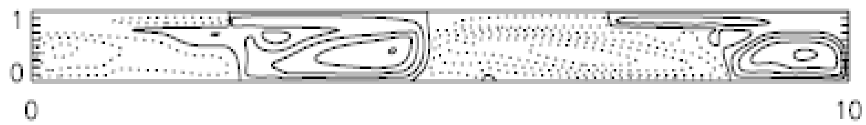


$\Delta T=-0.25$ $\Delta T=0.25$

Streamlines

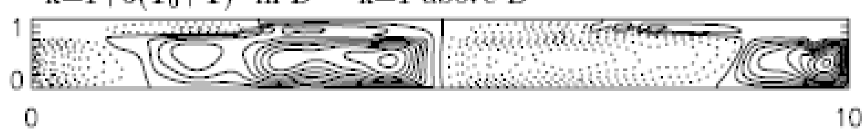
Old thermal expansivity P_{670}=-0.15 $P_{D''}$=0.10

k=1



$k=1+2(T_0+T)^3$ in D" k=1 above D"

$k=1+5(T_0+T)^3$ in D" k=1 above D"



$k=1+10(T_0+T)^3$ in D" k=1 above D"

$k=1+10(T_0+T)^3$ in the whole mantle

Superplumes Require Radiative Heat Transfer With Post-Perovskite Phase Transition

Temperatures with PPP
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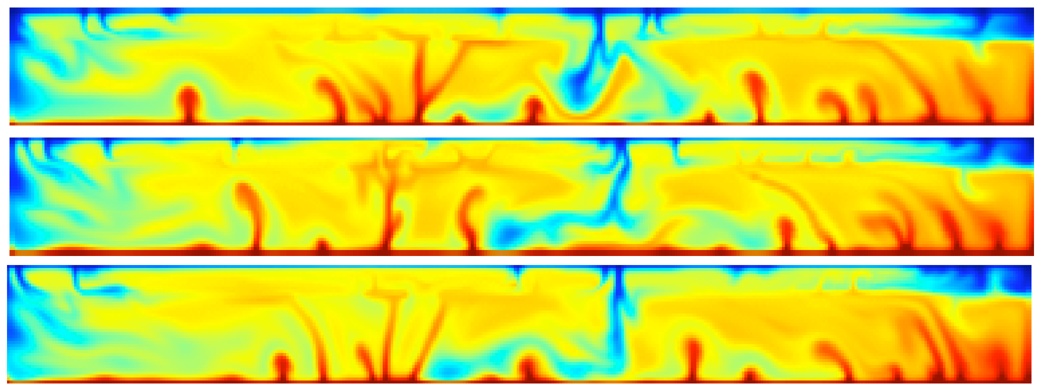
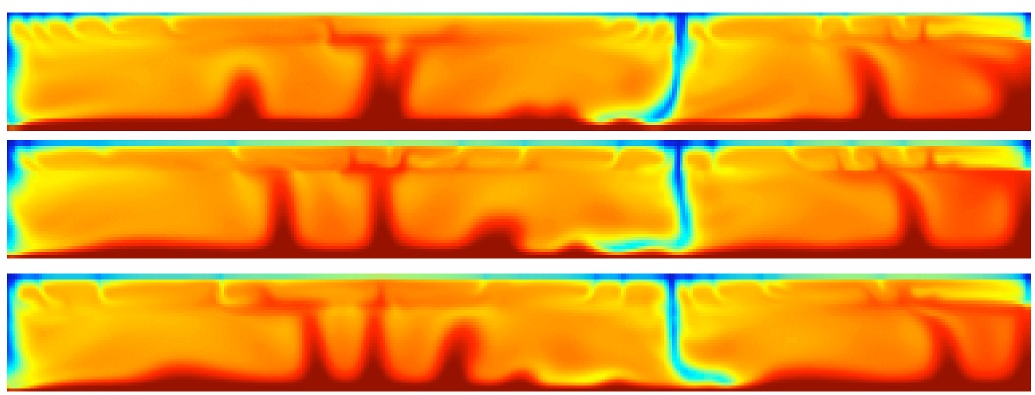
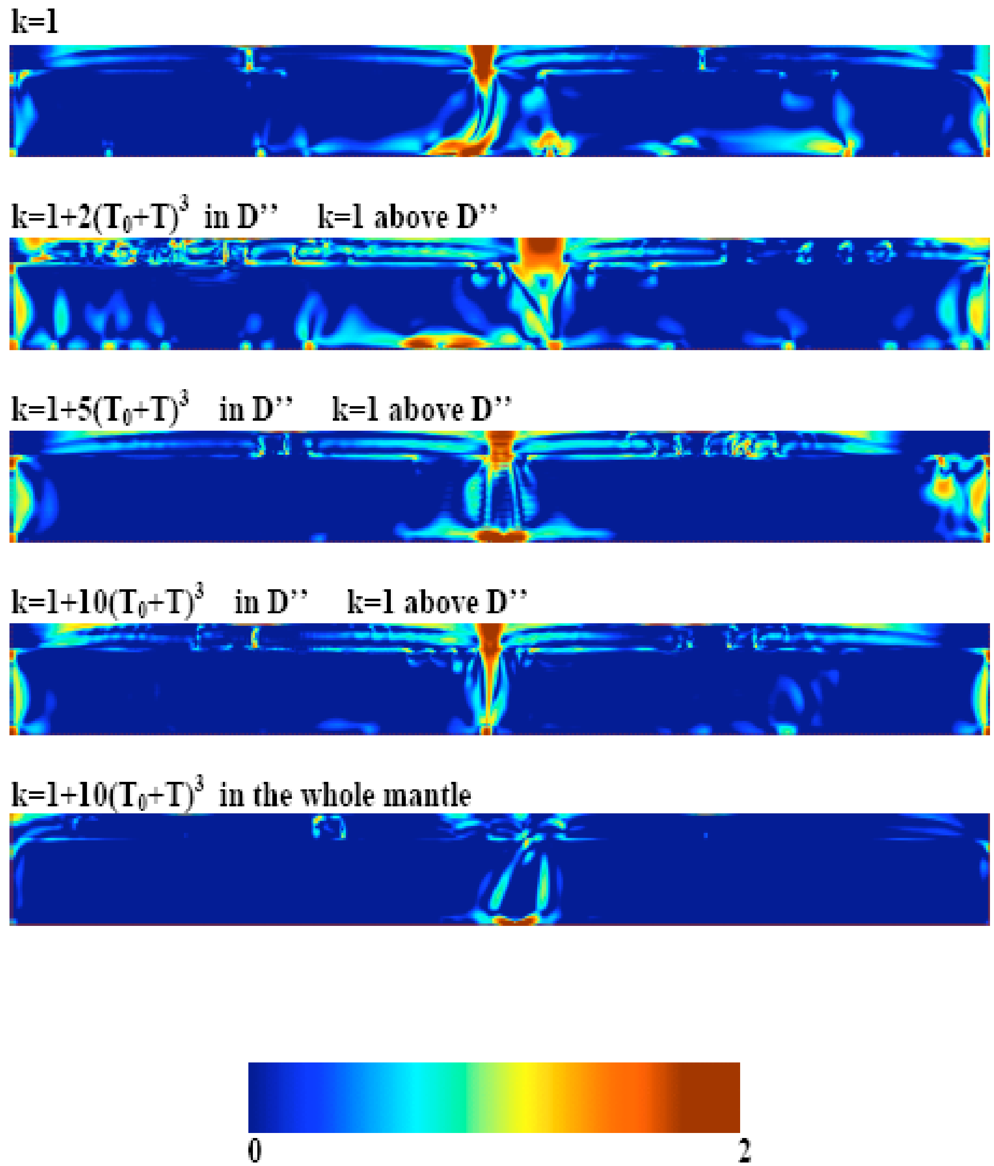


k=k(T)

