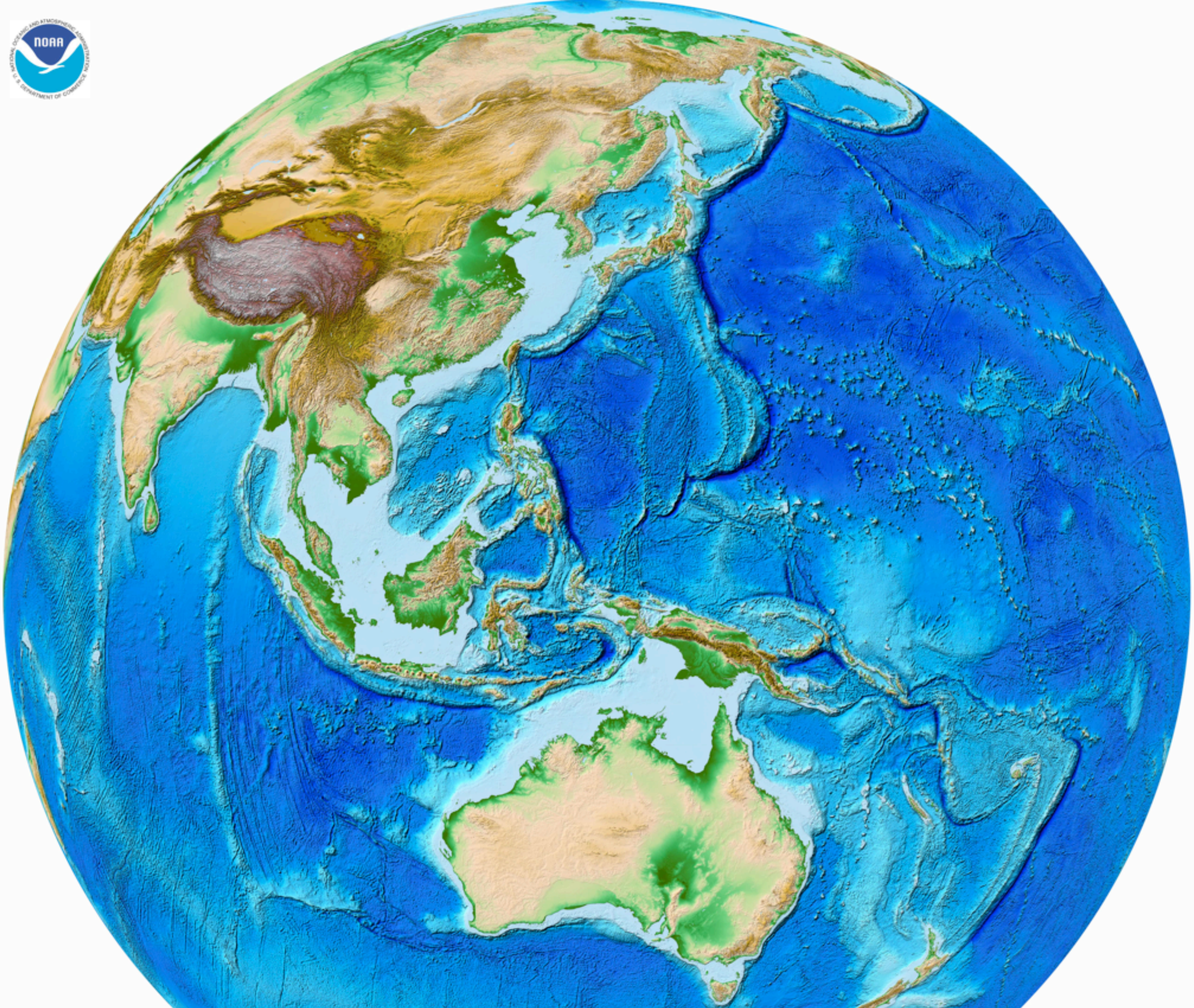
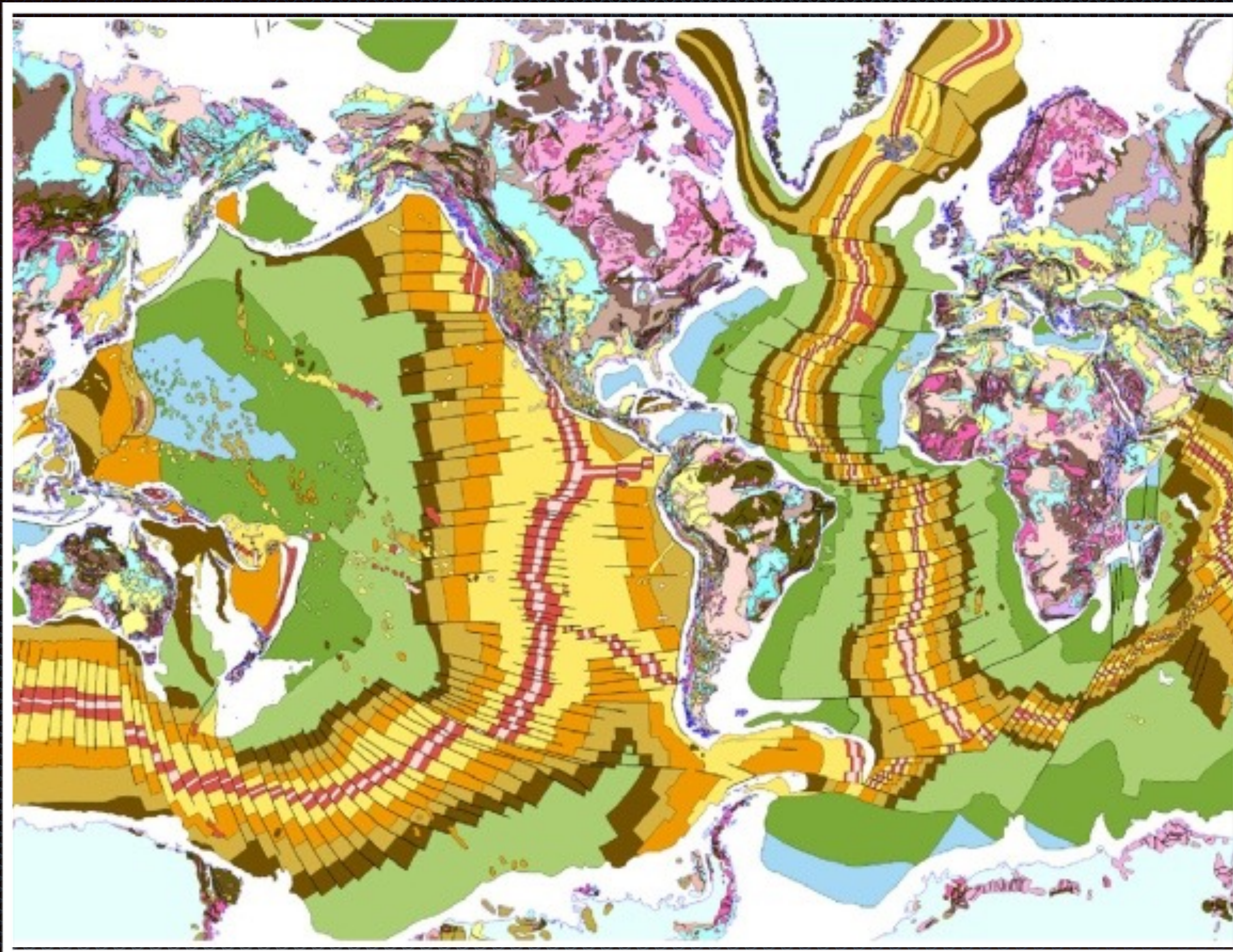
HeFESTo: a tool

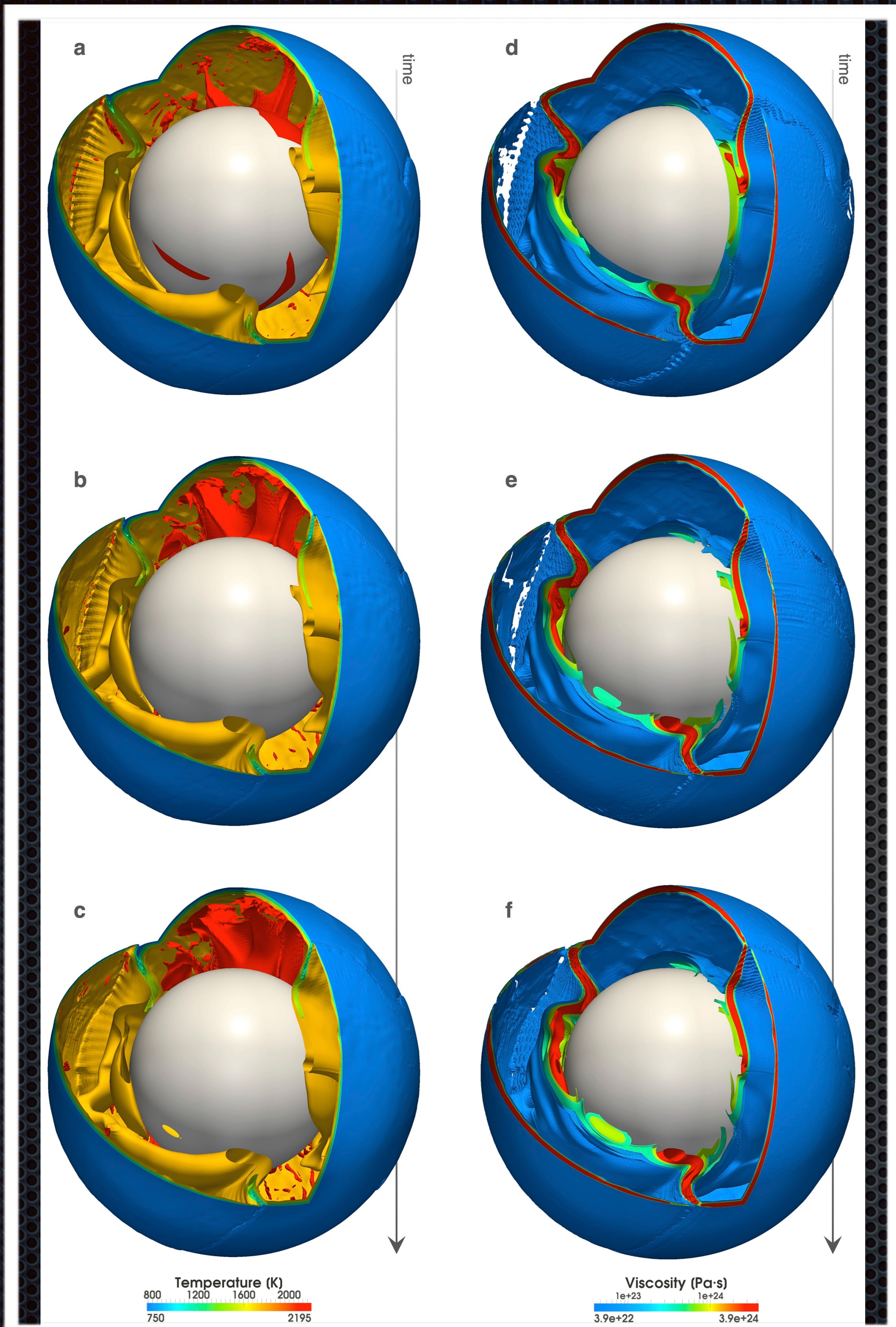
Carolina Lithgow-Bertelloni and Lars Stixrude





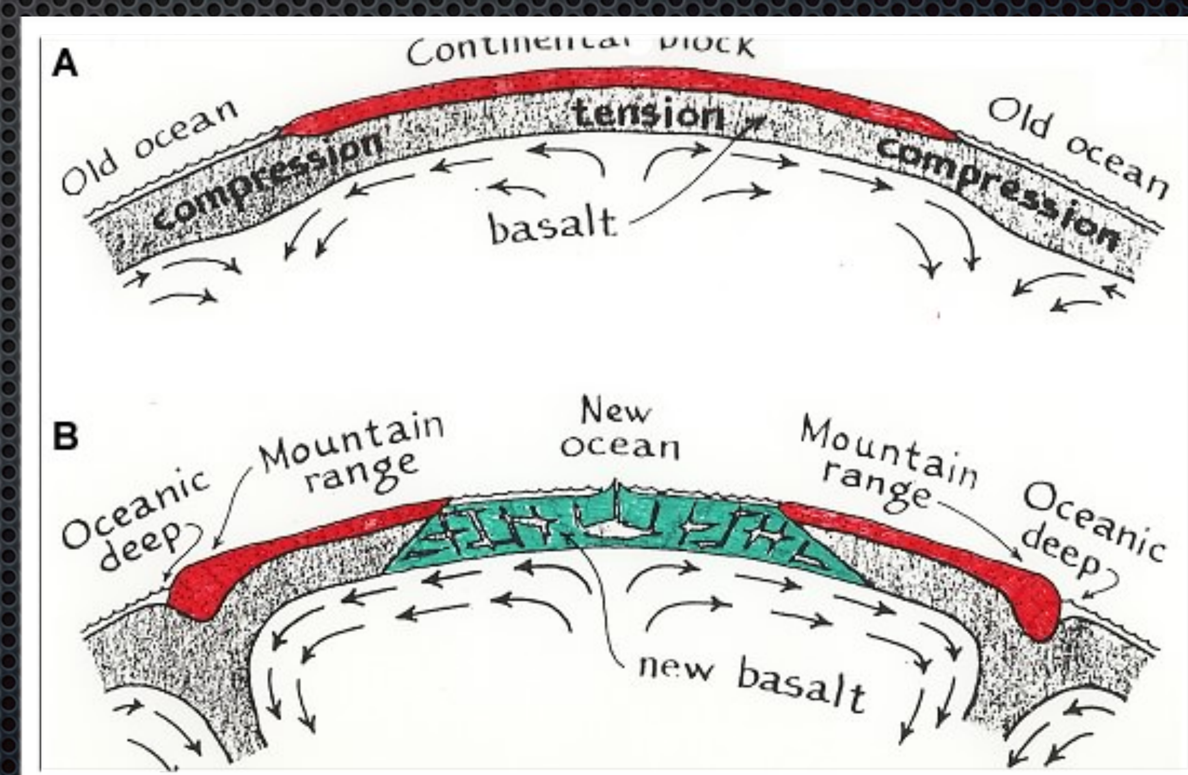
[*Geological Map of the World*, UNESCO, 1980’s]

