Lithosphere-upper mantle thermochemical modelling at global and regional scale



Lithosphere-upper mantle thermochemical structure: why bother?

✓ Mantle flow informing plate tectonics: density+ viscosity

✓ What supports the Earth's surface topography?

✓ Cooling of oceanic lithosphere: half-space vs plate model?

✓ Mid Oceanic Ridges: composition, temperature, spreading rate

✓ Mantle plumes: temperature and composition

✓ Stability of cratonic continental lithosphere

> Many techniques/observations, just ONE Earth...



Rock properties ->non linear functions of thermochemical structure...!



Why integrated modelling...?

A fundamental upper mantle discontinuity for plate tectonics: the lithosphereasthenosphere boundary (LAB) can be defined as **thermal, mechanical and chemical boundary.**

According to the property we focus on (e.g., **temperature, composition, Vs, Vp, anisotropy, electrical conductivity...**) there are many possible "LABs" (e.g. Eaton 2009):



Earth structure: what can we know?



What is the nature of the heterogeneity "observed" in the mantle?

Geophysical point of view



Shen et al., 2013, JGR

What is the nature of the heterogeneity "observed" in the mantle?

Petrological point of view



In mantle xenoliths

In outcrops



Courtesy of GEMOC

What is the nature of the heterogeneity "observed" in the mantle?

O

50 m

1) Av.

Representativeness of observed mantle samples (xenoliths, peridotite massifs etc..) on the lithospheric Forward modeling harzburgite foliation dip > 40° Iherzolite with websteritic layering breccias foliation in harzburgites Carbonate rocks foliation section localization in Iherzolites Depleted Depleted +metasomatised 2) Av. 6) Av. Middle 3) Av. 4) Av. 5) Av. UEVO Uarz La UI CO Occer floor Atlas (wt%)e

Geophysical data

	Harz.	HEXO	Harz. La	HLCO	Ocean floor	Atlas (wt%) ^e
	Lanzarote (wt%) ^a	Tenerife (wt%) ^b	Palma av. (wt%) ^c	Tenerife (wt%) ^b	peridot. (wt%) ^d	
SiO ₂	43.78	43.32	43.07	42.14	45.09	43.48
Al ₂ O ₃	0.7	0.61	0.53	0.73	2.33	2.38
FeO	7.79	8.04	8.43	8.8	8.4	8
MgO	46.1	45.31	45.19	44.14	41.23	42.6
CaO	0.6	0.81	0.68	1.68	1.32	2.83
Na ₂ O	0.1	0.14	0.17	0.18	0.23	0.24
Mg#	91.34	90.96	90.53	89.94	89.7	90.47

Mantle Depletion (partial melting)

scale

Mantle metasomatism (refertilization)

Mantle Geotherm: thermal lithosphere-asthenosphere boundary

Heat transport equation:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + H - \rho c_p \vec{u} \cdot \nabla T$$

Lithosphere: conductive mantle

Steady-state conduction equation: dT/dt=0and $U=0 \rightarrow Diffusion PDE$

 $\nabla \cdot [k(\vec{x}, T, P) \nabla T(\vec{x})] = -H(\vec{x})$





Sub-Lithosphere: mantle convection

Convection in the mantle (i.e. no heat interexchange with the surroundings). Fast heat transport mechanism compared to conduction

$$\left(\frac{\partial T}{\partial r}\right)_{S} = \frac{T\alpha g}{c_{P}}$$

Adiabatic gradient: typically 0.4-0.5 K/km in the uppermost mantle

Thermal field

✓ Mantle thermal conductivity dependent on T, P and C (numerical iteration)



- Sublithospheric geotherm: adiabatic gradient (usually 0.4-0.5 K/km) and potential temperature
- ✓ T@410 km =1520 -1600 ºC (Katsura 2022)

Surface heat Flow and lithospheric thickness



Isostasy

 Lithospheric isostasy: (absolute) elevation as a measure of the bouyancy of the lithosphere



$$\int_{LC} \Delta \rho(z) dz = 0$$

$$E = \frac{\rho_a - \rho_L}{\rho_a} \cdot L - L_0 \quad (E > 0)$$

$$E = \frac{\rho_a}{\rho_a - \rho_w} \cdot \left(\frac{\rho_a - \rho_L}{\rho_a} \cdot L - L_0\right) \quad (E < 0)$$

$$(E + z_0) + (z_0 - z_0) + (z_0 - z_0) = 0$$

$$\rho_{\rm L} = \frac{(E + z_{\rm c})\rho_{\rm c} + (z_{\rm L} - z_{\rm c})\rho_{\rm m}}{(E + z_{\rm L})}$$

(e.g. Lachenbruch & Morgan 1990)

Lithospheric mantle able to hold density contrasts over geological time scales...