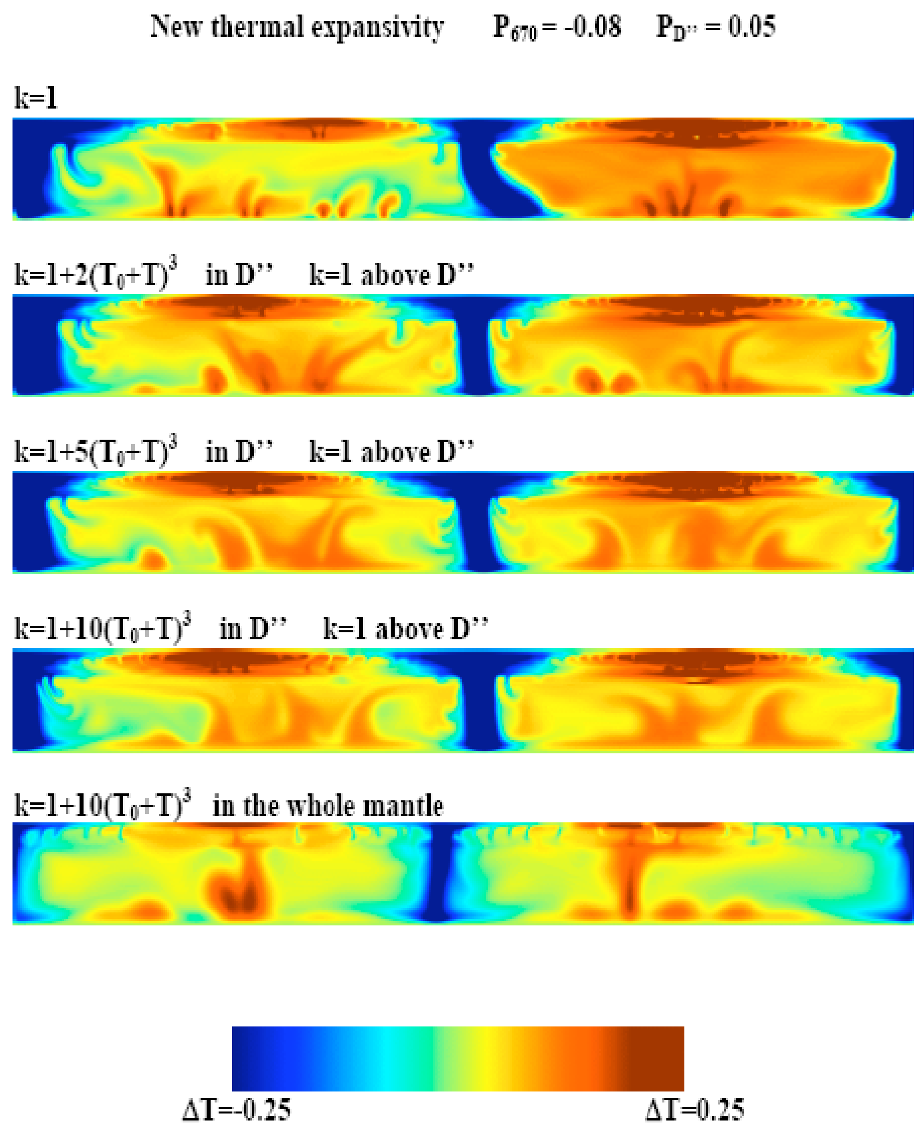


Decadic logarithm of shear heating

Old thermal expansivity $P_{670} = -0.15$ $P_{D''} = 0.10$

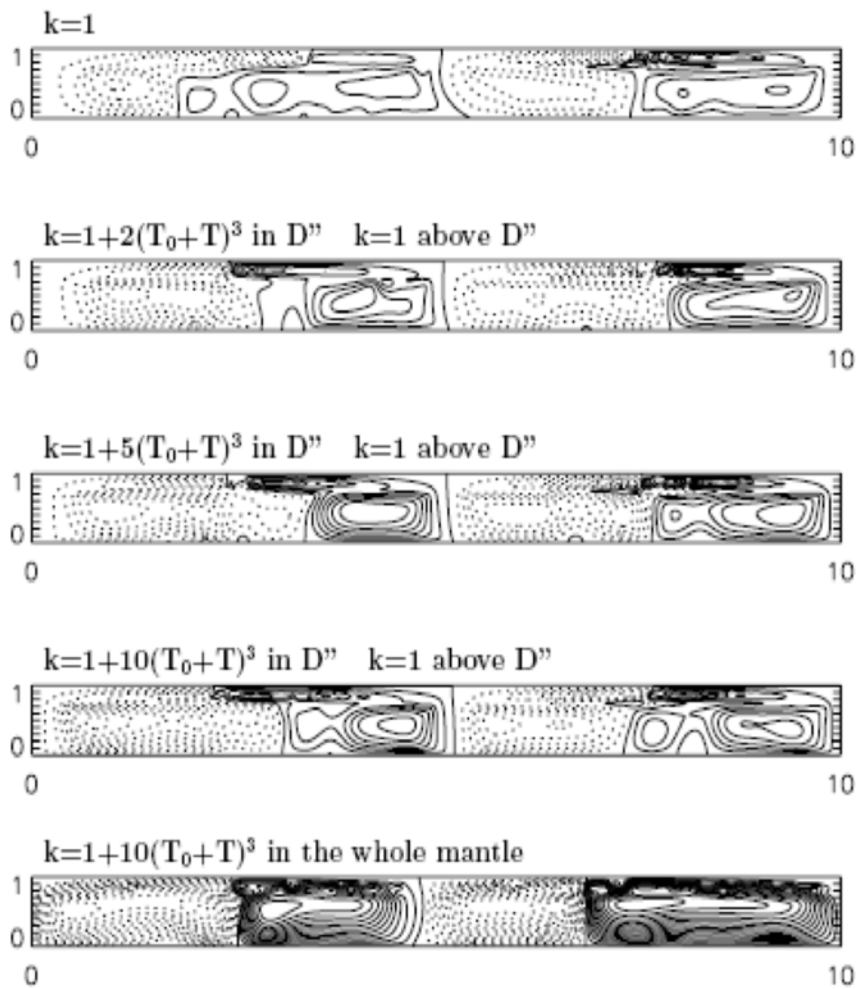