Mantle Convection

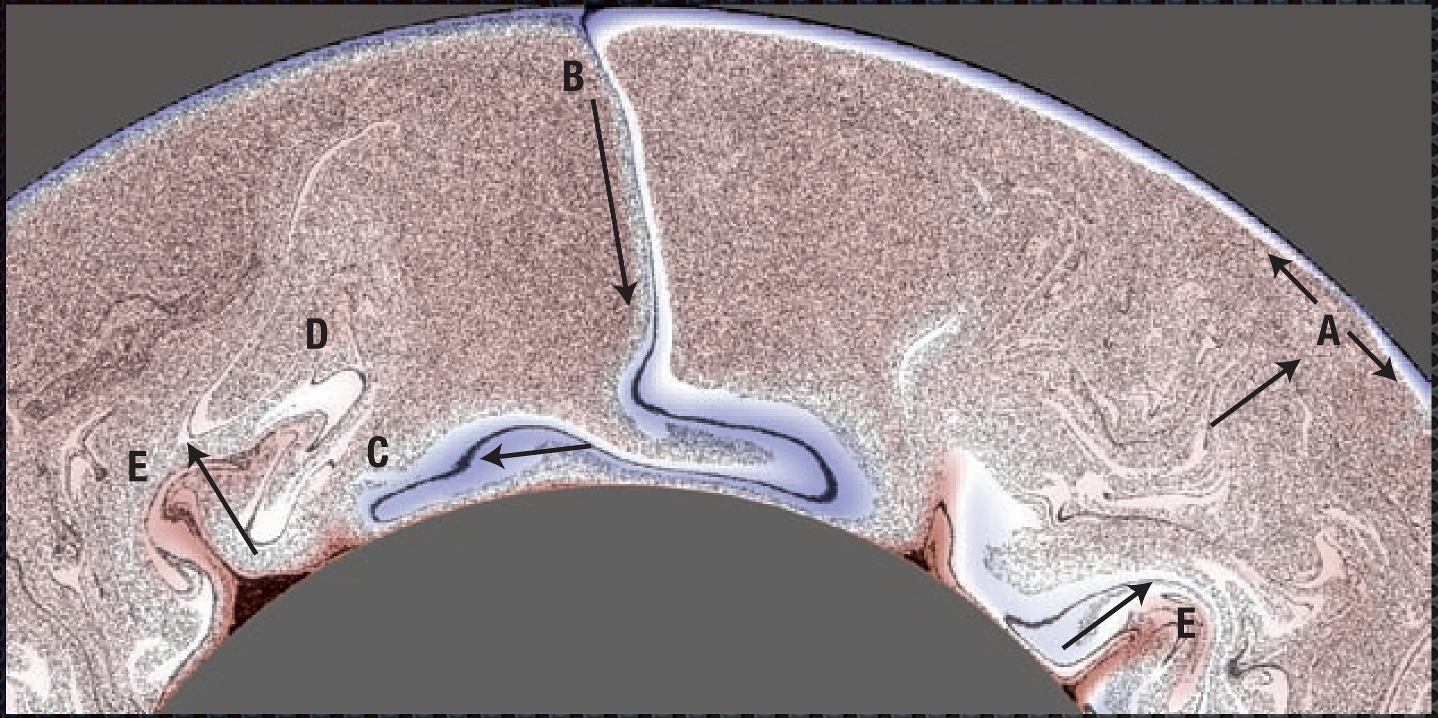


[*Crameri et al.*, 2011]

[*Holmes*, 1945]



Heterogeneity and Present-Day Mantle



[Brandenburg and van Keken, 2007]

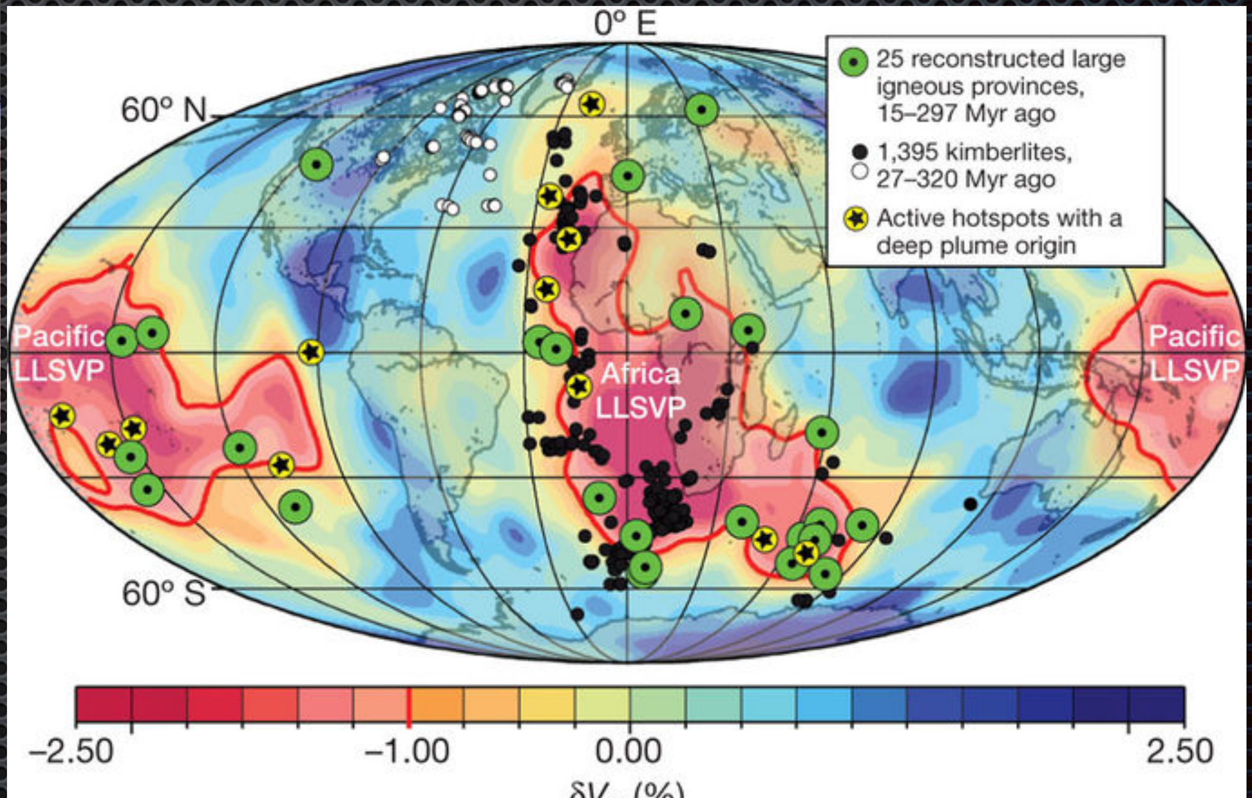


Figure 1. Reconstructed locations of LIPs and active hotspots and their relationship to the African and Pacific LLSVPs identified by the 2% contour of Vs

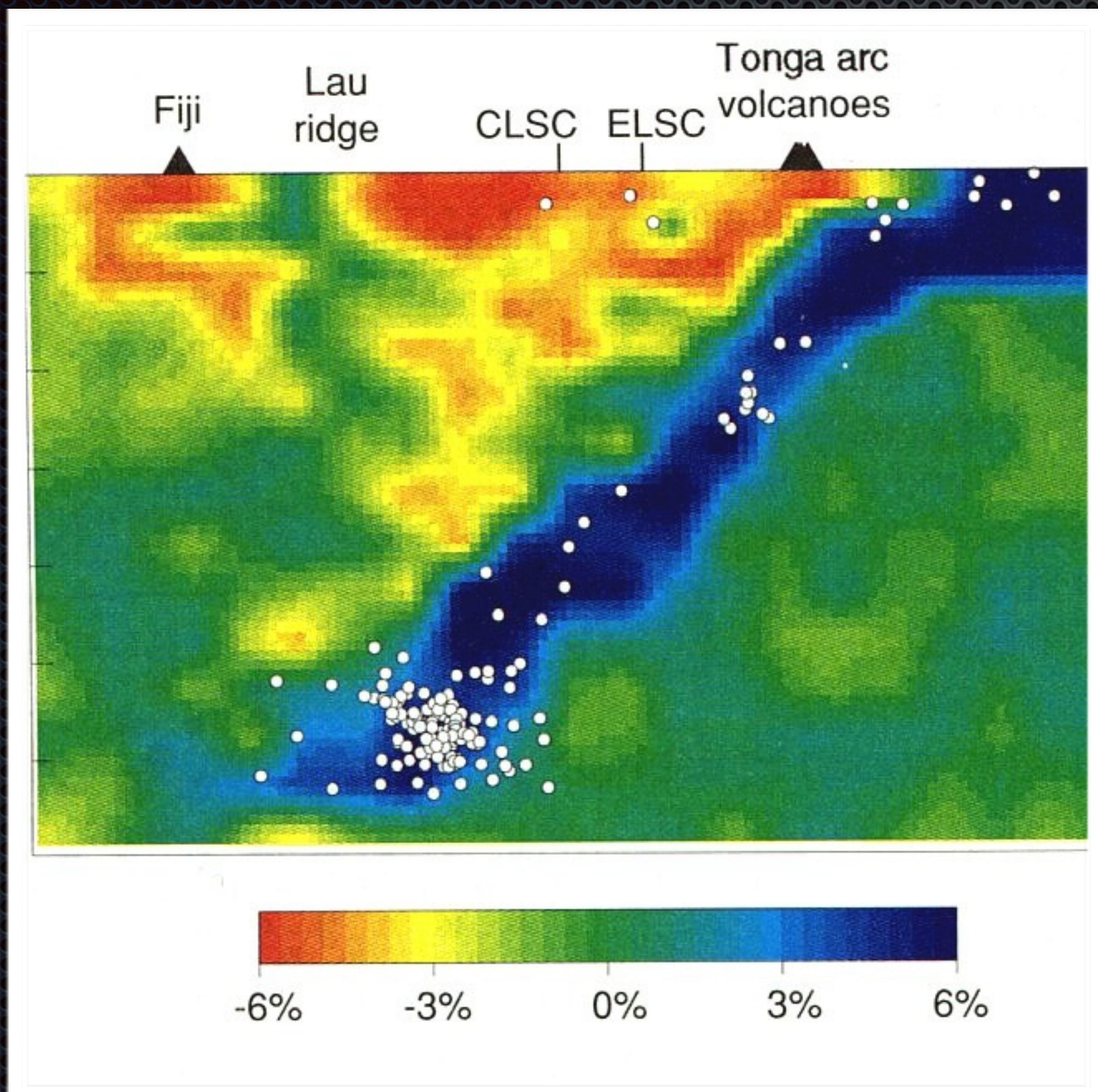
[*Torsvik et al.*, 2006]

- *Understand two separate but interrelated questions:*

  What is the origin of heterogeneity?

  What do seismic anomalies mean?

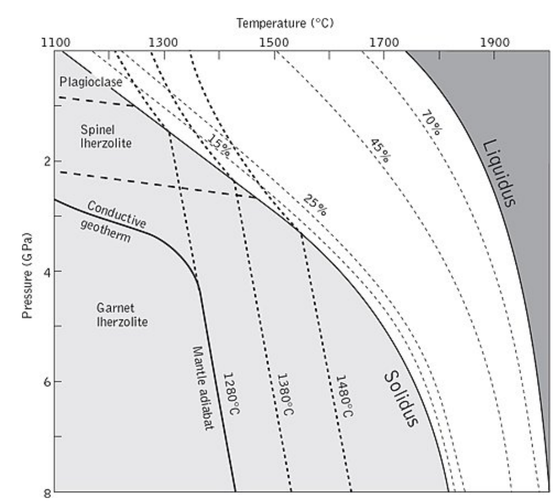
Melting and compositional heterogeneity



[*Zhao et al.*, 1997]

Melting

Decompression Melting



Melting forms oceanic crust (basalt)
and depleted residuum (harzburgite

Densities

basalt ~ 2.9 g/cm^3

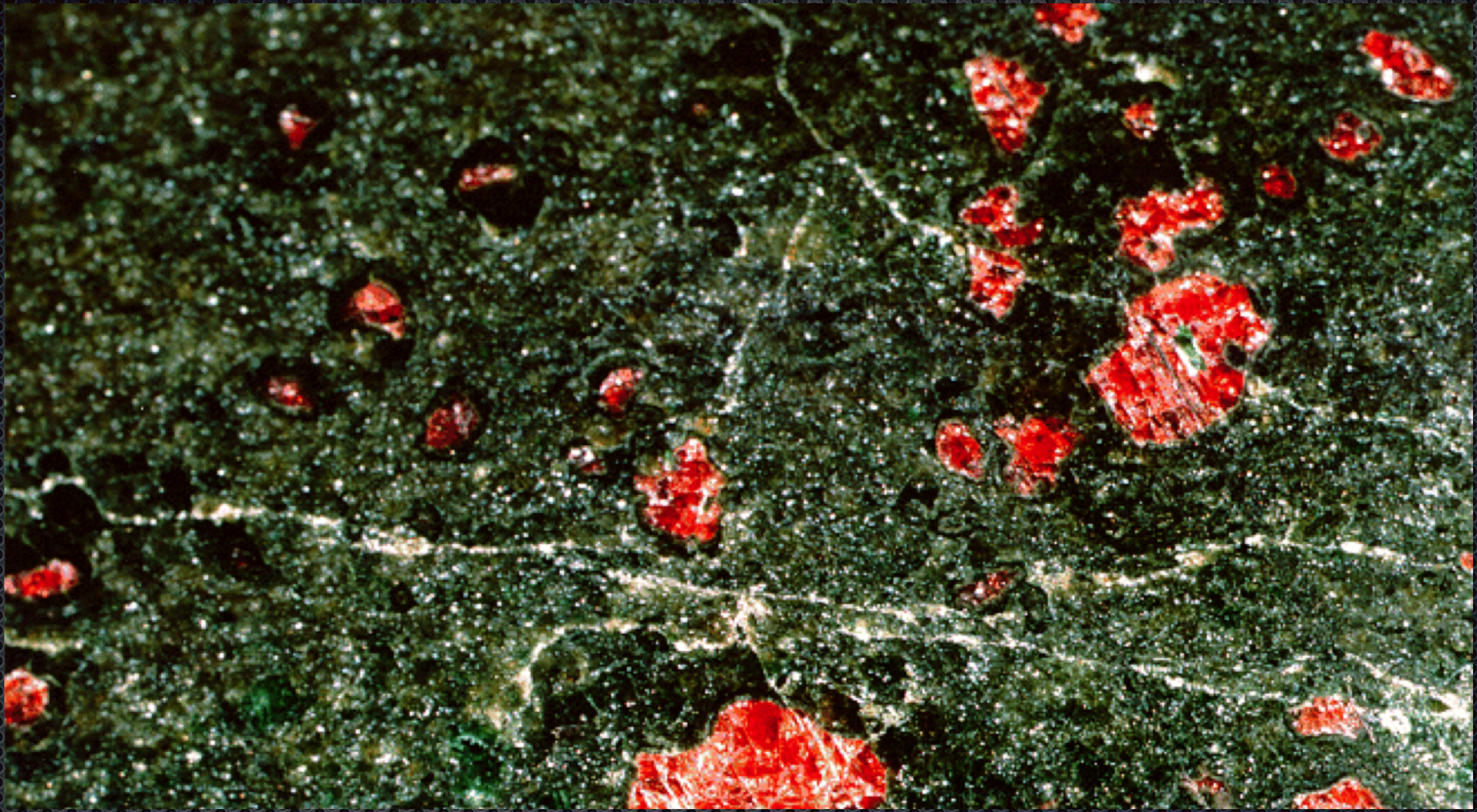
harzburgite ~ 3.2 g/cm^3

lherzolite ~ 3.3 g/cm^3

Oxburgh & Parmenti

[*Oxburgh and Parmentier*, 1978]

Heterogeneous Equilibria (i.e. Rocks!)