Local isostasy: average density of the lithosphere

Linear mantle density models (pressure effect neglected):

$$\rho_m(z) = \rho_a(1 + \alpha[T_a - T_m(z)])$$

 $\rho_m(z) = \rho_0(1 - \alpha[T_m(z)])$

Ta Lithosphere-asthenosphere boundary temperature (1200-1315 C typically), α thermal expansion coefficient, ρ_a asthenospheric density (typically 3200 kg/m3), ρ_0 mantle density at the surface (T=0)



Local isostasy: average density of the lithosphere



$$\int_{LC} \Delta \rho(z) dz = 0$$

$$E = \frac{\rho_a - \rho_L}{\rho_a} \cdot L - L_0 \quad (E > 0)$$
$$E = \frac{\rho_a}{\rho_a - \rho_w} \cdot \left(\frac{\rho_a - \rho_L}{\rho_a} \cdot L - L_0\right) \quad (E < 0)$$

$$\rho_{\rm L} = \frac{(E + z_{\rm c})\rho_{\rm c} + (z_{\rm L} - z_{\rm c})\rho_{\rm m}}{(E + z_{\rm L})}$$



Classical formulation of lithospheric isostasy (Lachenbruch & Morgan, 1990).

Includes variations in crustal and lithospheric thickness as well as crustal and mantle density.

A Mid Oceanic Ridge (MOR) is taken as the reference column (Lo)

Local isostasy: average density of the lithosphere



In terms of pressure, P, at the compensation level (CL), for an arbitrary reference column with E=0:

$$P_{ref} = \int_0^{z_{cREF}} \rho_c dz + \int_{z_{cREF}}^{z_{LREF}} \rho_m(z) dz + \int_{z_{LREF}}^{CL} \rho_{msub}(z) dz$$

For any other column at the CL the pressure must be the same. If the average lithospheric density is < reference lithospheric density the topography compensates the pressure deficit:

$$P_{c} = \int_{0}^{z_{c}} \rho_{c} dz + \int_{z_{c}}^{z_{L}} \rho_{m}(z) dz + \int_{z_{L}}^{CL} \rho_{msub}(z) dz + \int_{0}^{h_{cont}} \rho_{c} dz = P_{ref}$$

If the average lithospheric density is > reference lithospheric density the bathymetry compensates the pressure excess:

$$P_{c} = \int_{0}^{z_{c}} \rho_{c} dz + \int_{z_{c}}^{z_{L}} \rho_{m}(z) dz + \int_{z_{L}}^{CL} \rho_{msub}(z) dz + \int_{0}^{h_{bathy}} (\rho_{w} - \rho_{c}) dz = P_{ref}$$



Mantle density-pressure coupling

The lithostatic pressure, P, at any depth depends on the weight of the lithospheric column above:

 $P = \rho g z$

...

But in general $\rho = \rho(P)$, this coupling is solved numerically in a iterative scheme:

$$P_0(z) = P(z - \Delta z) + \rho(z - \Delta z)g\Delta z$$

$$\rho(z) = F(P_0(z)); \ \overline{\rho_1} = \frac{\rho(z) + \rho(z - \Delta z)}{2}$$

$$P_1(z) = P(z - \Delta z) + \overline{\rho_1}g\Delta z$$

$$\rho(z) = F(P_1(z)); \ \overline{\rho_2} = \frac{\rho(z) + \rho(z - \Delta z)}{2}$$

$$P_2(z) = P(z - \Delta z) + \overline{\rho_2} g \Delta z$$

✓ Easy density dependence: Cold = dense = less buoyant

 $\rho_m(z) = \rho_a \left(1 + \alpha \left[T_a - T_m(z) \right] \right)$



Summary of basic thermodynamic concepts

System: the region of interest, of sufficient size that average properties like temperature are well-defined; to be distinguished from the environment (i.e. the rest of the universe)

<u>Isolated system</u>: exchanges neither matter nor energy across its boundaries <u>Closed system</u>: may exchange energy across boundaries, but not matter <u>Open system</u>: may exchange matter and energy across boundaries

Phase: a physically homogeneous and mechanically separable part of the system, e.g. a vapor, liquid, or mineral. A system may be homogeneous (one phase) or heterogeneous (multiple phases). E.g. solid solution of Forsterite and Fayalite (Olivine end-member minerals).