From T. Katsura's Result on

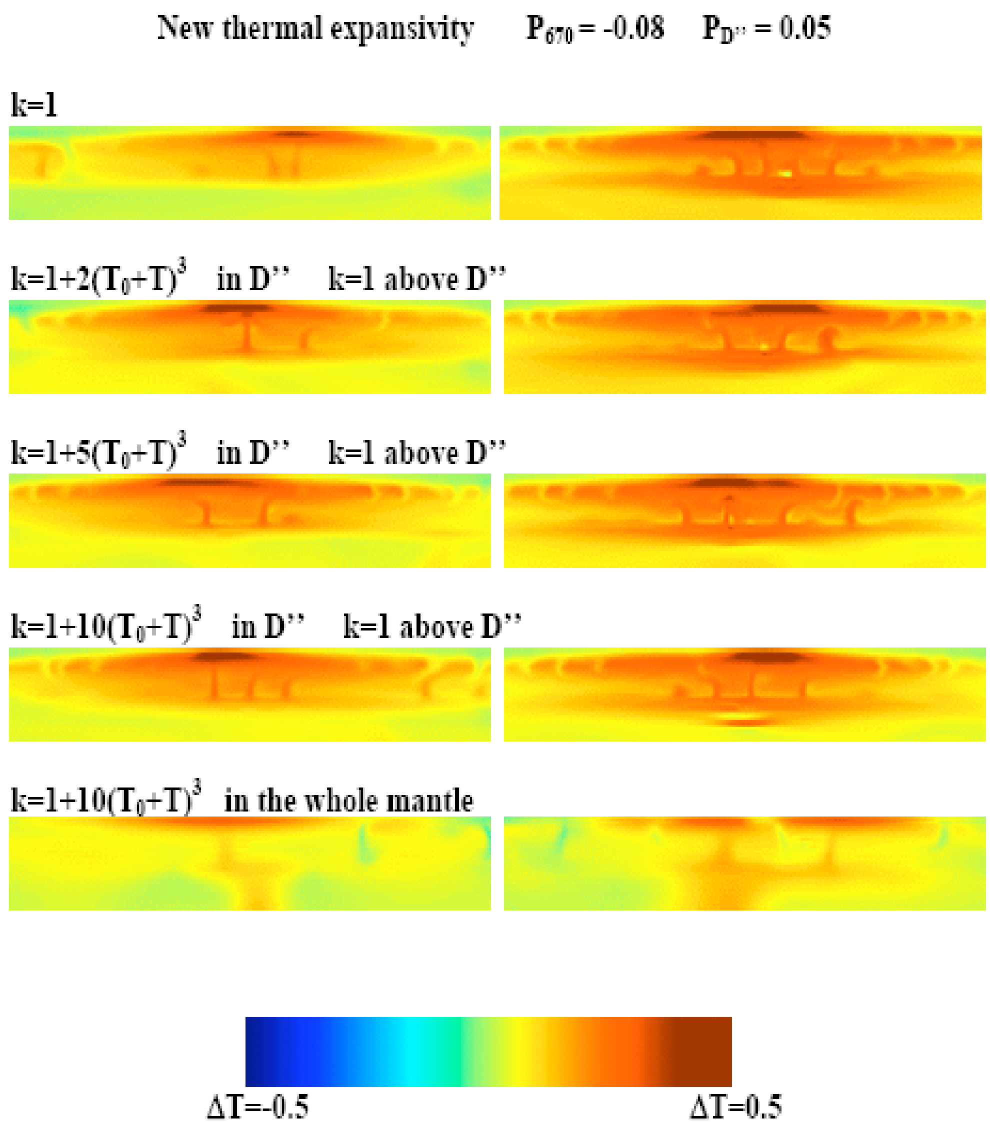


Katsura Streamlines

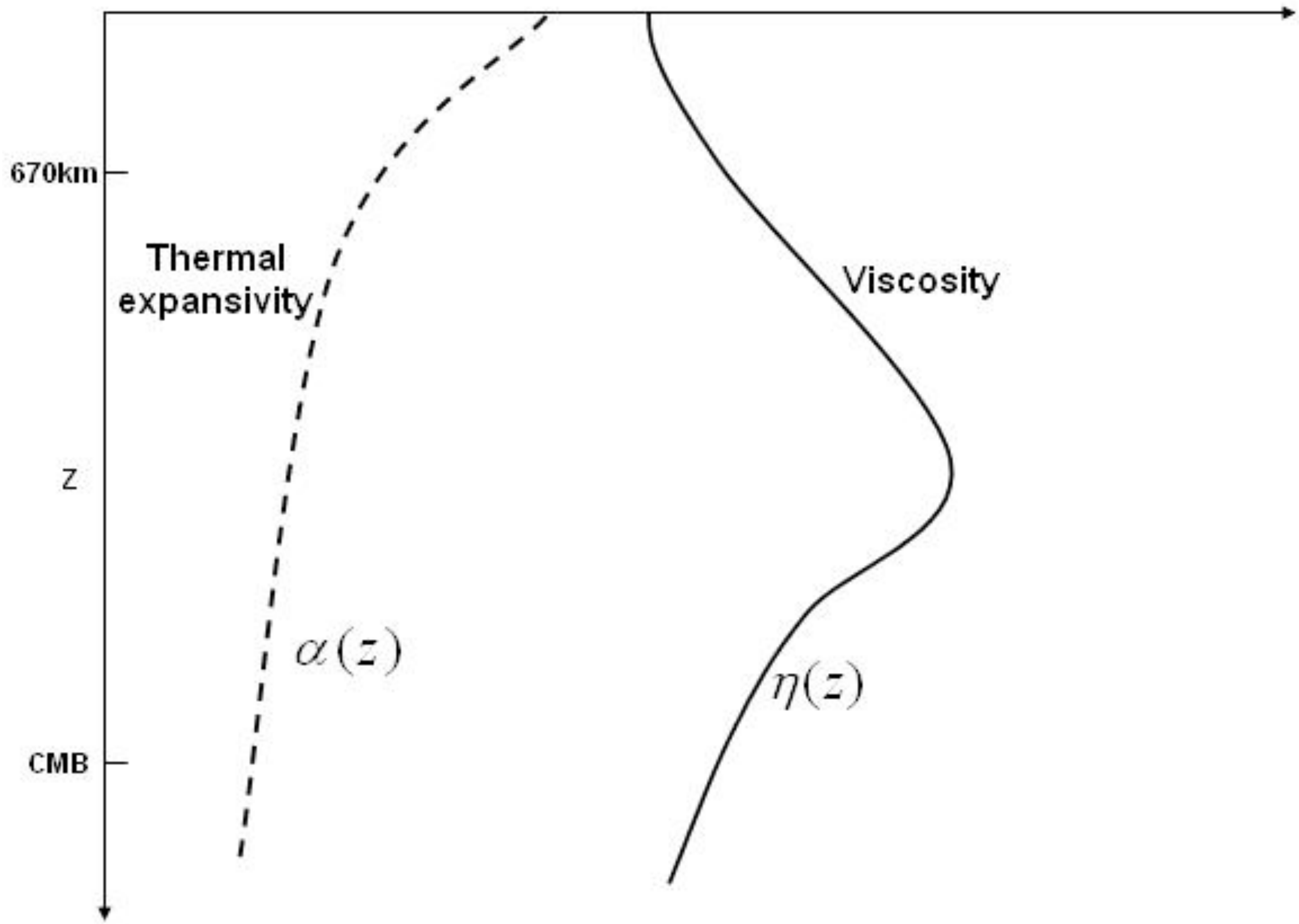
New thermal expansivity P_{670}=-0.08 $P_{D''}$=0.05