- *Multi-phase assemblages determined by the equilibrium thermodynamics*
- *Affects physical properties*

Governing Equations

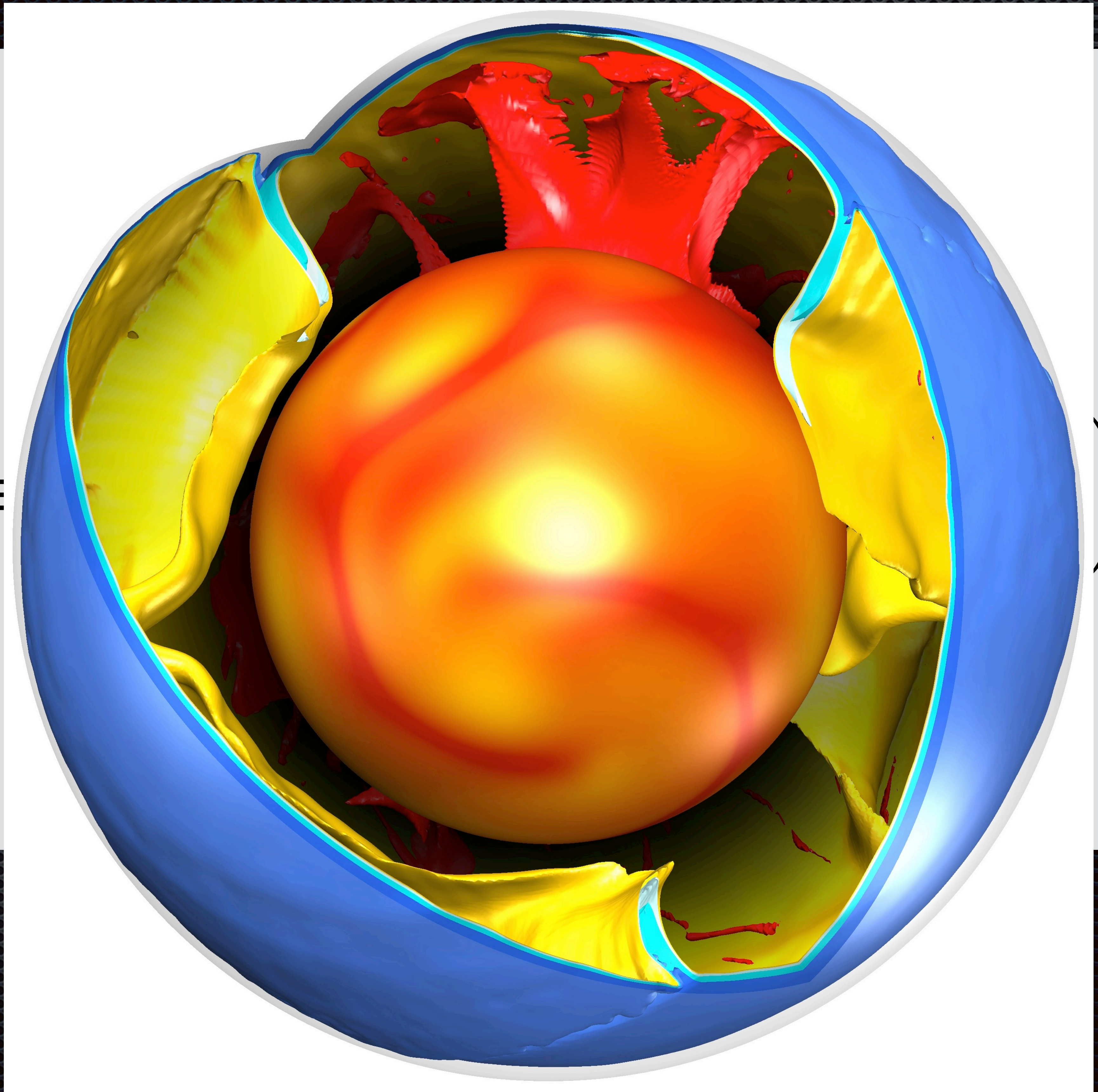
$$-\nabla \cdot \left[2\eta\left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1}\right)\right] + \nabla p = \rho \mathbf{g} \qquad \text{in } \Omega, \tag{1}$$

$$\nabla \cdot (\rho \mathbf{u}) = 0 \qquad \text{in } \Omega, \tag{2}$$

$$\begin{aligned} \rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T\right) - \nabla \cdot k \nabla T = \rho H & \\ + 2\eta\left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1}\right) : \left(\varepsilon(\mathbf{u}) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbf{1}\right) & \\ + \alpha T\left(\mathbf{u} \cdot \nabla p\right) & \\ + \rho T \Delta S\left(\frac{\partial X}{\partial t} + \mathbf{u} \cdot \nabla X\right) & \qquad \text{in } \Omega, \end{aligned} \tag{3}$$

CRUCIAL-Material Properties (equilibrium and transport)

Thermal Buoyancy



$\alpha \equiv$

$\Big)_P$

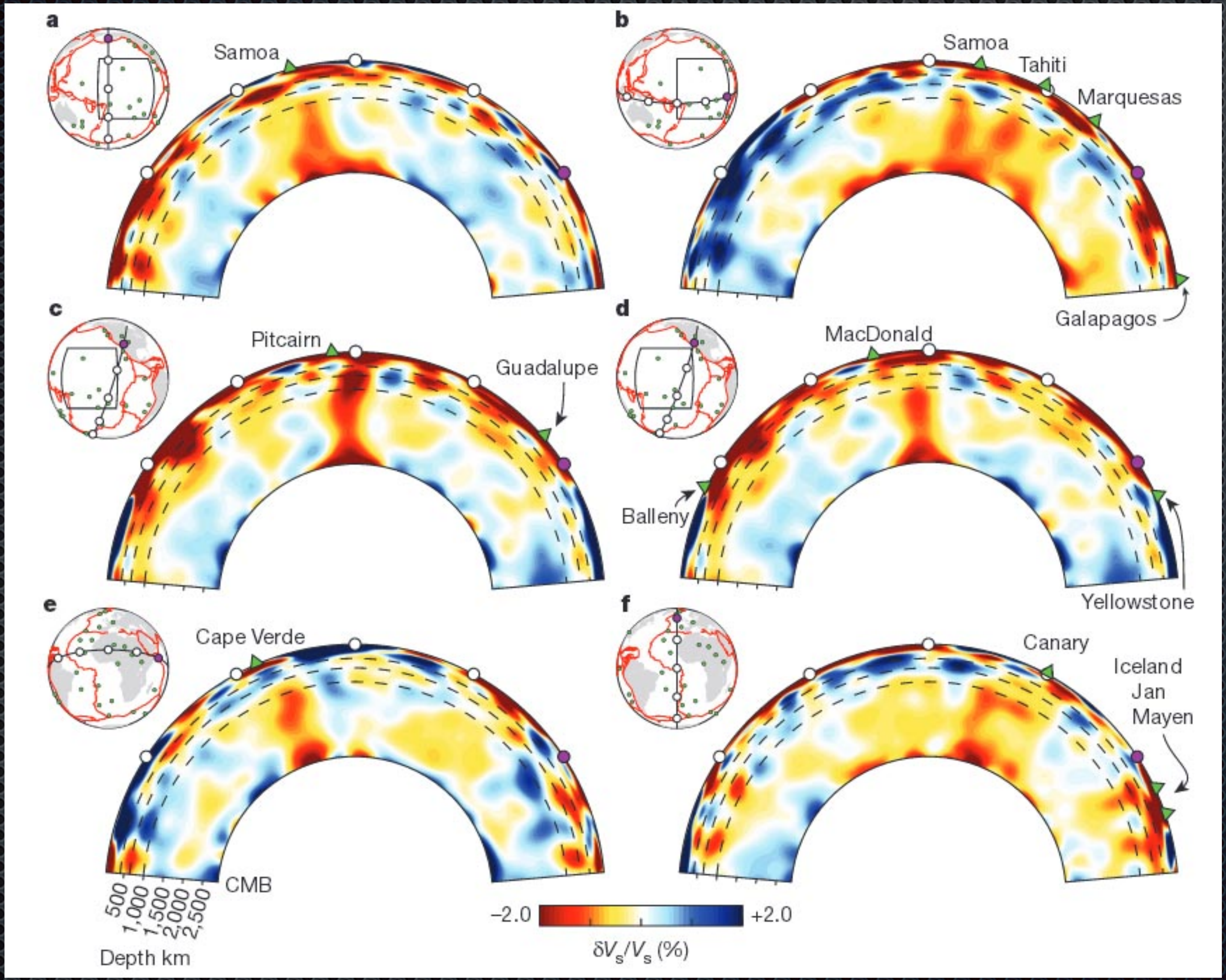
Lofty goals of HeFESTo

What is the origin of heterogeneity?

What do seismic anomalies mean?

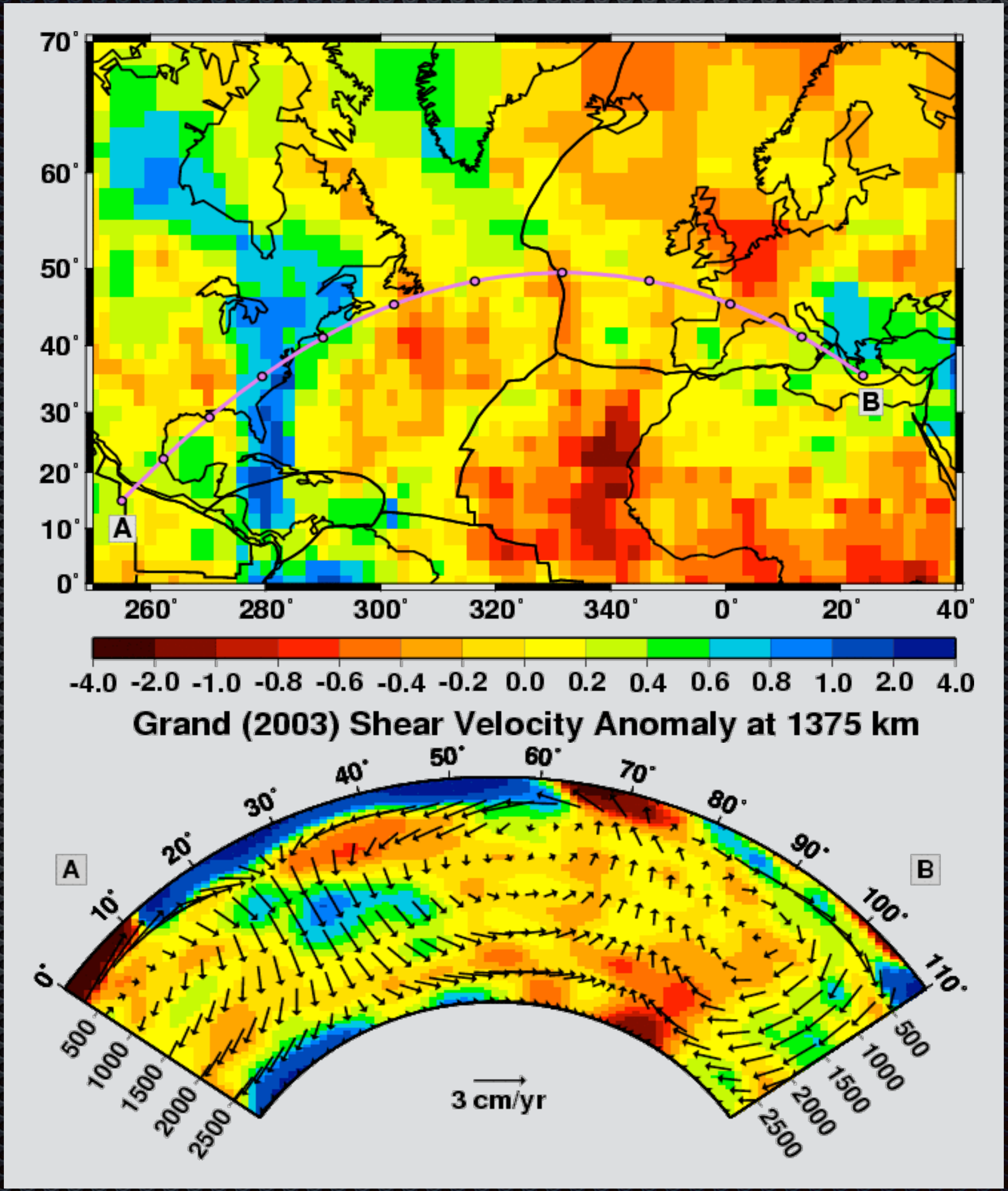
What effects on dynamics?

Convert Velocity to Density



[*French and Romanowicz*, 2015]

Compute Instantaneous Flow



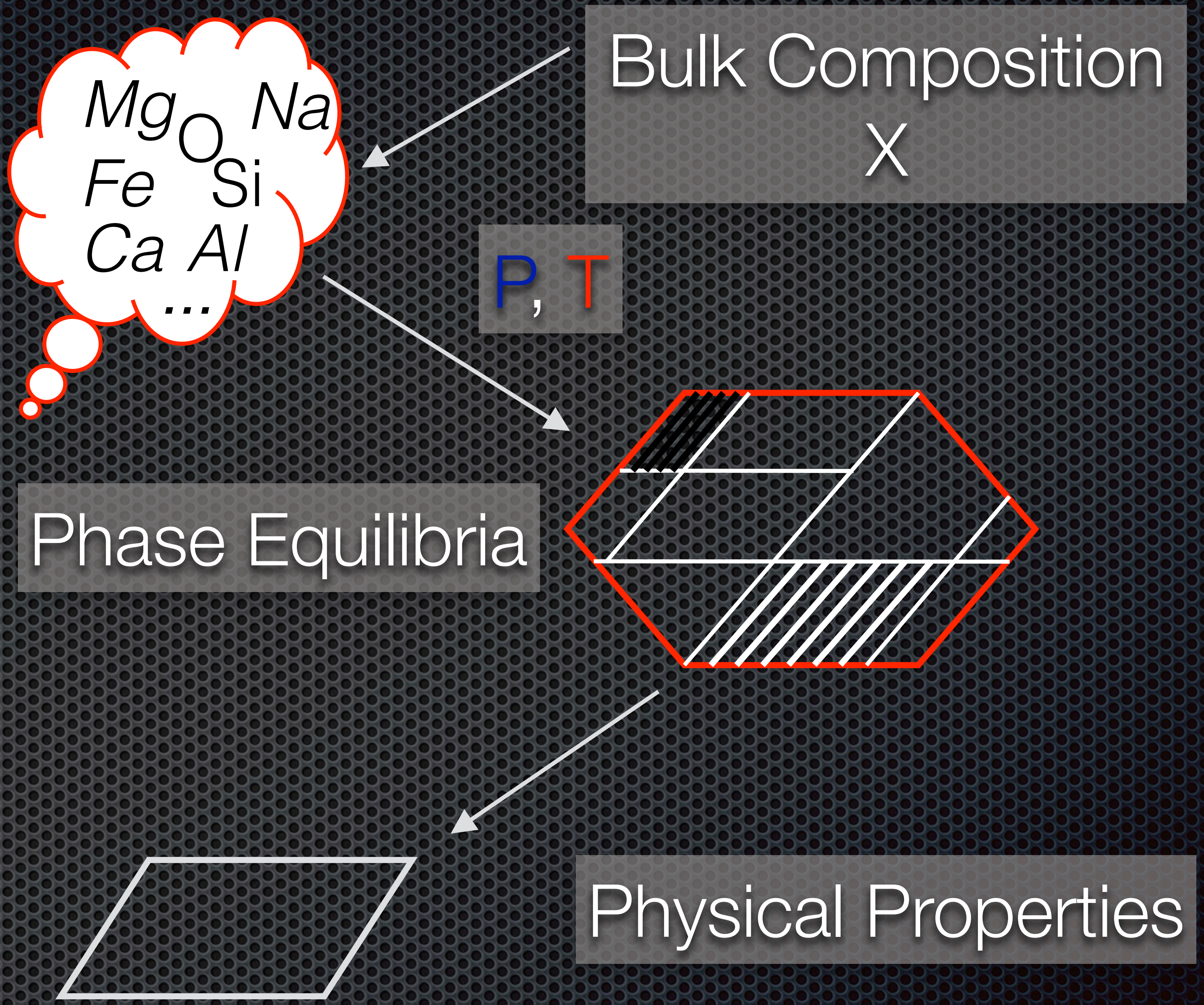
[*Conrad et al.*, 2004]