Olivine	Forsterite Mg ₂ SiO ₄		Fayalite	Fe ₂ SiO ₄
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Plagioclase Albite NaAlSi₃O₈ → Anorthite CaAl₂Si₂O₈

Component: a chemical formula; a basis vector for expressing compositional variations in thermodynamic systems; e.g., H_2O , SiO_2 , Fe, NaCl. Must be independently variable, but we choose the minimum set to span all phases. Main oxides in the mantle NCFMAS system (sometimes also Cr2O3)

Phase vs system component (e.g. oxide).





Synthetic wadsleyite II

Summary of basic thermodynamic concepts

Gibbs free energy: is the energy available for non-PV work (such as chemical work)

$$G = H - TS$$
(13)
$$dG = VdP - SdT$$
(15)

Note that $(dG/dT)_p = -S$ $(dG/dP)_T = V$

Since its independent variables are P and T, it is useful for equilibrium studies. It also contains the entropy term which can be used as an indication of the direction in which spontaneous reactions will occur.

Note that if P and T remain constant through any spontaneous change in state, then dG = 0 !!!!!!!!!

- Gibbs free energy is adequate for equilibrium studies because its independent variables are T and P, i.e. the ones we are usually interested in!

- Spontaneous reactions evolve to minimize the Gibbs free energy.

- At equilibrium, dG = 0 and $\Delta G = 0$. in other words, products and reactants are in equilibrium when their G are equal.

Summary of basic thermodynamic concepts

$$\Delta G_{T',P'} = \Delta G_{T_{ref},P_{ref}} + \int_{P_{ref}}^{P'} \Delta V_r dP - \int_{T_{ref}}^{T'} \Delta S_r dT$$

$$\left(\frac{\partial \Delta G}{\partial T}\right)_p = -\Delta S$$

$$\left(\frac{\partial \Delta G}{\partial P}\right)_T = \Delta V$$

Solve this system iteratively for discrete ΔT and ΔP and find the point where $\Delta G = 0$

$$\Delta S(T) = \Delta S_{T_{ref}} + \int_{T_{ref}}^{T} \frac{\Delta C_p}{T} dT$$

How do we get the fundamental parameters?

Two main categories:

*Analysis of each phase individually (calorimetry, electrochemical)

*Relate thermodynamic properties of minerals to each other (int. consist. dataset)

The "solution" is a combination of calorimetric data and additional constraints such as reaction reversal brackets.

A thermodynamic dataset compatible with calorimetry and reaction reversals alike is called an internally consistent thermodynamic dataset (e.g. Holland and Powel 98, Stixrude 05, etc.)

Ternary compositional plot for peridotites



Table 15.2 Mineralogy of Lherzolites						
	Spinel L	herzolite	Garnet Lherzolite			
Mineral	Average (wt. pct.)	Range (vol. pct.)	Average (vol. pct.)	Range (vol. pct.)		
Olivine	66.7	65-90	62.6	6080		
Orthopyroxene	23.7	5-20	30	20-40		
Clinopyroxene	7.8	3-14	2	0-5		
Spinel	1.7	0.2-3				
Garnet Phlogopite			5 0.4	3–10 0–0.5		

Peridotite as function of the stable mineral phases: Olivine (O), pyroxenes (cpx, opx), garnet(gnt) etc.

Maaløe and Aoki (1977).