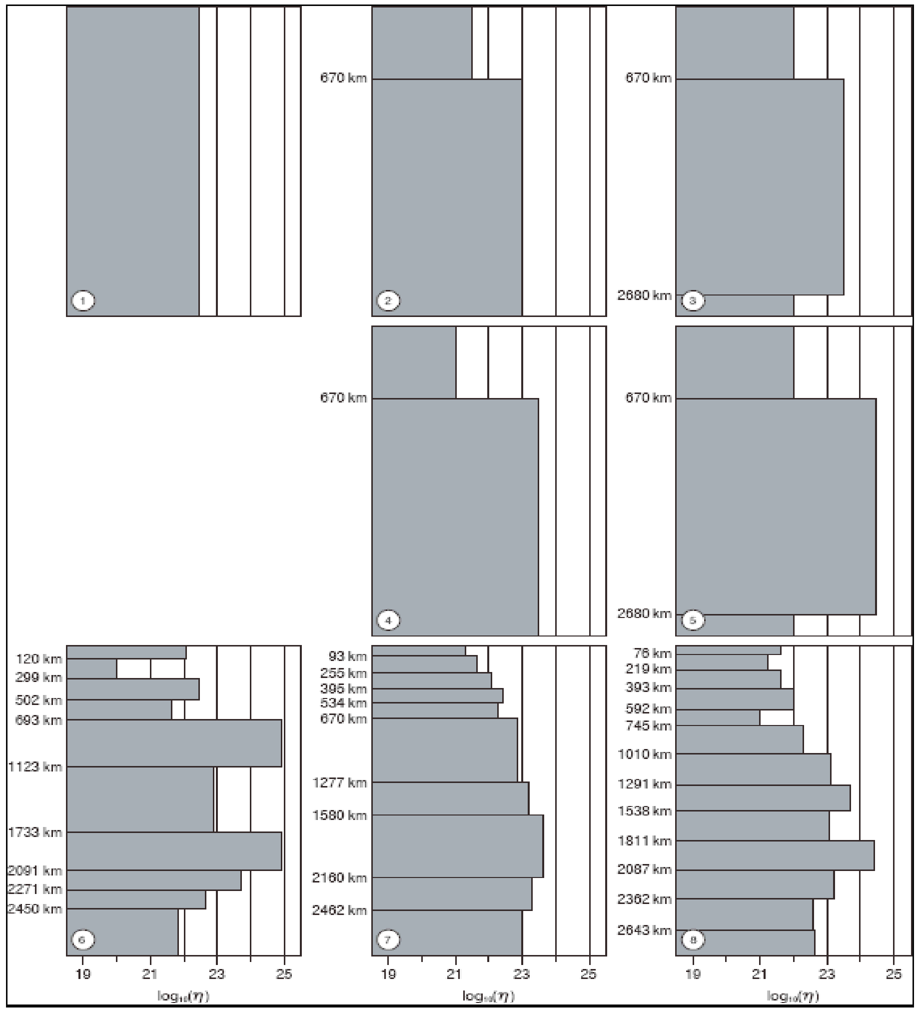
Zoom-in of Katsura Thermal Anomalies

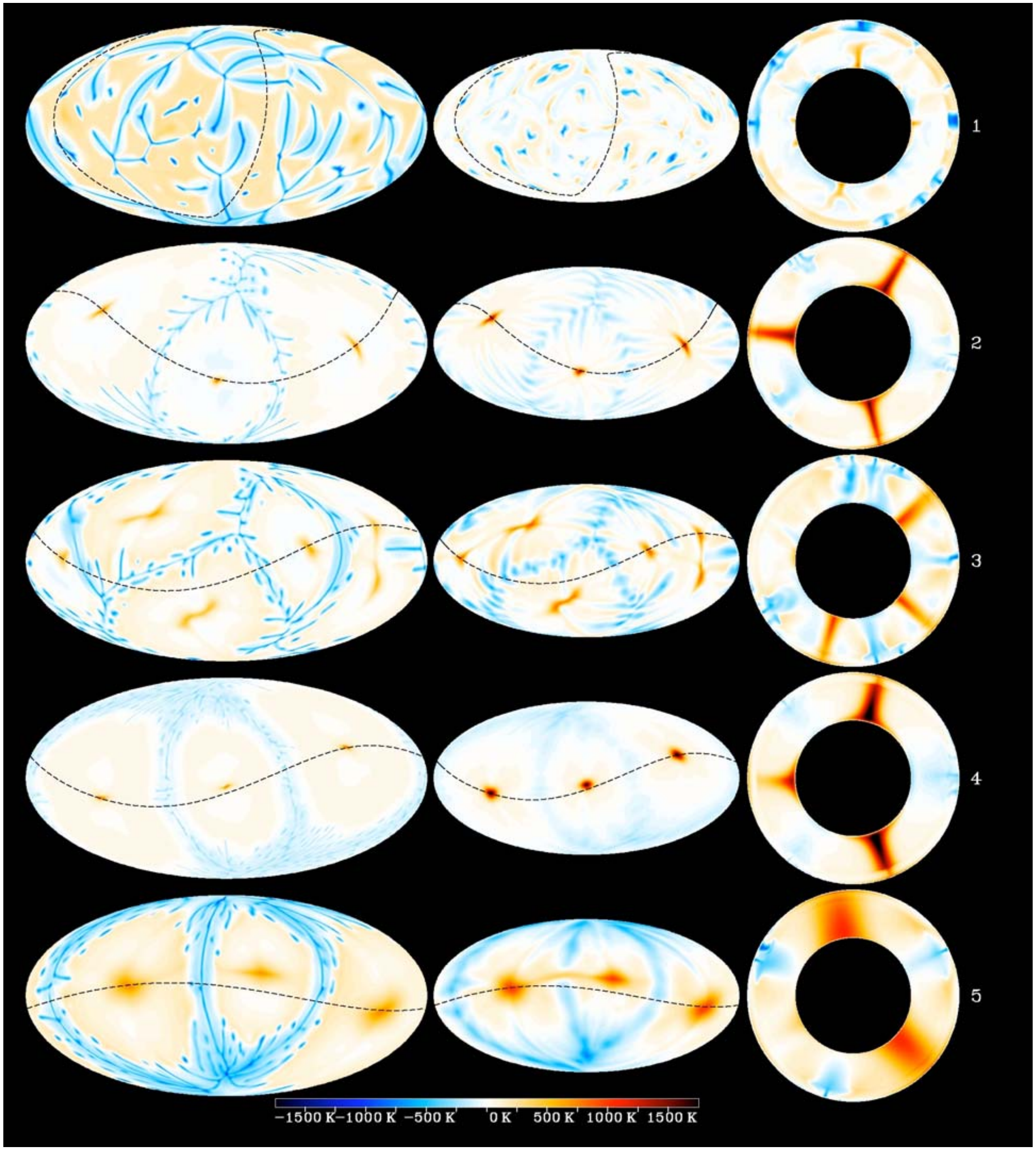


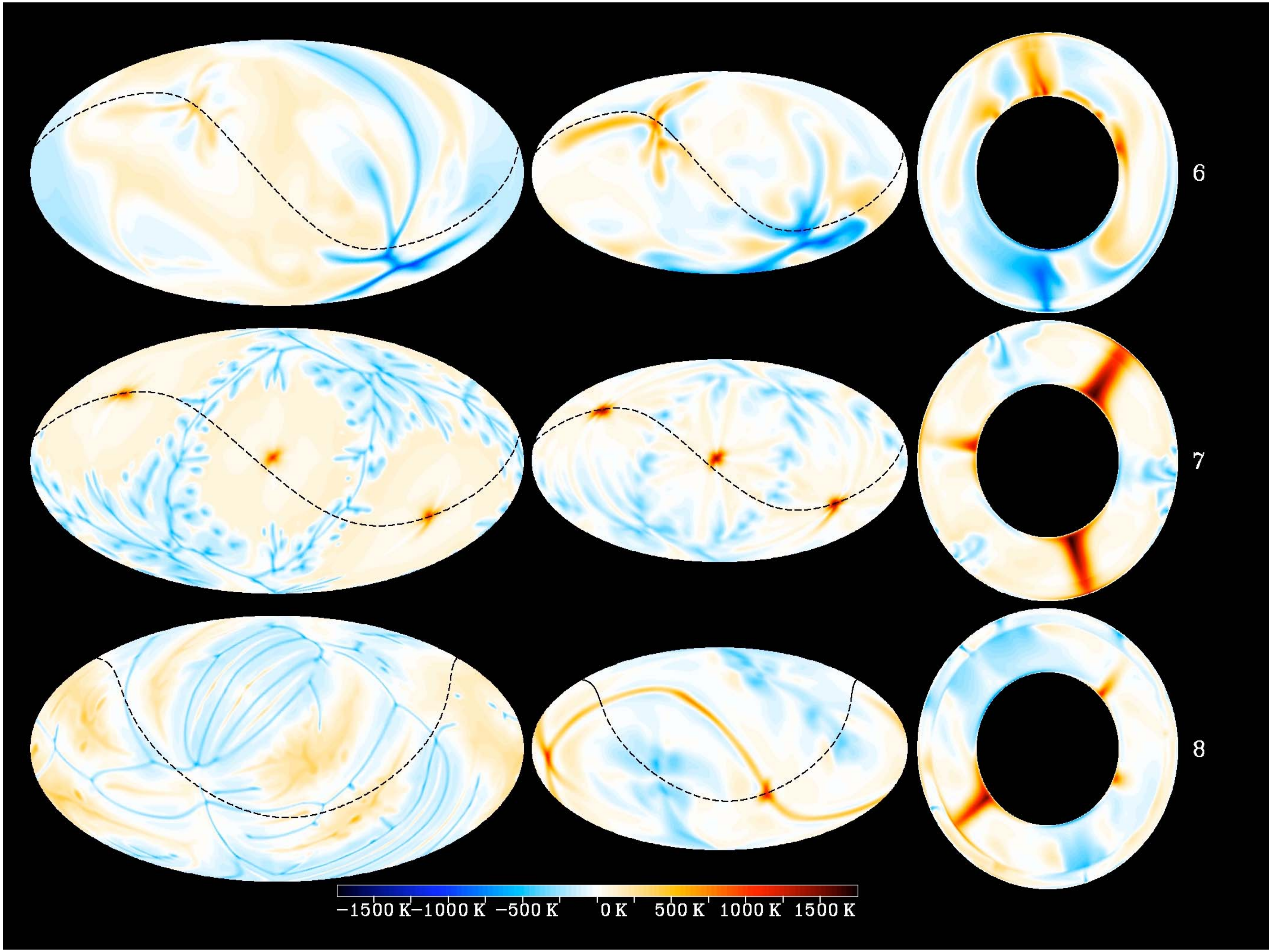
Influence of the Viscosity Profile



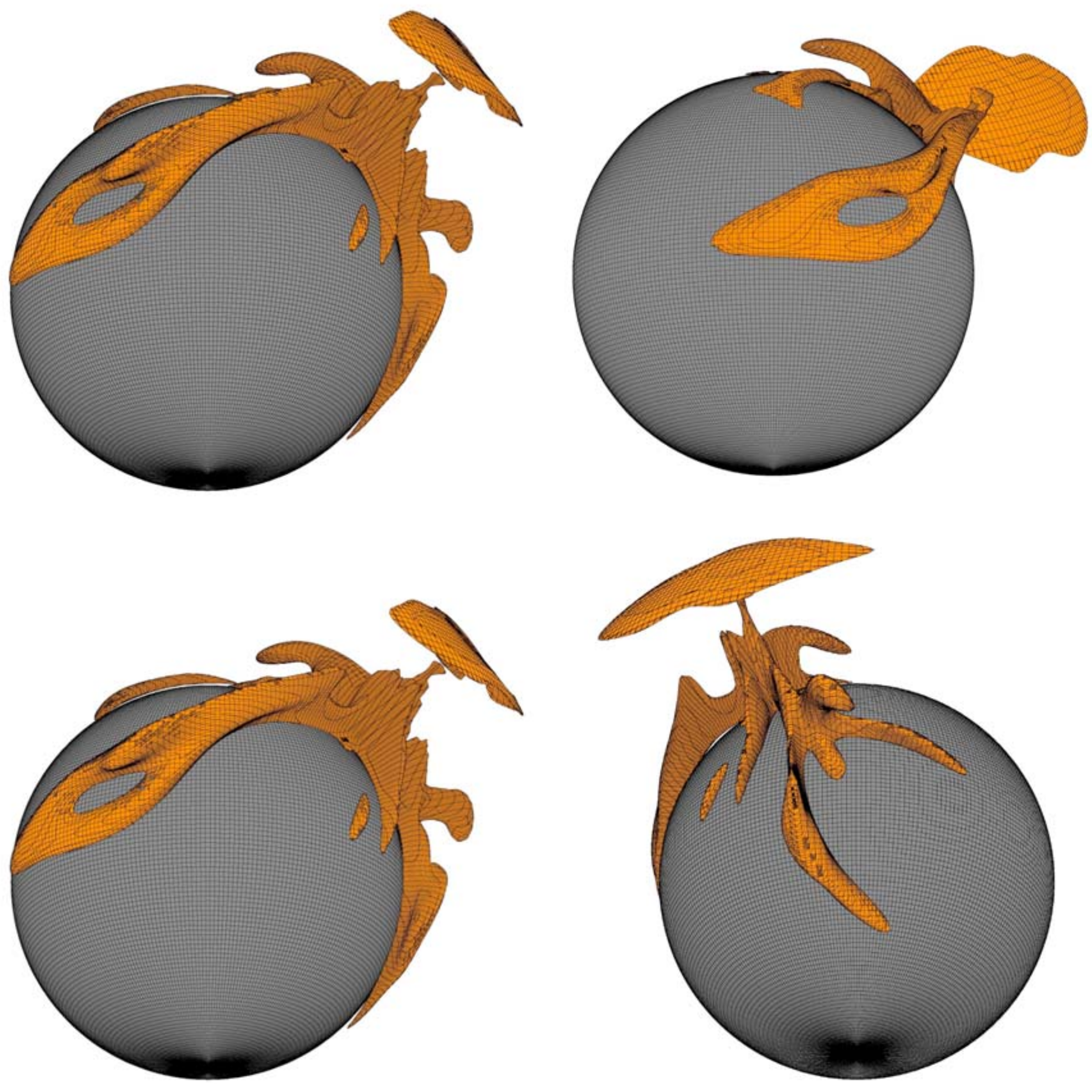
Families of Viscosity




1
2
3
4
5
−1500 K −1000 K −500 K 0 K 500 K 1000 K 1500 K


6
7
8
−1500 K
−1000 K
−500 K
0 K
500 K
1000 K
1500 K

Great Chinese Wall in Lower Mantle



Concluding Statement:

- The post-perovskite (PPV) transition together with the superplume concept, as advocated by S.D. Maruyama, can be used to understand about material properties in the deep mantle.