Thermodynamic Model

- *Bulk composition*
- *Pressure*
- *Temperature*

⬇

- *Phase Equilibria*
- *Physical Properties*
- *Self consistent*



$\rho, \alpha, C_P, V_P, V_S, \ldots \quad (X, P, T)$

[*Stixrude and Lithgow-Bertelloni*, 2005; 2011]

HeFESTo

- *Based on Fundamental Thermodynamic Relations*
- *Minimize Gibbs free energy over the amounts of all species n_i*

$$G(P,T,n_i) = \sum_{i=1}^{species} n_i\left[\mu_{0i}(P,T) + RT\ln a_i\right]$$

- *Subject to constraint of fixed bulk composition*

$$s_{ij}n_j = b_i$$

- *Full Anisotropic Generalization*

$$c_{ijkl} = \frac{1}{V}\left(\frac{\partial^2 F}{\partial E_{ij}\partial E_{kl}}\right)_{S'_{ij},T} + P\left(\delta_{ij}\delta_{kl} + \delta_{il}\delta_{jk} + \delta_{jl}\delta_{ik}\right)$$

- *Many previous efforts, however*

  Full self-consistency between phase equilibria and physical properties (not only one or the other)

  Anisotropic generalization and robust thermal extrapolation for shear properties

HeFESTo

GitHub

(https://github.com/stixrude/HeFESToRepository).

Perple_X

BurnMan

LARS' CIDER LECTURES

https://seismo.berkeley.edu/wiki_cider/Mineral_Physics

Stixrude and Lithgow-Bertelloni, 2005 GJI
Stixrude and Lithgow-Bertelloni, 2011 GJI

First Law of Thermodynamics

$$dU = TdS - PdV + \sum_{i=1}^{N} \mu_i dn_i$$ Internal Energy

$$T = \left(\frac{\partial U}{\partial S}\right)_{V,n_i}$$ Temperature

$$P = -\left(\frac{\partial U}{\partial V}\right)_{S,n_i}$$ Pressure

$$\mu_i = \left(\frac{\partial U}{\partial n_i}\right)_{S,V,n_{j\neq i}}$$ Chemical Potential

Euler Form

$$U(\lambda S, \lambda V) = \lambda U(S, V)$$

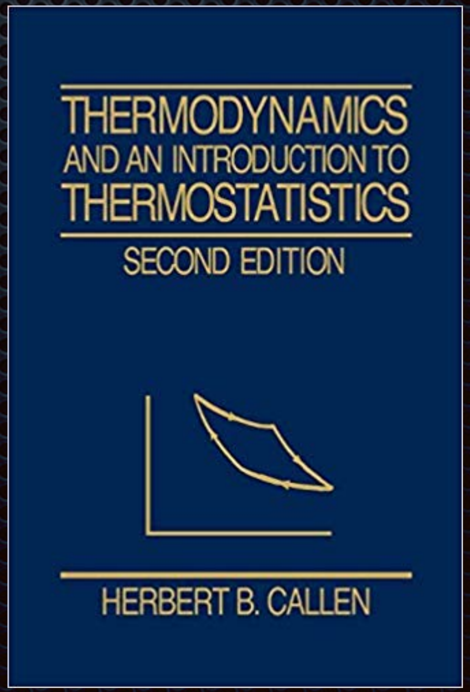
$$U(S, V) = \frac{\partial U}{\partial(\lambda S)}\frac{\partial(\lambda S)}{\partial \lambda} + \frac{\partial U}{\partial(\lambda V)}\frac{\partial(\lambda V)}{\partial \lambda}$$

$$U\left(S, V, n_i\right) = TS - PV + \sum_{i=1}^{N} \mu_i n_i$$

Fundamental Thermodynamic Relation

A single function that contains complete information of all properties of all equilibrium states of a system

$$U(S, V, n_i) = TS - PV + \sum_{i=1}^{N} \mu_i n_i$$



Formulation

Euler Form

$$U(S,V,n_i) = TS - PV + \sum_{i=1}^{N} \mu_i n_i$$

Legendre Transform

$$F(T,V,n_i) = U - TS = -PV + \sum_{i=1}^{N} \mu_i n_i$$

$$G(T,P,n_i) = F + PV = \sum_{i=1}^{N} \mu_i n_i$$

Anisotropic Generalization

$$F = F(T, E_{\alpha\beta}, n_i)$$

$$G = G(T, \sigma_{\alpha\beta}, n_i)$$

HeFESTo: Phase Equilibria

Minimize with respect to n_i at fixed P, T

$$G\left(P,T,n_i\right) = \sum_{i=1}^{species} n_i\left\{\mu_{i0}(P,T) + RT\ln\left[a_i(P,T,n_i)\right]\right\}$$

Subject to constant bulk composition

$$r_{ij}n_j = b_i$$

HeFESTo: Phase Equilibria

Search over null space of the linear problem (SVD)

$$\left[\ \mathbf{r}\ \right] \times \left[\ \mathbf{n}\ \right] = \left[\ \mathbf{b}\ \right]$$

Stoichiometric Coefficient Matrix

Amount of Species

Bulk Composition

Check for phase addition based on chemical affinity

$$A_\phi = \min_{x_i}\left[\sum_{i=1}^{species\ \phi} x_i\left(\mu_i - r_{ij}\varepsilon_j\right)\right]$$

$$r'_{ij}\varepsilon_j = \mu'_i$$

HeFESTo: Physical Properties

Cold Part

Start from fundamental relation
Helmholtz free energy

$$F = F(V, T, n_i)$$

Isotherm, fixed composition

$$F = F(V)$$

Taylor series expansion
Expansion variable must be V or function of V

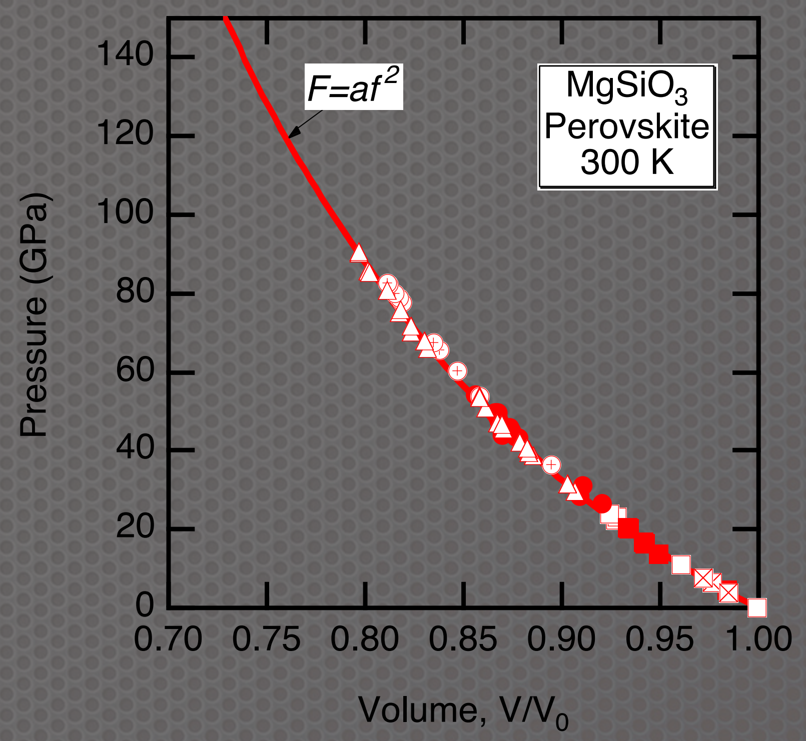
$$F = af^2 + bf^3 + \cdots$$

Eulerian finite strain

$$f = f(V)$$

$$a = 9K_0V_0$$

$$f = \frac{1}{2}\left[\left(\frac{V}{V_0}\right)^{-2/3} - 1\right]$$



Data: Knittle and Jeanloz (1986) Science, Ross and Hazen (1989) PCM, Mao et al. (1991) JGR, Wang et al. (1994) PEPI, Utsumi et al. (1995) JGR, Funamori et al. (1996) JGR, Fiquet et al. (1998) GRL, Saxena et al. (1999) Am. Min.

HeFESTo: Physical Properties

Full

$$\boxed{F(\varepsilon_{ij},T,\vec{n}) = F_0 + F_C(\varepsilon_{ij},T_0,\vec{n}) + \Delta F_{TH}(\varepsilon_{ij},T,\vec{n})}$$

- V_0 Volume: x-ray diffraction
- K_0, G_0 Elastic moduli: Brillouin data, DFTheory
- K_0', G_0' P-derivatives: Brillouin data, DFTheory
- θ_0 Debye temperature: calorimetry, phase equilibria
- γ_0 Grüneisen parameter: thermal expansion
- q_0 V-derivative of γ_0: K(T) from Brillouin or DFTheory
- η_S T-derivative of G: G(T) from Brillouin or DFTheory
- F_0 Reference free energy: phase equilibria
- Landau terms: V_{max}, S_{max}

Parameters

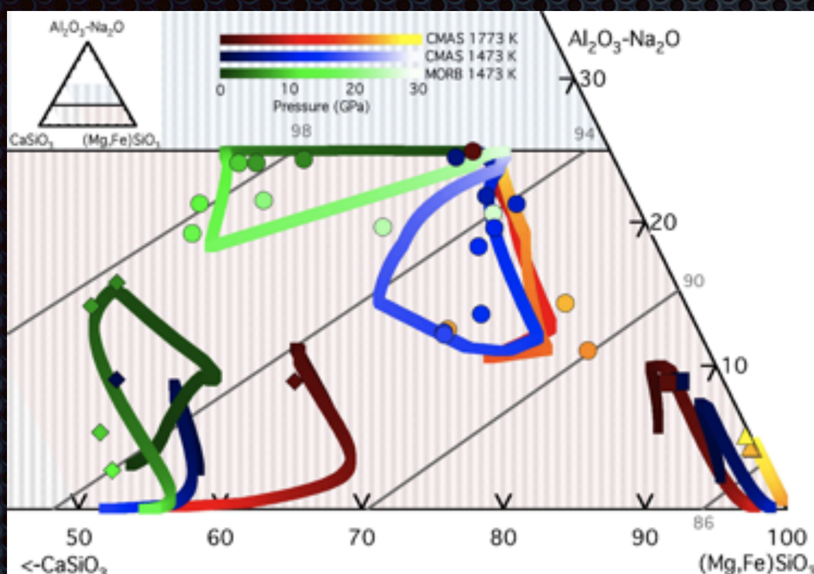
Table A1. Properties of mantle species.