Ternary compositional plot for peridotites

(a) a

Coort



Table 15.3 Compositions of peridotites and pyroxenites								
		Lherzolit	es					
	Spi	inel	Garnet	Dunite	Pyroxenite		Peridoti	tes
Oxide	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)
SiO ₂	44.15	44.40	44.90	41.20	48.60	44.14	46.36	42.1
Al ₂ O ₃	1.96	2.38	1.40	1.31	4.30	1.57	0.98	
FeO	8.28	8.31	7.89	11.0	10.0	8.31	6.56	7.10
MgO	42.25	42.06	42.60	43.44	19.10	43.87	44.58	48.3
CaO	2.08	1.34	0.82	0.80	13.60	1.40	0.92	
Na ₂ O	0.18	0.27	0.11	0.08	0.71	0.15	0.11	
K ₂ O	0.05	0.09	0.04	0.016	0.28			
MnO	0.12	0.17	0.11	0.15	0.18	0.11	0.11	
TiO ₂	0.07	0.13	0.06	0.06	0.83	0.13	0.05	
P ₂ O ₅	0.02	0.06		0.10	0.10			
NiO	0.27	0.31	0.26					
Cr ₂ O ₃	0.44	0.44	0.32			0.34	0.33	
H ₂ O	—	_		0.50	0.90	—	—	

Peridotite as function of the major oxide composition

1.11

1.2.4

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12.0

Magnesium number: Mg#= MgO/(MgO+FeO)

Mg# low→ fertile mantle (enriched in Al2O3 and CaO, depleted in MgO)

Mg# high→ refractory mantle (enriched in MgO, depleted in Al2O3 and CaO)



Meting trend

Meting trend

5 4 3 3 2 1 1 0	(a) PM + 5% Mg	Melting (Mg# 10% 20% 42 44 MgO	increase 46 48 50	Ol Orthop Ol Orth	Harzburgite ivine byroxenite	Ol Dunite 90 Lherzolite Olivine Websterite Websterite	Wherlite PERID 40 Olivine Clinopyroxenite PYRO) 10 Cpx Clinopyroxenite	°OTITE - XENITE
		¥						
		1) Av.	2) Av.	3) Av.	4) Av.	5) Av.	6) Av. Middle	
		Harz.	HEXO	Harz. La	HLCO	Ocean floor	Atlas (wt%) ^e	
		Lanzarote	Tenerite	Palma av.	Tenerite	peridot.		
		(wt%)"	(wt%)*	(wt%)*	(wt%)*	(wt%)*		
	<u>S1O2</u>	43.78	43.32	43.07	42.14	45.09	43.48	
	Al ₂ O ₃	0.7	0.61	0.53	0.73	2.33	2.38	
	FeO	7.79	8.04	8.43	8.8	8.4	. 8	
	MgO	46.1	45.31	45.19	44.14	41.23	42.6	
	CaO	0.6	0.81	0.68	1.68	1.32	2.83	
	Na ₂ O	0.1	0.14	0.17	0.18	0.23	0.24	
	Mg#	91.34	90.96	90.53	89.94	89.7	90.47	

Mantle Depletion (partial meltina)

Mantle metasomatism (refertilization)

Compositional space: world petrological data bases

*Five major oxides (CFMAS (CaO-FeO-MgO-Al2O3-SiO2).

* A priori petrological data base (>2900 samples from xenoliths, perid. massifs and ophiolites)



Correlation between oxides regardless of tectonic age or facies.

Al2O3 is strong compositional indicator, mainly through its control of modal garnet.



Possible bias in database (e.g. double peaks) due to sampling



(From Ed Garnero's webpage)

(Modified from Xu et al., 2008)



> Mantle density is anti-correlated with Mg#...



Bulk mant	le compositions used in this work fr					
	1) Av. tecton gnt, perid, (wt%) ^a	2) Harz, inver (wt.%) ^b	3) Lherz, inver (wt.%) ^b	 Derbyshire av. (wt%)^c 	5) Fidra av. (wt%) ^d	6) PUM M&S95 (wt.%)e
SiO ₂ TiO ₂ Al-O ₂	45 0.16 3.9	41.7 - 2.65	45.84 - 3.92	43.4 0.02 2	44.31 0.15 3.5	45 0.201 4.45
Cr ₂ O ₃ FeO MnO MgO CaO	0.41 8.1 0.07 38.7 3.2	- 8.32 - 44.86 0.77	- 7.19 - 38.05 2.72	0.51 7.4 0.22 44.5 1.5	- 8.6 0.14 38.5 3.3	0.384 8.05 0.135 37.8 3.55
Na ₂ O NiO Total Mg#	0.28 0.24 100.06 89.5	0.05 - 90.58	0.21 - 90.42	0.08 0.32 99.95 91.47	0.3 - 99.8 87.73	0.36 - 99.93 89.3

> Mantle density is a complex function of T and C (no shortcuts...)