- (radiative heat transfer, viscosity, thermal expansion coefficient)
- Onset of post-perovskite transition would have an influence on mode of heat transfer by superplume.
- We must not forget that we can learn something about material propertiesin the deep mantle from putting geophysical constraints together.

computational

Methods

--- *Density Functional Theory*

(Hohenberg and Kohn, 1964)

--- *LDA and GGA*

(Ceperley and Alder, 1985)
(Perdue at al.,1996)

--- *Plane wave basis – pseudopotential*

(Troullier and Martins, 1991
von Bar and Car)

--- *Variable Cell Shape Molecular Dynamics*

(Wentzcovitch, 1991)

--- *Density Functional Perturbation Theory for phonons*

(Baroni et al., 1987)

--- *LDA+U with internally consistent U for strongly correlated systems*

(Cococcioni and de Gironcoli

<u>Thermodynamics Method</u>

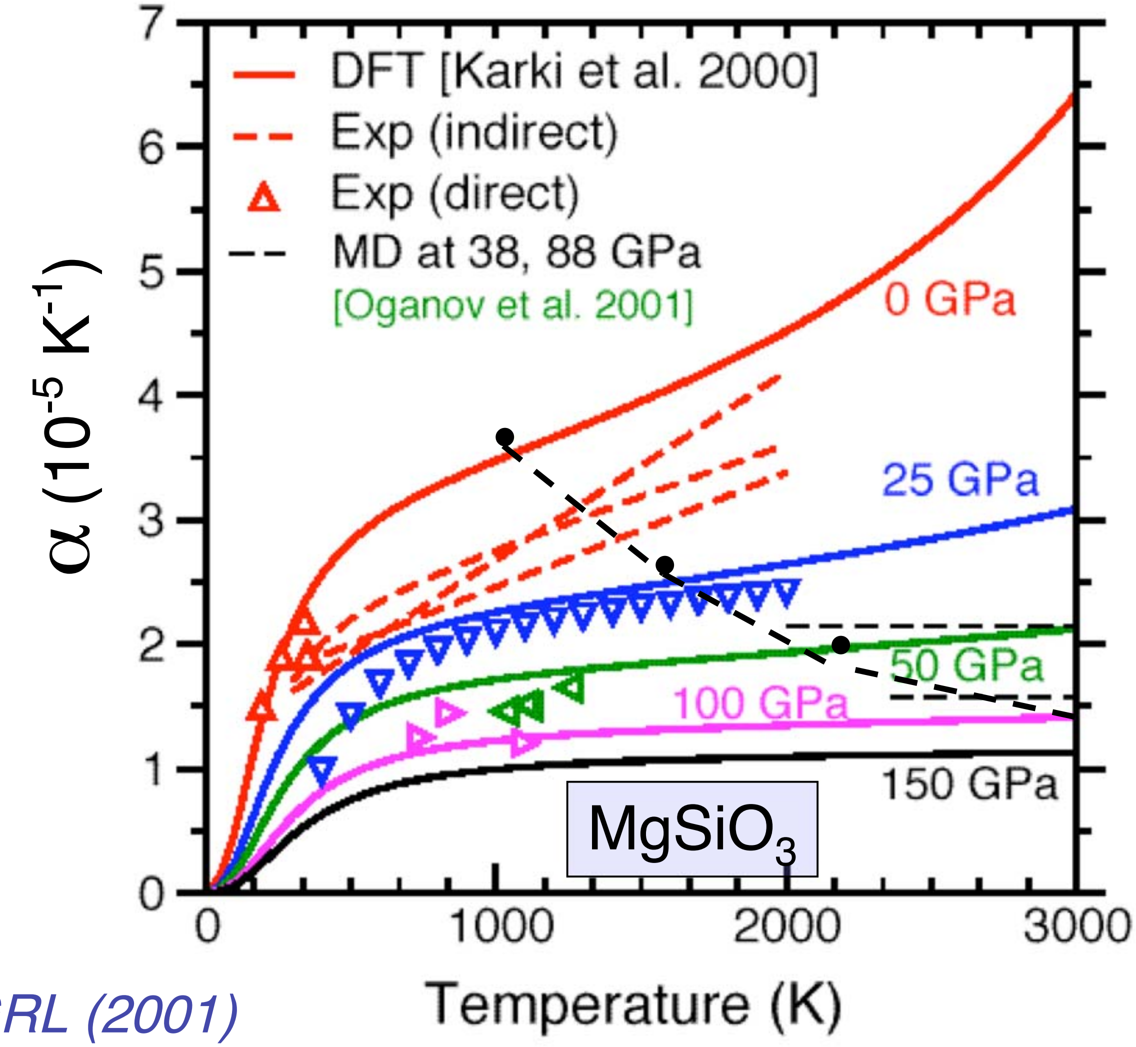
- VDoS and F(T,V) within the QHA

N-th (N=3,4,5…) order *isothermal* (eulerian or logarithm) finite strain EoS

<u>IMPORTANT</u>: crystal structure and phonon frequencies depend on *volume* alone!!….