Phase	Species	Formula	$\mathcal{F}_0$ (kJ mol^{-1})	V_0 (cm^3 mol^{-1})	K_{T0} (GPa)	K'_{T0}	θ_0 (K)	γ_0	q_0	G_0 (GPa)	G'_0	η_{S0}	Ref.
feldspar (plg)	Anorthite (an)	$Ca\,[Al_2Si_2]\,O_8$	−4015 (4)	100.61	84 (5)	*4.0* (10)	752 (2)	0.39 (5)	*1.0* (10)	40 (3)	*1.1* (5)	*1.6* (10)	1-6
feldspar	Albite (ab)	$Na\,[Al\,Si_3]\,O_8$	−3719 (5)	100.45	60 (5)	*4.0* (10)	716 (13)	0.57 (3)	*1.0* (10)	36 (5)	*1.4* (5)	*1.0* (10)	1,6,7
spinel (sp)	Spinel (sp)	$(Mg_3Al)(Al_7Mg)O_{16}$	−8668 (32)	159.05	197 (1)	5.7 (2)	843 (33)	1.02 (4)	2.7 (6)	108 (10)	0.4 (5)	2.7 (6)	1,8-10
spinel	Hercynite (hc)	$(Fe_3Al)(Al_7Fe)O_{16}$	−7324 (35)	163.37	209 (2)	*5.7* (10)	763 (32)	1.22 (7)	*2.7* (10)	84 (13)	*0.4* (5)	*2.8* (10)	1,2,11
olivine (ol)	Forsterite (fo)	$Mg_2Si\,O_4$	−2055 (2)	43.60	128 (2)	4.2 (2)	809 (1)	0.99 (3)	2.1 (2)	82 (2)	1.5 (1)	2.3 (1)	1,10,12–14
olivine	Fayalite (fa)	$Fe_2Si\,O_4$	−1371 (1)	46.29	135 (2)	4.2 (10)	619 (2)	1.06 (7)	3.6 (10)	51 (2)	*1.5* (5)	1.0 (6)	1,2,6,10,13,15,16
wadsleyite (wa)	Mg-Wadsleyite (mgwa)	$Mg_2Si\,O_4$	−2028 (2)	40.52	169 (3)	4.3 (2)	844 (7)	1.21 (9)	2.0 (10)	112 (2)	1.4 (2)	2.6 (4)	1,6,17-20
wadsleyite	Fe-Wadsleyite (fewa)	$Fe_2Si\,O_4$	−1365 (7)	42.80	169 (13)	*4.3* (10)	665 (21)	*1.21* (30)	*2.0* (10)	72 (12)	*1.4* (5)	*1.0* (10)	17,21
ringwoodite (ri)	Mg-Ringwoodite (mgri)	$Mg_2Si\,O_4$	−2017 (2)	39.49	185 (2)	4.2 (2)	878 (8)	1.11 (10)	2.4 (4)	123 (2)	1.4 (1)	2.3 (5)	1,6,22–24
ringwoodite	Fe-Ringwoodite (feri)	$Fe_2Si\,O_4$	−1363 (2)	41.86	213 (7)	*4.2* (10)	679 (8)	1.27 (23)	*2.4* (10)	92 (10)	*1.4* (5)	*1.8* (10)	22,25,26
orthopyroxene (opx)	Enstatite (en)	$Mg\,Mg\,Si_2O_6$	−2913 (2)	62.68	107 (2)	7.0 (4)	812 (4)	0.78 (4)	3.4 (4)	77 (1)	1.5 (1)	2.5 (1)	1,27–32
orthopyroxene	Ferrosilite (fs)	$Fe\,Fe\,Si_2O_6$	−2226 (4)	65.94	101 (4)	7.0 (5)	674 (10)	0.72 (8)	*3.4* (10)	52 (5)	*1.5* (5)	*1.1* (10)	1,2,27,33,34
orthopyroxene	Mg-Tschermaks (mgts)	$Mg\,Al\,[Si\,Al]\,O_6$	−3003 (9)	59.14	*107* (10)	*7.0* (10)	784 (24)	*0.78* (30)	*3.4* (10)	*97* (10)	*1.5* (5)	*2.5* (10)	35
orthopyroxene	Ortho-Diopside (odi)	$Ca\,Mg\,Si_2O_6$	−3016 (3)	68.05	*107* (10)	*7.0* (10)	745 (9)	*0.78* (30)	*3.4* (10)	*60* (10)	*1.5* (5)	*1.4* (10)	36
clinopyroxene (cpx)	Diopside (di)	$Ca\,Mg\,Si_2O_6$	−3030 (2)	66.04	112 (5)	5.2 (18)	782 (3)	0.96 (5)	1.5 (20)	67 (2)	*1.4* (5)	*1.6* (10)	1,2,6,13,37,38
clinopyroxene	Hedenbergite (he)	$Ca\,Fe\,Si_2O_6$	−2677 (45)	67.87	119 (4)	5.2 (10)	702 (2)	0.94 (6)	*1.5* (10)	61 (1)	*1.2* (5)	*1.6* (10)	1,6,13,16,39
clinopyroxene	Clinoenstatite (cen)	$Mg\,Mg\,Si_2O_6$	−2906 (3)	62.50	*112* (10)	*5.2* (10)	805 (10)	*0.96* (30)	*1.5* (10)	*81* (10)	*1.7* (5)	*1.7* (10)	36
clinopyroxene	Ca-Tschermaks (cats)	$Ca\,Al\,(Si\,Al)O_6$	−3120 (5)	63.57	*112* (10)	*5.2* (10)	804 (5)	0.78 (0)	*1.5* (10)	*76* (10)	*1.6* (5)	*2.0* (10)	40,41
clinopyroxene	Jadeite (jd)	$Na\,Al\,Si_2O_6$	−2855 (3)	60.51	142 (2)	*5.2* (10)	821 (12)	0.90 (8)	0.4 (14)	85 (2)	*1.4* (5)	*2.2* (10)	1,6,42–44
HP-clinopyroxene (hpcpx)	HP-Clinoenstatite (hpcen)	$Mg_2Si_2O_6$	−2905 (3)	60.76	116 (1)	6.2 (3)	824 (7)	1.12 (5)	0.2 (5)	88 (1)	1.8 (1)	2.1 (5)	45
HP-clinopyroxene	HP-Clinoferrosilite (hpcfs)	$Fe_2Si_2O_6$	−2222 (4)	63.85	*116* (10)	*6.2* (10)	692 (11)	*1.12* (30)	*0.2* (10)	*71* (10)	*1.8* (5)	*0.8* (10)	46
Ca-perovskite (cpv)	Ca-Perovskite (capv)	$Ca\,Si\,O_3$	−1463 (8)	27.45	236 (4)	3.9 (2)	796 (44)	1.89 (7)	0.9 (16)	157 (12)	2.2 (5)	*1.3* (10)	1,47-49
akimotoite (ak)	Mg-Akimotoite (mgak)	$Mg\,Si\,O_3$	−1410 (2)	26.35	211 (4)	5.6 (8)	934 (12)	1.19 (13)	2.3 (8)	132 (8)	1.6 (5)	*2.8* (10)	1,2,6,50,51
akimotoite	Fe-Akimotoite (feak)	$Fe\,Si\,O_3$	−1068 (21)	26.85	*211* (10)	*5.6* (10)	888 (120)	*1.19* (30)	*2.3* (10)	*150* (10)	*1.6* (5)	*3.5* (10)	52
akimotoite	Corundum (co)	$Al\,Al\,O_3$	−1582 (1)	25.58	253 (5)	4.3 (2)	933 (3)	1.32 (4)	1.3 (2)	163 (2)	1.6 (1)	2.8 (2)	1,6,10,13,53
garnet (gt,mj)	Pyrope (py)	$Mg_3Al\,Al\,Si_3O_{12}$	−5936 (10)	113.08	170 (2)	4.1 (3)	823 (4)	1.01 (6)	1.4 (5)	94 (2)	1.4 (2)	1.0 (3)	1,13,54–56
garnet	Almandine (al)	$Fe_3Al\,Al\,Si_3O_{12}$	−4935 (29)	115.43	174 (2)	4.9 (2)	741 (5)	1.06 (6)	*1.4* (10)	96 (1)	1.4 (1)	*2.1* (10)	1,13,55,57
garnet	Grossular (gr)	$Ca_3Al\,Al\,Si_3O_{12}$	−6278 (11)	125.12	167 (1)	3.9 (2)	823 (2)	1.05 (6)	1.9 (2)	109 (4)	1.2 (1)	2.4 (1)	1,10,29,55,57,58
garnet	Mg-Majorite (mgmj)	$Mg_3Mg\,Si\,Si_3O_{12}$	−5691 (10)	114.32	165 (3)	4.2 (3)	822 (4)	0.98 (7)	1.5 (5)	85 (2)	1.4 (2)	1.0 (3)	1,13,23,56,59,60
garnet	Jd-Majorite (jdmj)	$(Na_2Al)Al\,Si\,Si_3O_{12}$	−5519 (14)	110.94	177 (7)	*4.1* (10)	896 (18)	*1.01* (30)	*1.4* (10)	125 (4)	*1.4* (5)	*3.3* (10)	61
quartz (qtz)	Quartz (qtz)	$Si\,O_2$	−859 (1)	23.67	50 (1)	4.3 (1)	816 (31)	*0.00* (5)	*1.0* (10)	45 (1)	1.0 (1)	*2.4* (10)	1,6,62–64
coesite (coes)	Coesite (coes)	$Si\,O_2$	−855 (1)	20.66	114 (1)	*4.0* (10)	857 (9)	0.39 (5)	*1.0* (10)	62 (1)	*1.2* (5)	*2.4* (10)	1,6,65
stishovite (st)	Stishovite (st)	$Si\,O_2$	−819 (1)	14.02	314 (8)	3.8 (1)	1108 (13)	1.37 (17)	2.8 (22)	220 (12)	1.9 (1)	*4.6* (10)	1,6,66–68
seifertite (seif)	Seifertite (seif)	$Si\,O_2$	−794 (2)	13.67	328 (2)	4.0 (1)	1141 (16)	*1.37* (30)	*2.8* (10)	227 (2)	1.8 (1)	*5.0* (10)	36,67
perovskite (pv)	Mg-Perovskite (mgpv)	$Mg\,Si\,O_3$	−1368 (1)	24.45	251 (3)	4.1 (1)	905 (5)	1.57 (5)	1.1 (3)	173 (2)	1.7 (0)	2.6 (3)	1,69-74
perovskite	Fe-Perovskite (fepv)	$Fe\,Si\,O_3$	−1041 (6)	25.49	272 (40)	*4.1* (10)	871 (26)	*1.57* (30)	*1.1* (10)	133 (40)	1.4 (0)	*2.3* (10)	52,75,76
perovskite	Rh_2O_3-II (rh2o3)	$Al\,Al\,O_3$	−1534 (2)	24.94	258 (10)	4.1 (5)	886 (7)	*1.57* (30)	*1.1* (10)	171 (10)	1.5 (1)	2.5 (5)	77–79
post-perovskite (ppv)	Mg-Post-Perovskite (mppv)	$Mg\,Si\,O_3$	−1348 (3)	24.42	231 (1)	4.0 (1)	855 (7)	1.89 (3)	1.1 (1)	150 (4)	2.0 (1)	1.2 (2)	80-82
post-perovskite	Fe-Post-Perovskite (fppv)	$Fe\,Si\,O_3$	−982 (21)	25.46	*231* (10)	*4.0* (10)	782 (52)	*1.89* (30)	*1.1* (10)	129 (5)	1.4 (1)	*1.4* (10)	83,84
post-perovskite	Al-Post-Perovskite (appv)	$Al\,Al\,O_3$	−1378 (4)	23.85	249 (20)	4.0 (1)	762 (9)	1.65 (2)	*1.1* (10)	92 (10)	1.8 (1)	2.8 (2)	79,85,86
magnesiowüstite (mw)	Periclase (pe)	$Mg\,O$	−569	11.24	161 (3)	3.8 (2)	767 (9)	1.36 (5)	1.7 (2)	131 (1)	2.1 (1)	2.8 (2)	1,9,10,13,54,87,88
magnesiowüstite	Wüstite (wu)	$Fe\,O$	−242 (1)	12.26	179 (1)	4.9 (2)	454 (21)	1.53 (13)	*1.7* (10)	59 (1)	1.4 (1)	*−0.1* (10)	6,13,89–92
Ca-ferrite (cf)	Mg-Ca-Ferrite (mgcf)	$Mg\,Al\,Al\,O_4$	−2122 (4)	36.18	211 (1)	4.1 (1)	838 (16)	*1.31* (30)	*1.0* (10)	130 (1)	1.8 (1)	*2.1* (10)	93,94
Ca-ferrite	Fe-Ca-Ferrite (fecf)	$Fe\,Al\,Al\,O_4$	−1790 (25)	37.26	*211* (10)	*4.1* (10)	804 (69)	*1.31* (30)	*1.0* (10)	*152* (10)	*1.8* (5)	*3.0* (10)	36
Ca-ferrite	Na-Ca-Ferrite (nacf)	$Na\,Al\,Si\,O_4$	−1851 (11)	36.27	158 (1)	4.3 (1)	812 (51)	*1.17* (30)	*1.0* (10)	121 (1)	2.1 (1)	*1.6* (10)	94,95
kyanite (ky)	Kyanite (ky)	$Al_2Si\,O_5$	−2446 (4)	44.23	160 (1)	4.0 (0)	943 (8)	0.93 (7)	*1.0* (10)	*121* (10)	*1.7* (5)	*3.0* (10)	1,96–98
nepheline (neph)	Nepheline (neph)	$Na\,Al\,Si\,O_4$	−1993 (3)	54.67	53 (1)	*4.0* (10)	701 (13)	0.69 (3)	*1.0* (10)	31 (1)	*1.3* (5)	*0.6* (10)	2,13,100,101

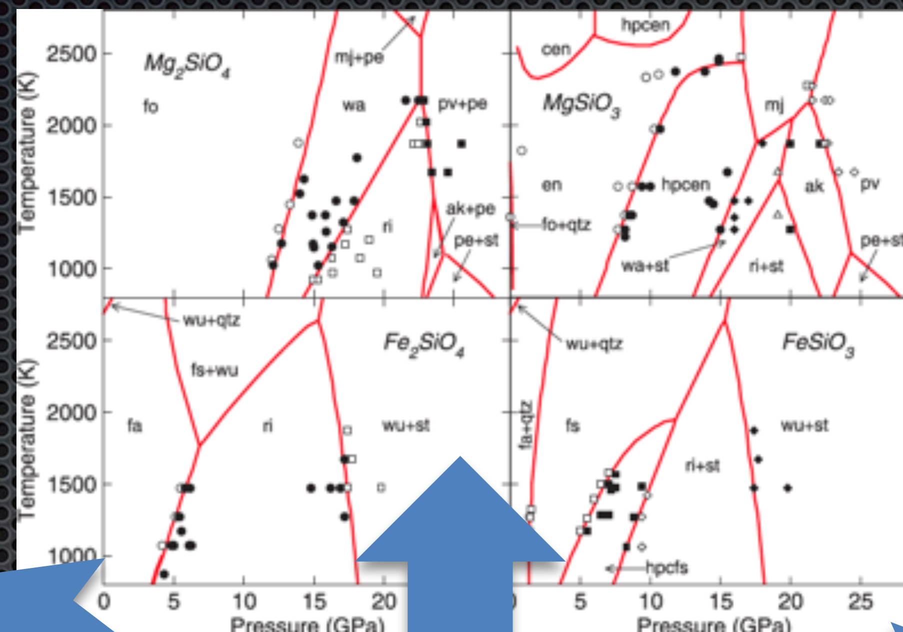
[*Stixrude & Lithgow-Bertelloni*, 2011]

Stixrude & Lithgow-Bertelloni (2005 JGR; 2005 GJI; 2011 GJI)

HeFESTo

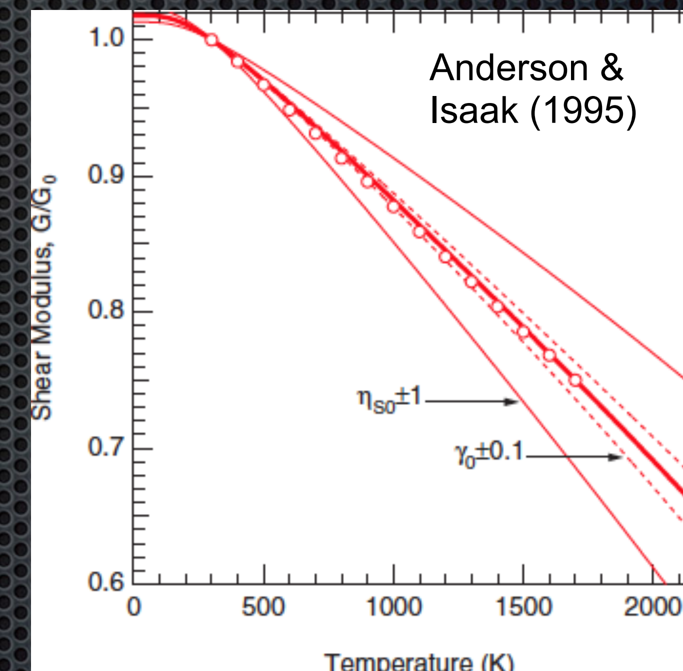


Sen (1985); Irifune et al. (1986); Irifune (1987, 1994); Klemme & O'Neill (2000)