Density=f(T,P,C)



Fig 7

Upper mantle phase transitions

Differences in synthetic Bouguer anomaly due to shallow phase transitions (Al-bearing minerals)



P-wave anomaly seismic tomography model (*Villaseñor et al., 2003*) ^{350°} ^{352°} ^{354°} ^{356°} ^{358°} ^{0°}

 36° 36° 3

-1.5%

Depth (km)

500

+1.5%

+2.0%

-2.0%

Simplified slab with ΔT =-400 K with respect to ambient mantle based on geodynamic modelling of the Alboran Sea since upper Oligocene (Fullea et al. 2015)



Simplified slab with ΔT =-400 K with respect to ambient mantle based on geodynamic modelling of the Alboran Sea since upper Oligocene (Fullea et al. 2015)

Sublithospheric thermal anomaly effect on gravity field



Weaker effect in xy and yy in components

Complex parameter space

* Trade-offs between Temperature and Composition

* T has a greater effect than C in most of the observables

* Non uniqueness of compositional field (worse in the lithosphere than in the sublithosphere)

$$\sigma(\mathbf{m}) = k\rho(\mathbf{m})L(\mathbf{m}) \qquad \qquad L(\mathbf{m}) \propto \exp\left\{-\frac{1}{2}[g(\mathbf{m}) - \mathbf{d}_{obs}]^T C_D^{-1}[g(\mathbf{m}) - \mathbf{d}_{obs}]\right\}$$



Integrated forward modelling: work flow



Integrated modelling Magnetotelluric data (Kaapvaal craton)

Kaapvaal craton (S. Africa): 2D magnetotelluric (MT) model



Magnetotellurics (MT)



Electrical conductivity: lab experiments and mineral physics

Experimental measurements of conductivity in single crystals or mineral aggregates



Electrical conductivity: the water problem

Pressure (GPa)

Laboratory uncertainties/discrepancies

Peridotite solidus





From Asimow et al. (2004)



Electrical condutivity of the upper mantle: lab mineral studies (dry)



Electrical conductivity of the upper mantle: Kaapvaal (dry)





(Peslier, 2009; Grant et al., 2007)

(Zhao et al., 2004; Mierdel et al., 2007; Gavrilenko, 2008; Lu and Keppler, 1997)

Electrical conductivity of the upper mantle: Kaapvaal (wet)



Electrical conductivity of the upper mantle: Sensitivity tests







Lithosphere-asthenosphere boundary depth (thermal): 230-260 km



(Griffin et al., 2003; O'Reilly et al. 2010; Fullea et al., 2011)

Integrated modelling surface wave data (Central Mongolia)

LitMod1D : Surface waves



Pairs of stations, detailed dispersion curves

North Central Mongolia



Mantle composition

	a) Aver.	b) PUM
	Central	M&S95
	Mongolia	
	and	
	Baikal	
SiO ₂	44.59	45
TiO ₂	0.14	0.2
Al_2O_3	3.48	4.5
Cr ₂ O ₃	0.4	0.38
FeO	8.25	8.1
MnO	0.14	0.14
MgO	39.56	37.8
CaO	2.85	3.6
Na ₂ O	0.31	0.36
Mg#	89.7	89.3
-		•



Lebedev et al. EPSL 2006 Surface wave seismic tomography

(Purely) Seismic models



Lebedev et al. EPSL 2006

Range of preferred models fitting surface wave data. Seismic velocities and densities computed as function of *T*, *P* and composition (LitMod)



Seismic attenuation



Integrated inversion: Xenolith data



→Integrated modelling effectively reduce the uncertainties of purely seismic inversions →Thermobarometric estimates from Cenozoic mantle xenoliths in central Mongolia confirm estimated geotherms



Summary of results

- 80-90 km LAB
- dense and mafic lower crust
- fertile-moderately depleted
 lithospheric mantle
- isostatically compensated topography

Fullea et al., 2012

Surface-wave sensitivity kernels



Depth