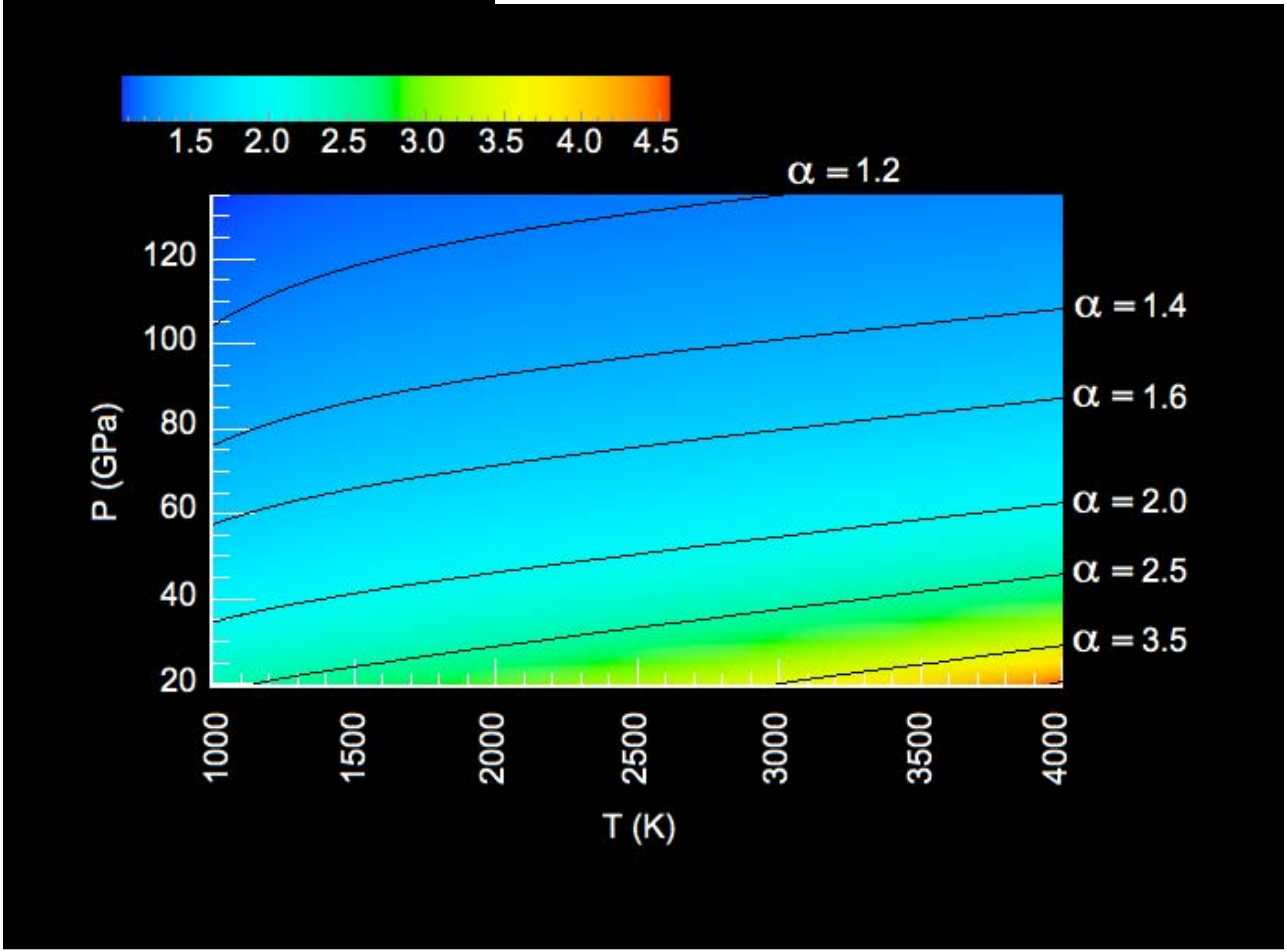
Thermal expansivity and the QHA

α provides an *a posteriori* criterion for the validity of the QHA

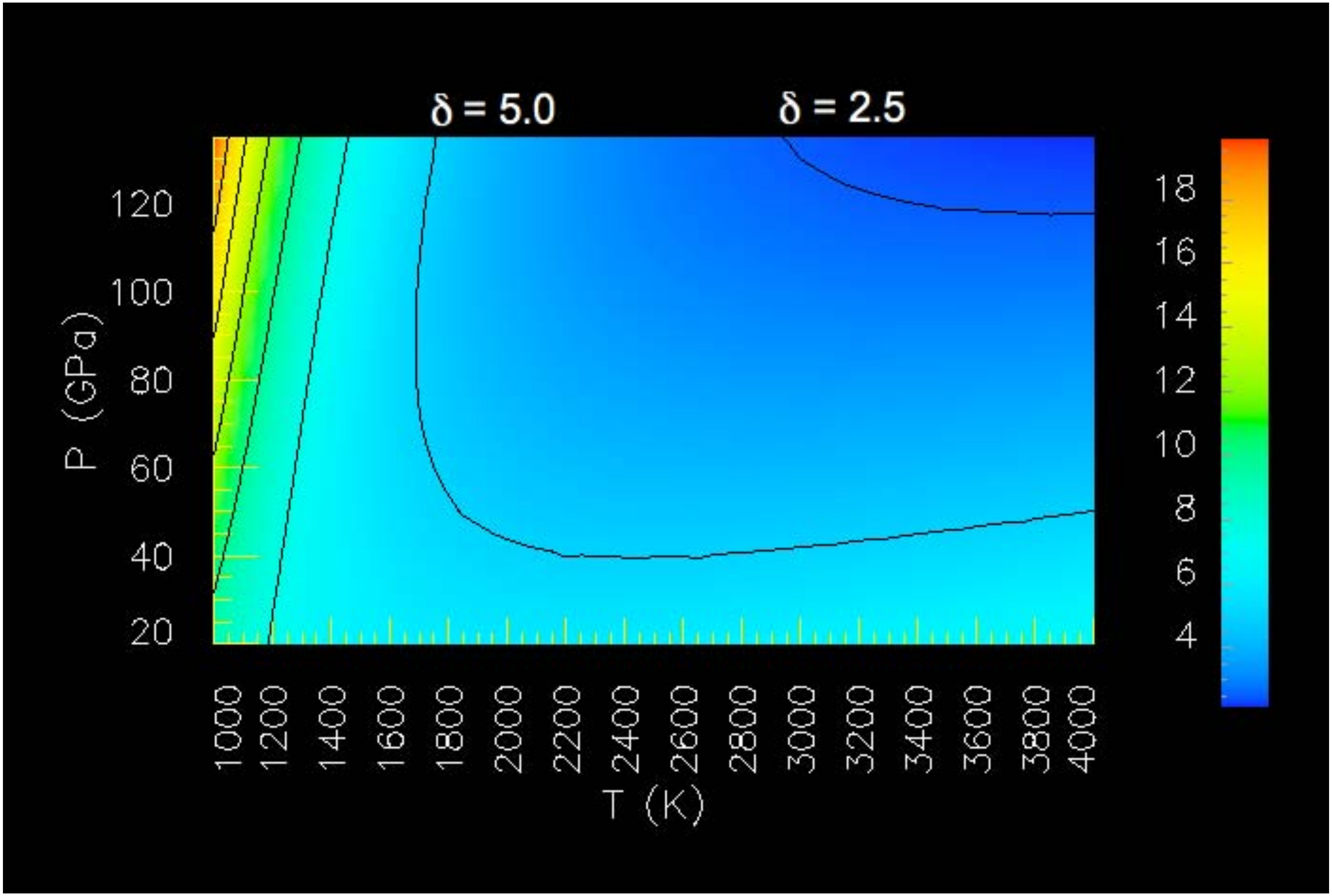


Karki et al, GRL (2001)