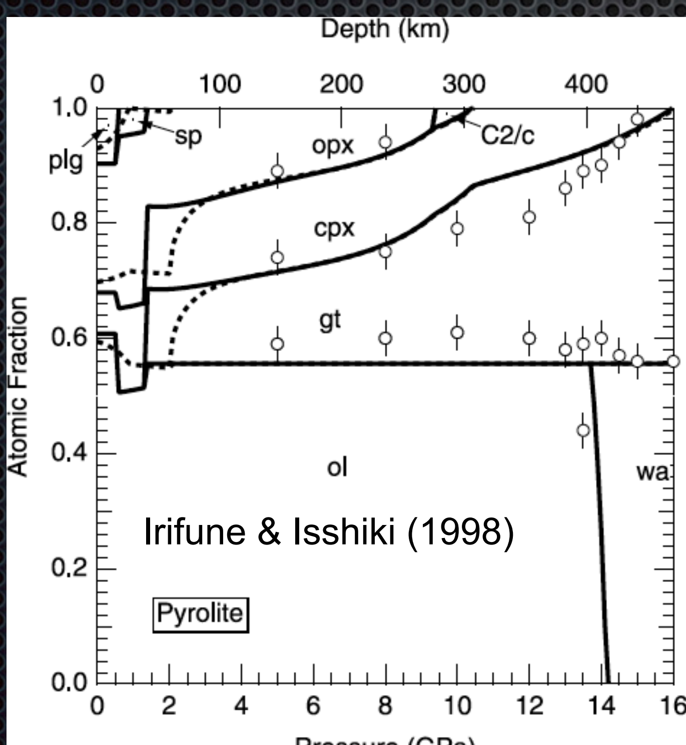


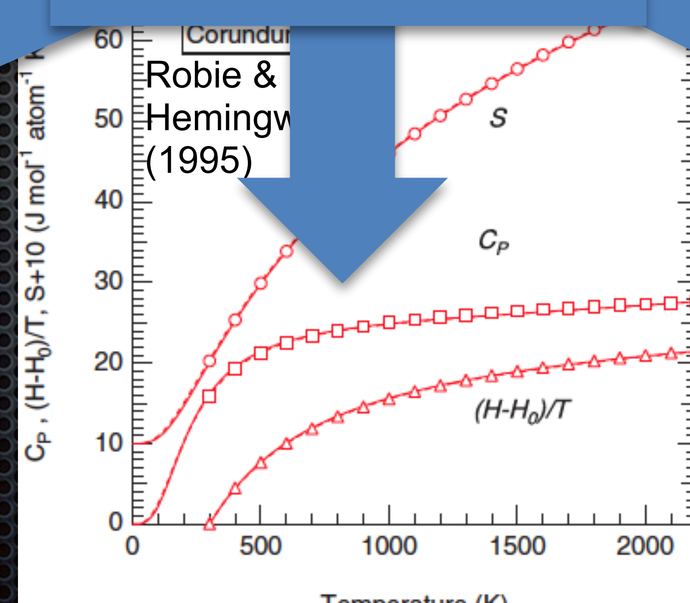
Morishim… Ghose (19… et al. (1998… Angel (199… et al. (1998…

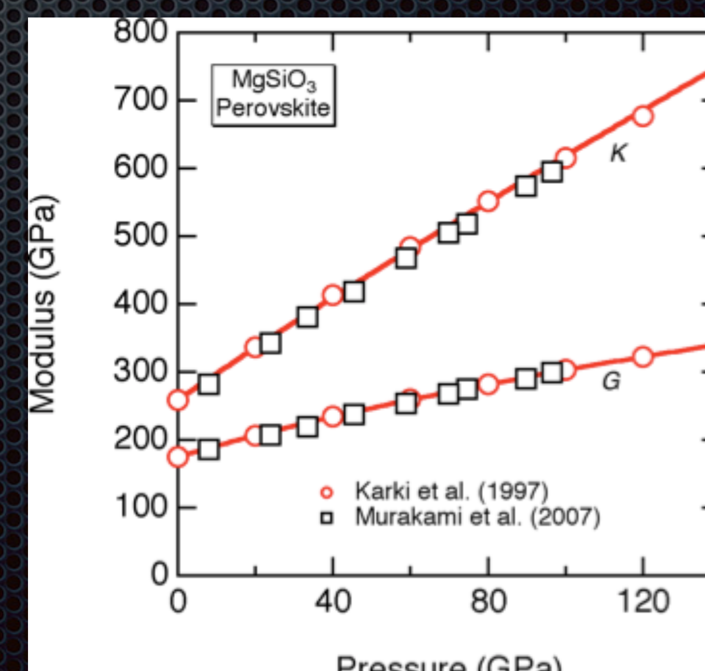
…& …resnall …Woodland & …0); Katsura



$$F\left(E_{ij}, T, \vec{n}\right)$$

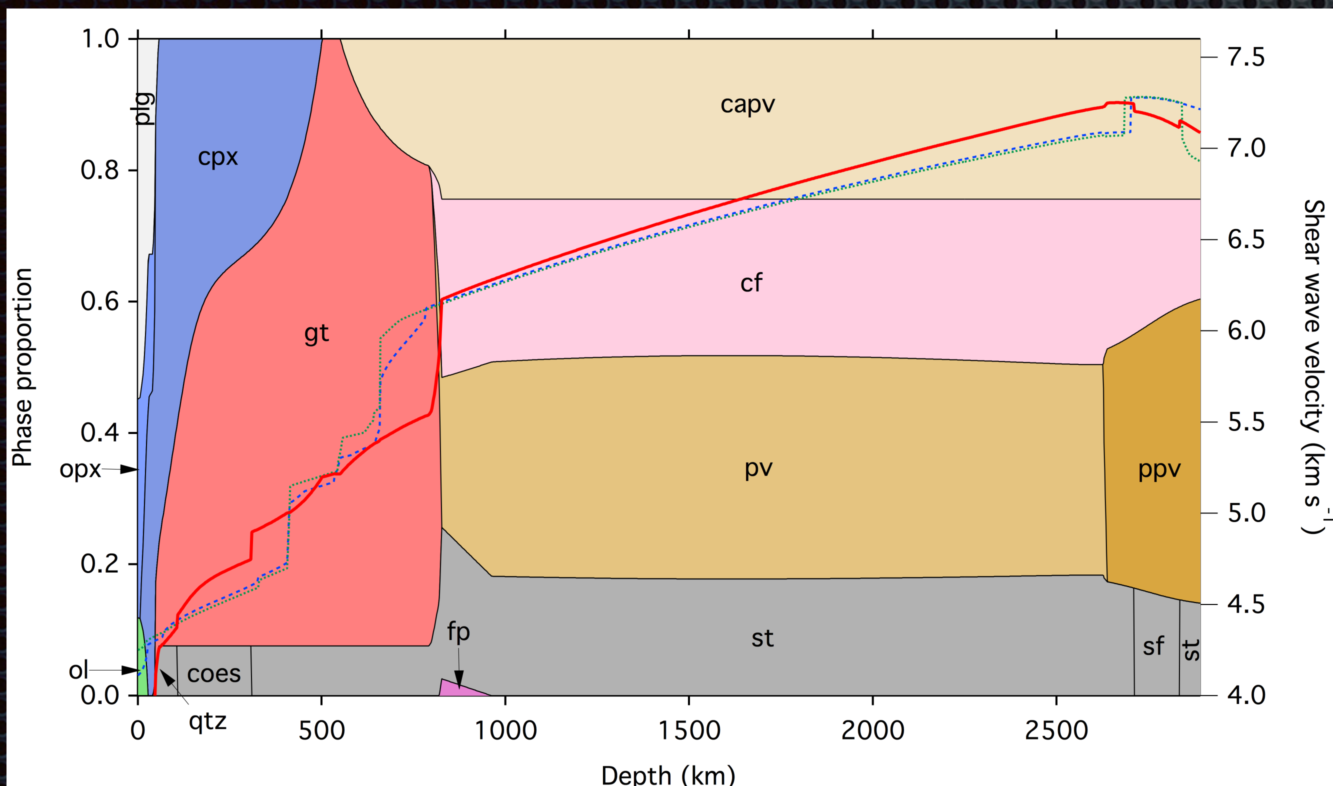




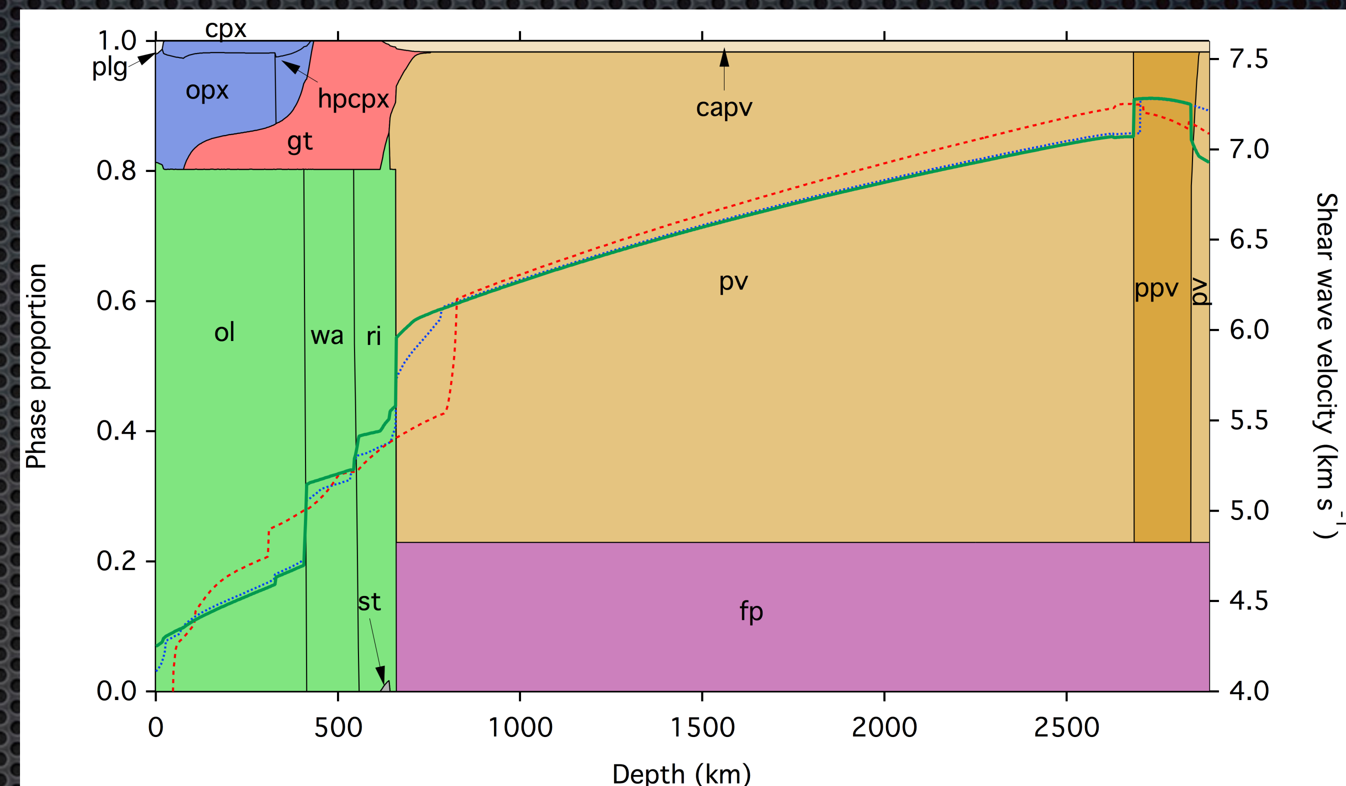


Multiphase Mantle

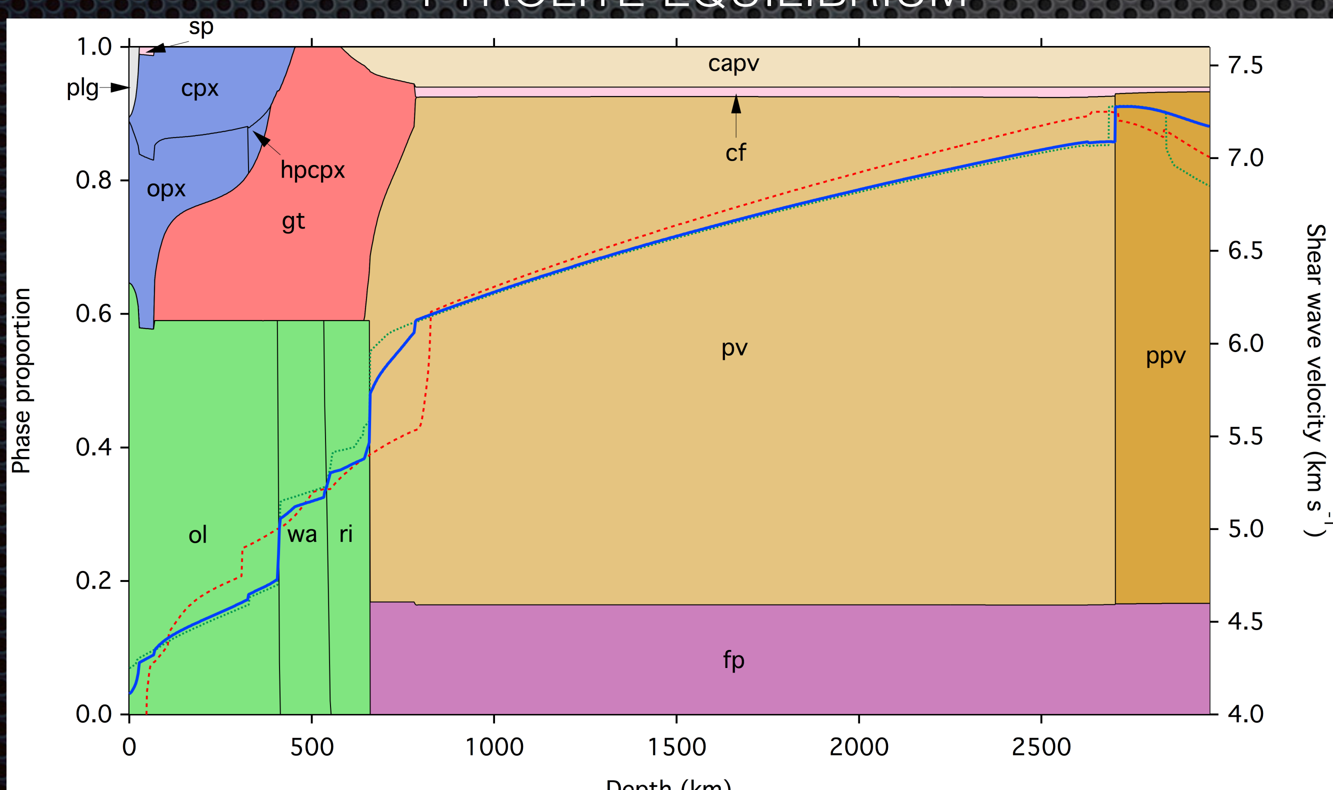
BASALT



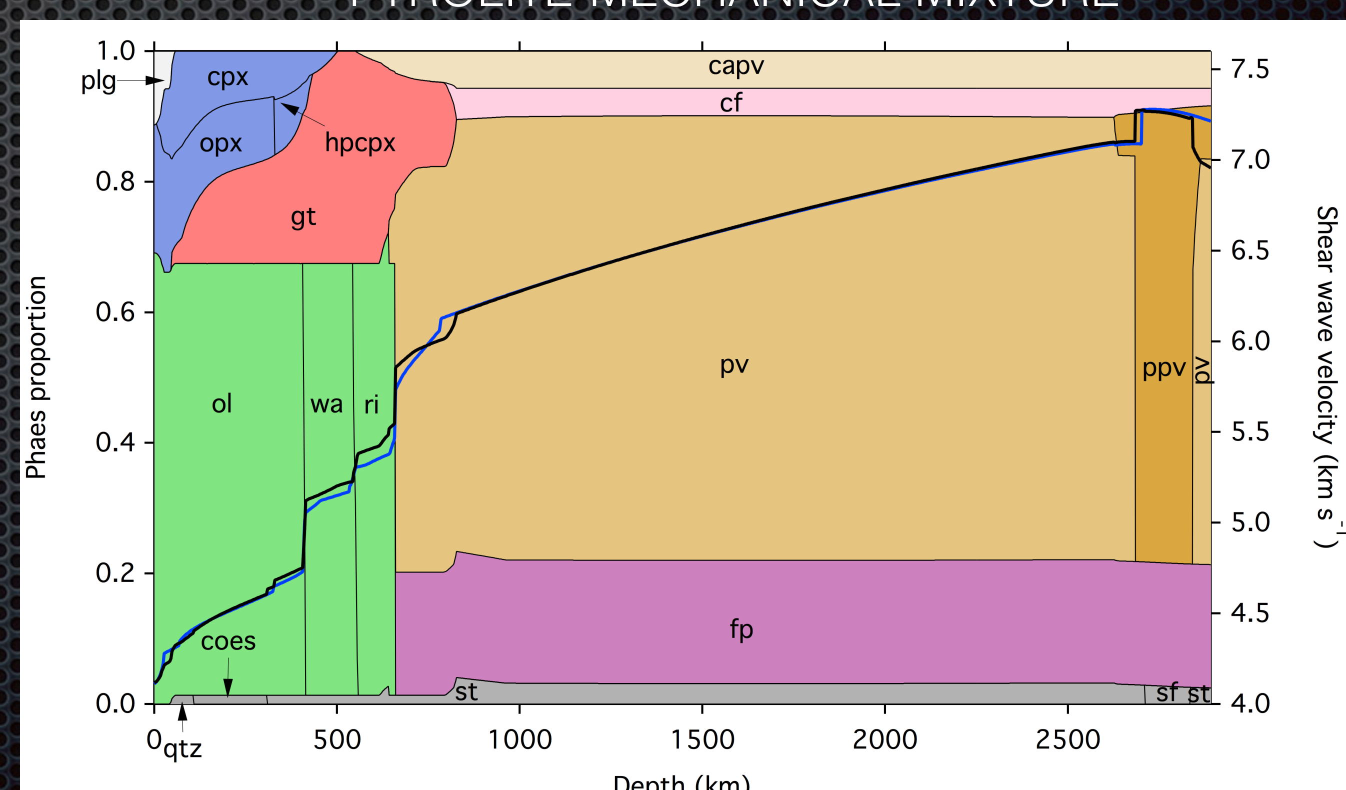
HARZBURGITE



PYROLITE-EQUILIBRIUM



PYROLITE-MECHANICAL MIXTURE



[*Stixrude and Lithgow-Bertelloni*, 2012]

HeFESTo

GitHub

(https://github.com/stixrude/HeFESToRepository).

Perple_X

BurnMan

Thermal expansivity

$$G(P,T,n_i) = \sum_{i=1}^{species} n_i \mu_i$$

$$V = \left(\frac{\partial G}{\partial P}\right)_{T,n_i} = \sum_{i=1}^{species} n_i \left(\frac{\partial \mu_i}{\partial P}\right)_{T,n_i} \equiv \sum_{i=1}^{species} n_i V_i$$

Metamorphic

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P = \frac{1}{V}\sum_{i=1}^{species} n_i \left(\frac{\partial V_i}{\partial T}\right)_P + \left(\frac{\partial n_i}{\partial T}\right)_P V_i$$

Isomorphic

[*Stixrude & Lithgow-Bertelloni* , 2007] EPSL

Thermal expansivity

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P = \frac{1}{V}\sum_{i=1}^{species} n_i\left(\frac{\partial V_i}{\partial T}\right)_P + \left(\frac{\partial n_i}{\partial T}\right)_P V_i$$

$$\left(\frac{\partial n_i}{\partial T}\right)_P = \sum_{j=1}^{species}\left(\frac{\partial n_i}{\partial \mu_j}\right)_P\left(\frac{\partial \mu_j}{\partial T}\right)_P = \sum_{j=1}^{species} H_{ij}^{-1}\left(\frac{\partial \mu_j}{\partial T}\right)_P$$

$$H_{ij} = \left(\frac{\partial^2 G}{\partial n_i \partial n_j}\right)_{P,T}$$

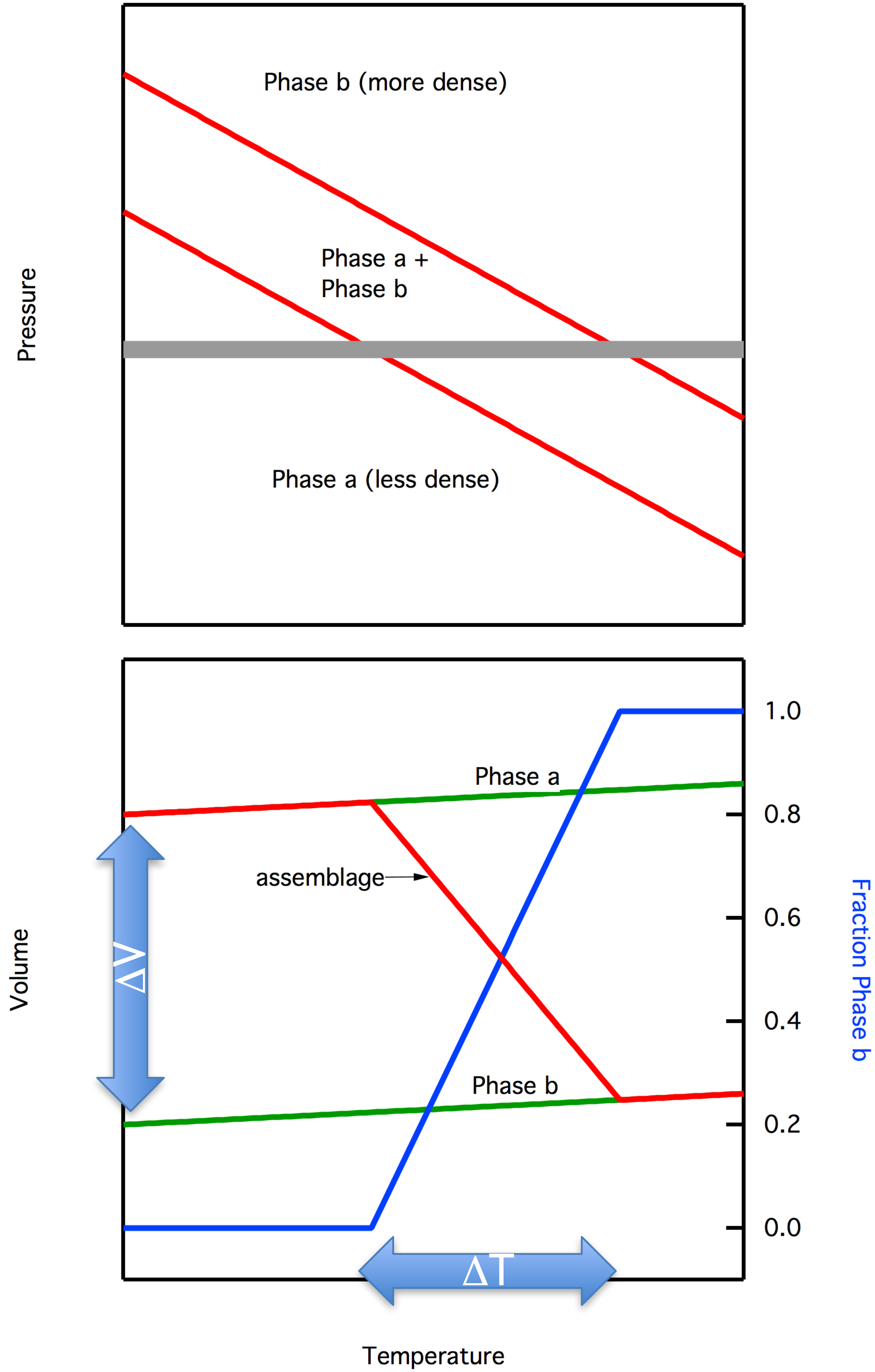
Schematic

Fractional volume
(density)
contrast

$$\alpha \approx \frac{1}{V}\frac{\Delta V}{\Delta T} = \Gamma \frac{\left|\Delta \ln V\right|}{\Delta P}$$