Another depiction of α(P,T) in 10^{-5} K^{-1}



$$\delta = -\left(\frac{\partial \ln \alpha}{\partial \ln \rho}\right)_P = -\frac{\rho}{\alpha}\left(\frac{\partial \alpha}{\partial \rho}\right)_P$$

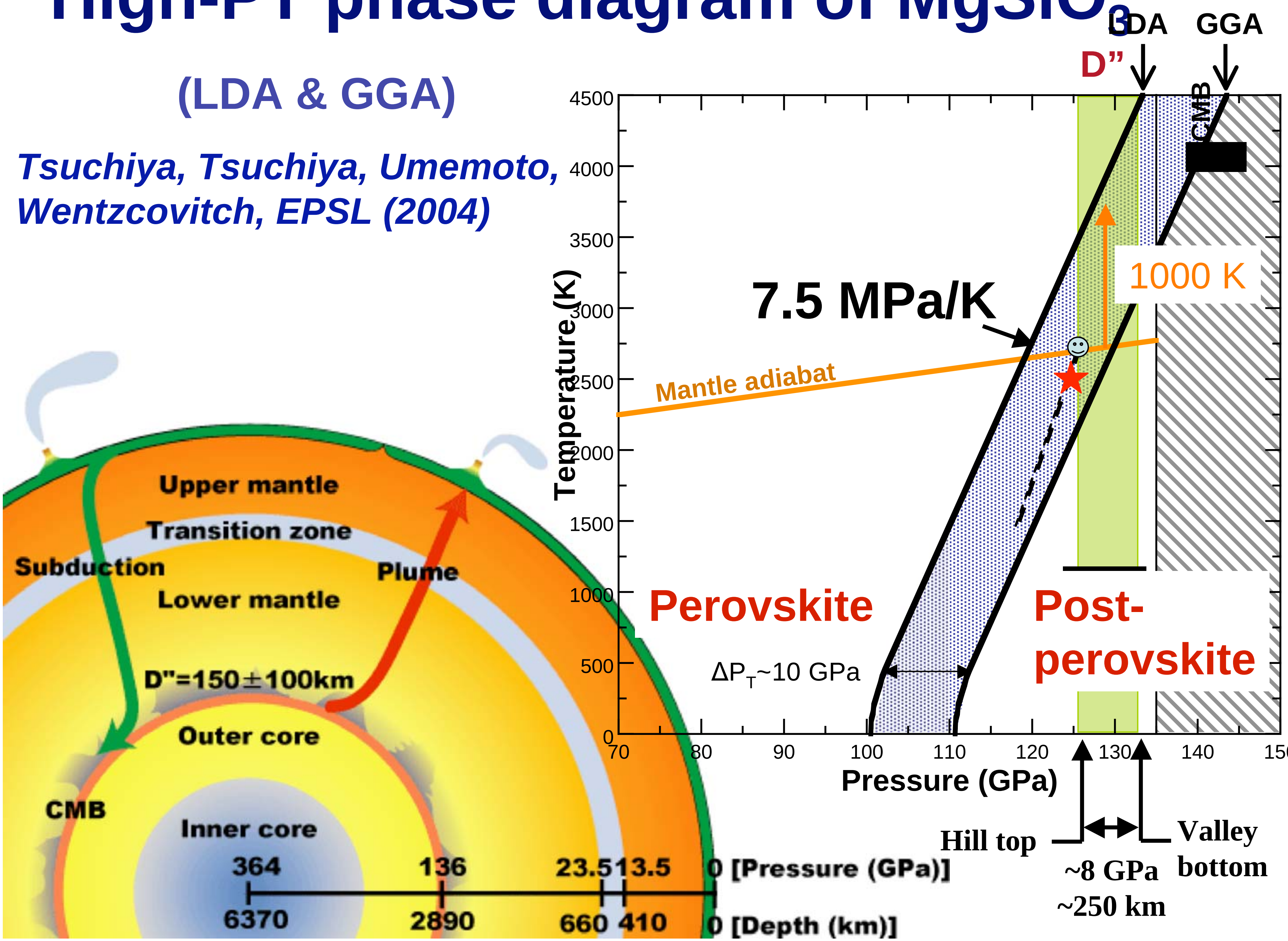


Impact of Mineral Physics on Geodynamics

High-PT phase diagram of $MgSiO_3$

(LDA & GGA)

Tsuchiya, Tsuchiya, Umemoto, Wentzcovitch, EPSL (2004)



http://www.vlab.msi.umn.edu

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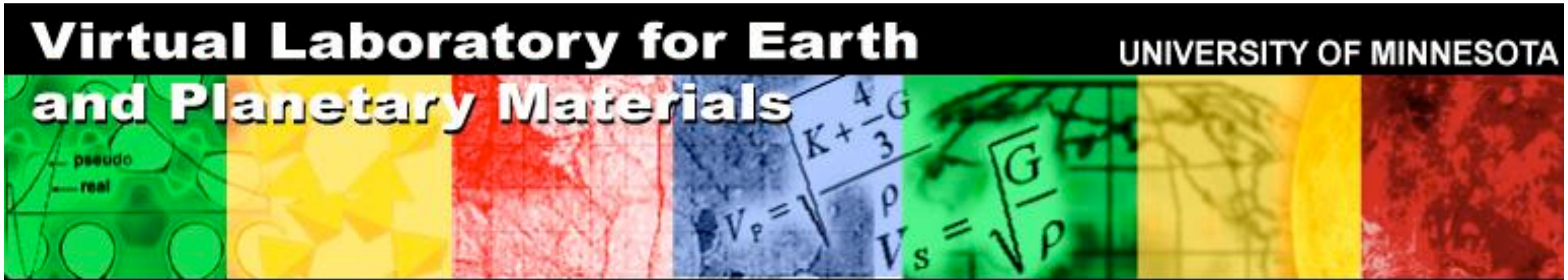
The Virtual Laboratory for Earth and Planetary Materials, VLab, funded by the National Science Foundation and hosted by the Supercomputing Institute for Digital Simulations and Advanced Computation at the University of Minnesota, is an interdisciplinary consortium dedicated to the development and promotion of the theory of planetary materials. Computational determination of geophysically important materials properties at extreme conditions provides today, and maybe for a long time to come, the most accurate information to a) interprete seismic data in the context of likely geophysical processes and b) be used as input for more sophisticated and reliable modeling of planets. The laboratory aims to accelerate developments in this emergent area by:

- Addressing materials physics and physical chemistry issues of importance to planetary sciences.
- Developing and improving first principles simulations methodologies, integrating highly tested first principles software with utility programs, and creating novel human/software interfaces to facilitate and automate time-consuming human tasks.
- Developing an educational program to provide training and bridge the gap between mineral physicists and materials theorists.

VLab



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