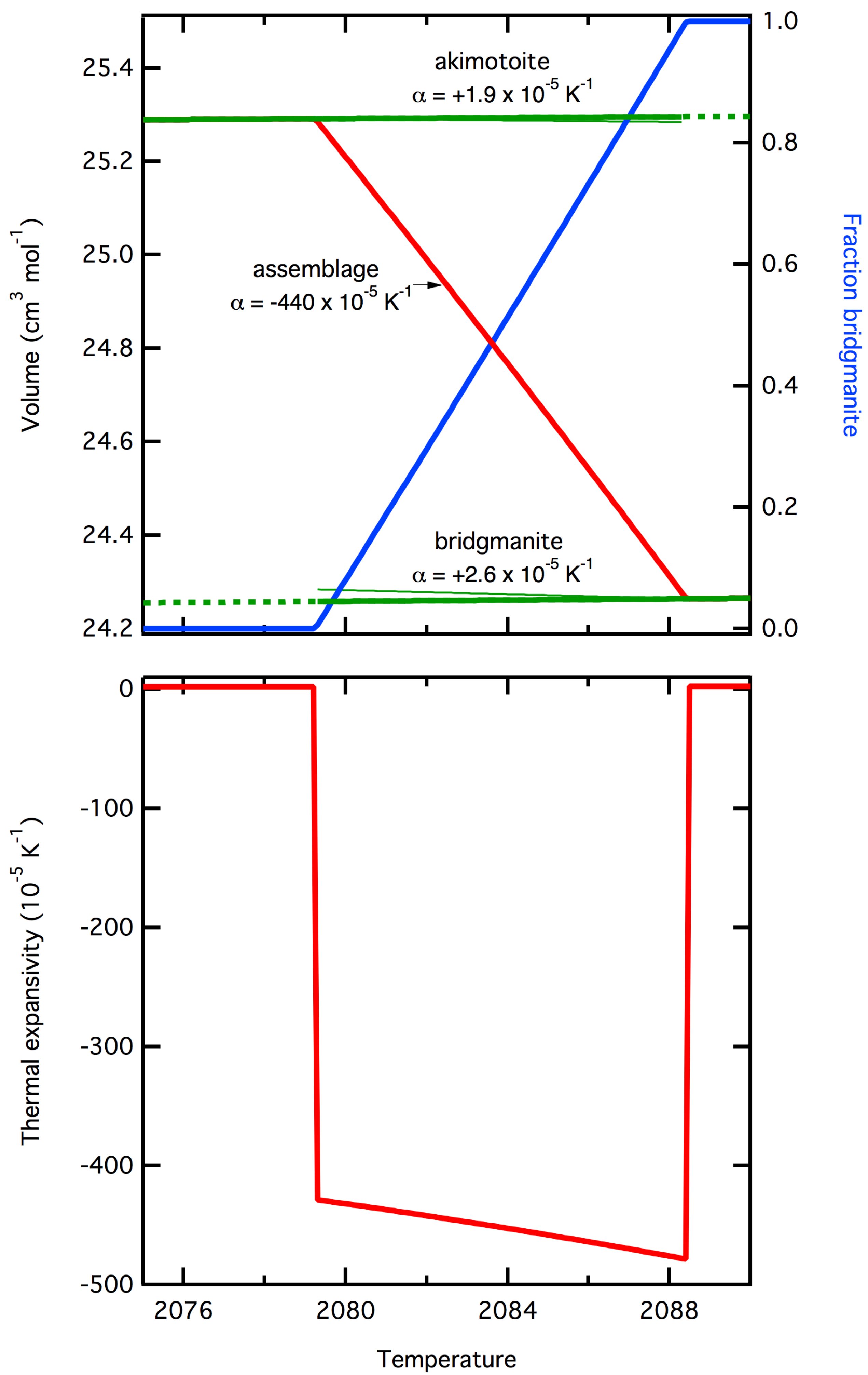
Clapeyron
slope

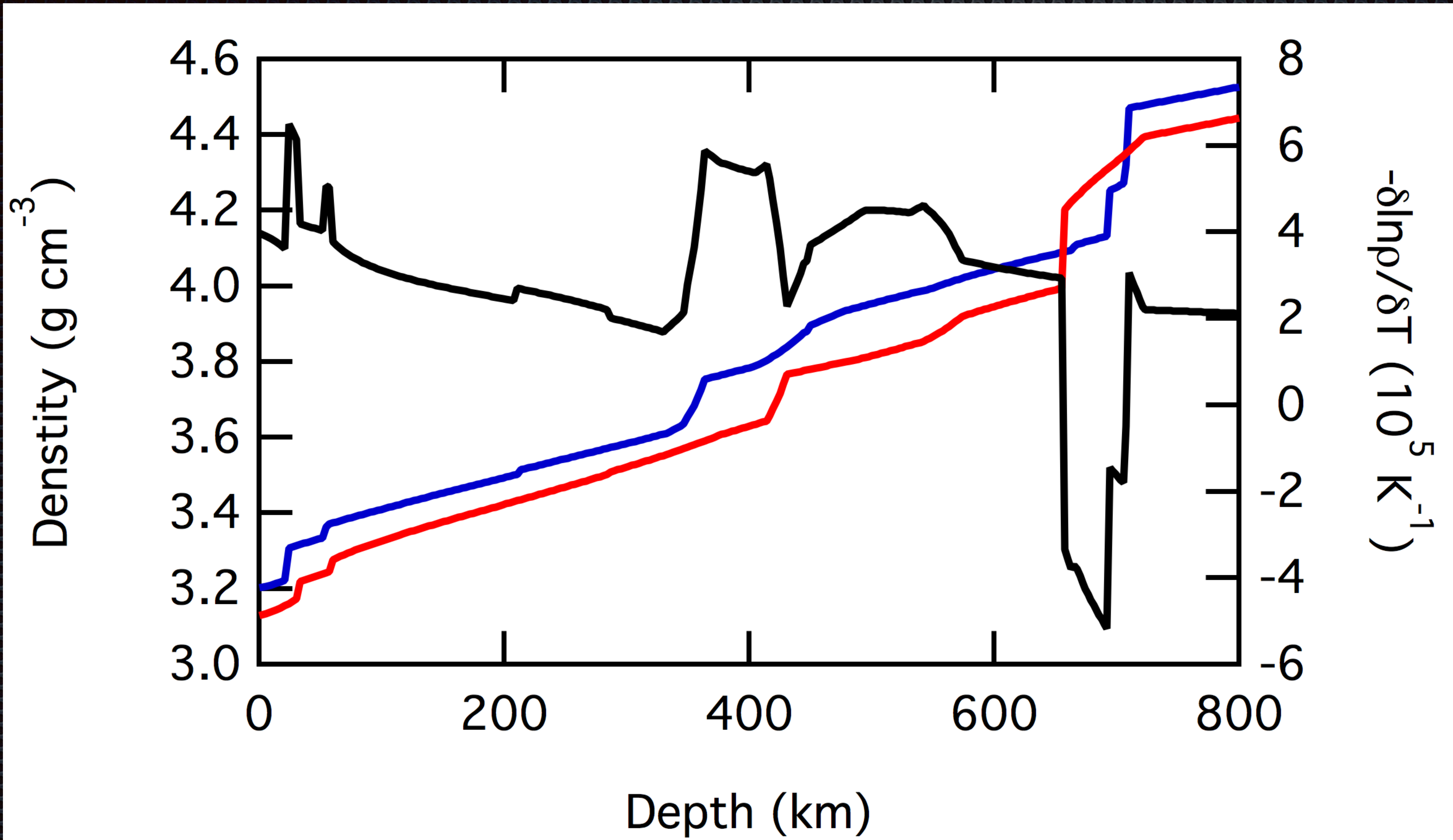
Width of
transition



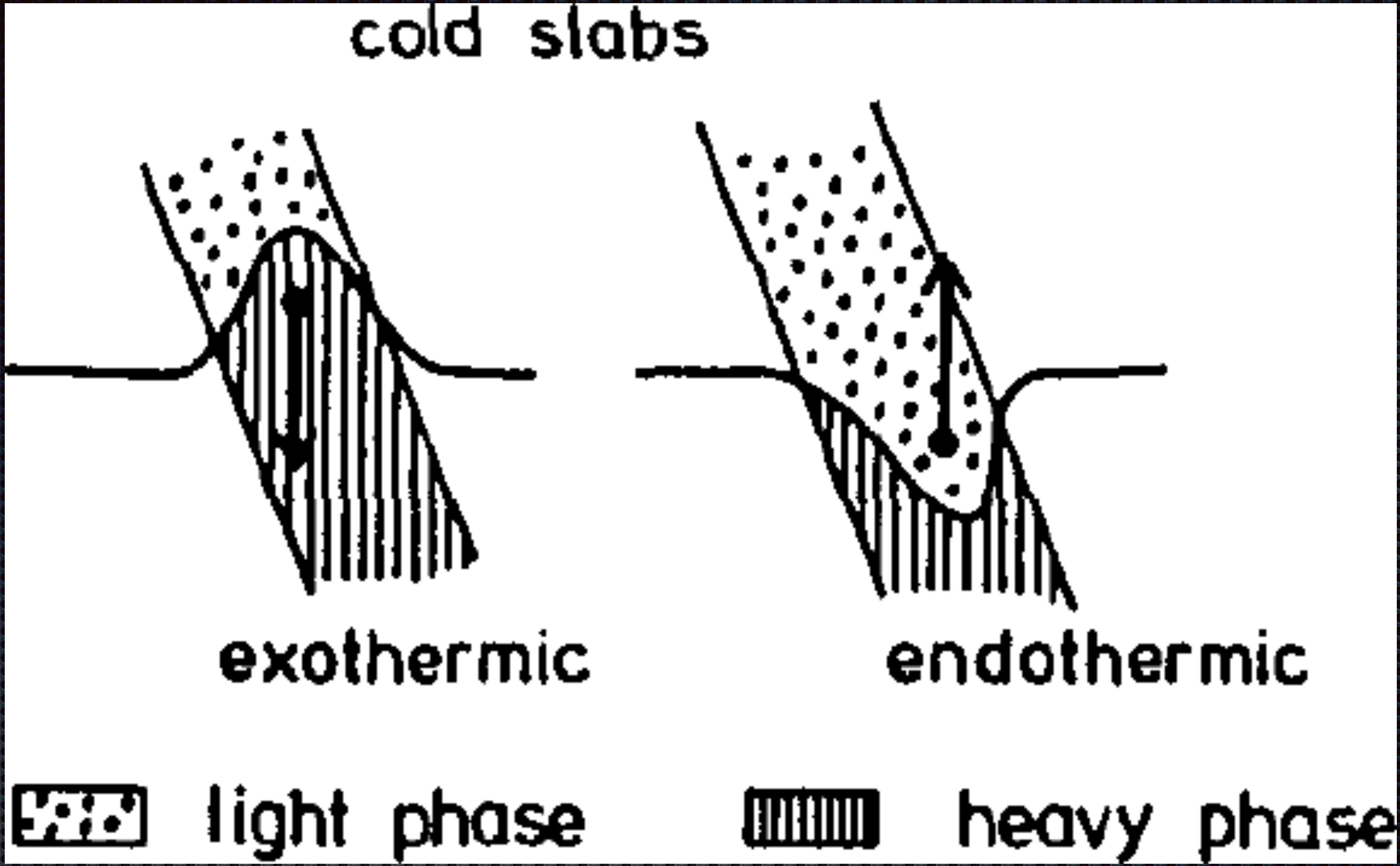
HeFESTo

Super-colossal negative thermal expansivity?



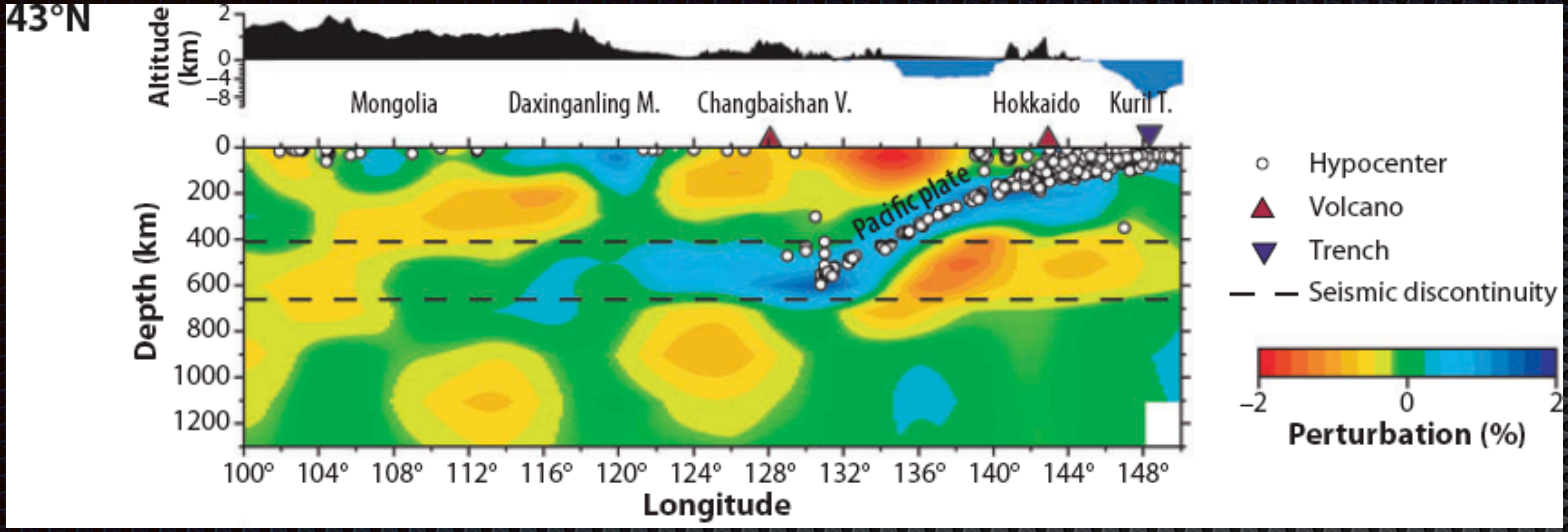


[*Stixrude & Lithgow-Bertelloni*, 2007]

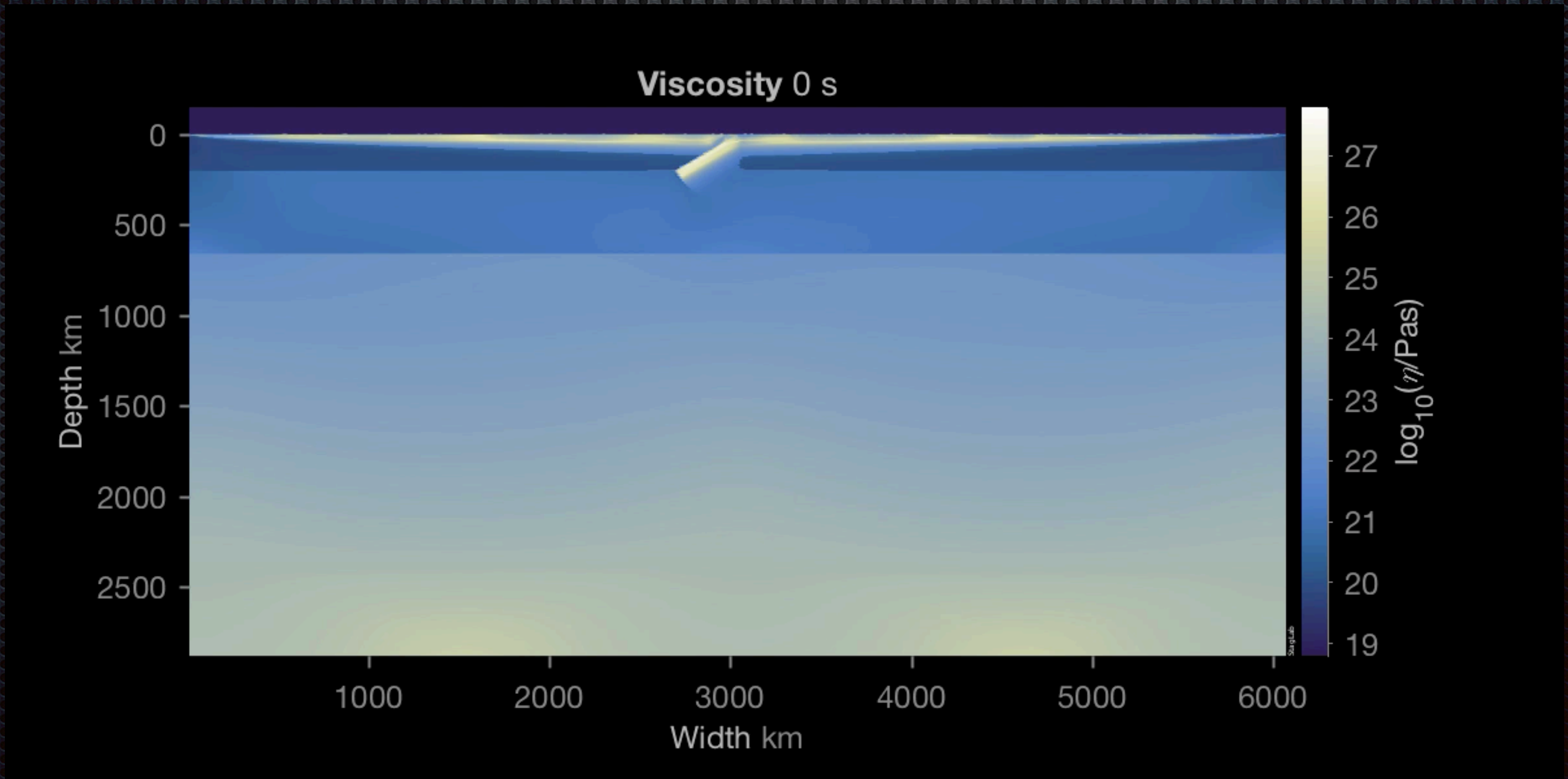


$$\left(\frac{\partial \ln\rho}{\partial x}\right)_P = \left(\frac{\partial \ln\rho}{\partial T}\right)_P \left(\frac{\partial T}{\partial x}\right)_P = -\alpha\left(\frac{\partial T}{\partial x}\right)_P$$

[*Christensen*, 2005] *AREPS*

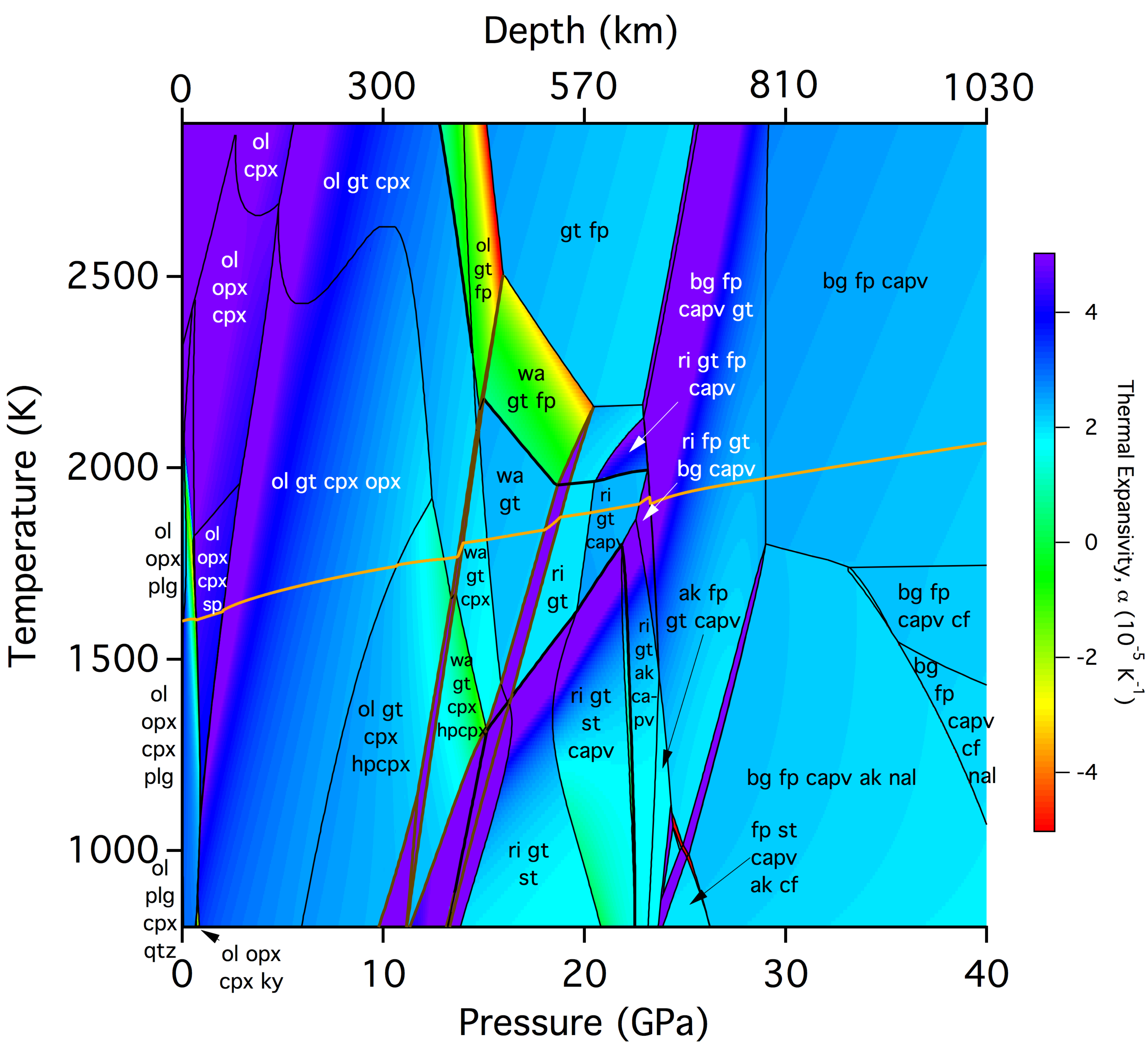


Fukao (2009) AREPS



Thermal Expansivity

[THIS PHASE DIAGRAM IS UNPUBLISHED DO NOT USE!]



Some Conclusions

Negative thermal expansion appears in heterogeneous systems

May be super-colossal

Tends to stabilize the mantle against convection