PHYS3070 Physics of the Earth: from seismic structure to geodynamics

‘Geophysics … has the rigour of physics and the vigour of geology’

C. M. R. Fowler

Goal: to connect the seismological investigation of the Earth’s internal structure (Hrvoje Tkalcic’s segment) with Paul Tregoning’s component concerning geodetic observations of surface deformations

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WebCT

http://rses.anu.edu.au/people/jackson_i/PHYS3070/
Part I: Elasticity, equations-of-state & interpretation of seismological models

Tensor stress & strain
Constitutive law & elastic waves
Elasticity & interatomic forces
Geophysical thermodynamics
Lattice vibrations & thermal energy
Anharmonicity & thermal expansion
Finite strain & cohesive energy @ high pressure
Mie-Grüneisen equation-of-state & thermal pressure
Anelasticity & seismic wave attenuation
Interpretation of seismological models

The End
References


Inversion of traveltime versus angular distance & free-oscillation data for spherically averaged structure
Seismological models for the transition zone of the Earth’s mantle

Seismological models for bulk sound speed $V_\phi = (K_\phi/\rho)^{1/2}$ vs depth

Jackson & Rigden, In The Earth’s Mantle, 1998
Lateral variations of seismic wave speeds in the upper mantle

Surface-wave tomographic model of Fishwick et al. (2005)
$V_S$ variations (%) at 200 km depth
Recap on elasticity: tensor strain

Displacement
gradient tensor

\[ e_{ij} = \frac{\partial u_i}{\partial x_j} (i, j = 1, 2, 3) \]

\[ u_i = e_{ij}x_j \] for homogeneous deformation

Rigid-body rotation:

\[ e_{21} = -e_{12} = \delta \theta \neq 0 \]

\[ \therefore \text{define strain as symmetrical part of } e_{ij} \]

\[ \varepsilon_{ij} = \frac{1}{2}(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}) \]
Recap on elasticity: tensor stress

\( \sigma_{ij} \) is the component of force parallel to \( x_i \) per unit area oriented normal to \( x_j \) (exerted on the infinitesimal element by the surrounding medium; tension +ve)

Rotational equilibrium requires \( \sigma_{ji} = \sigma_{ij} \)

Translational equilibrium ➔ the wave equation

\[ \rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j} \]
Elasticity: constitutive law & elastic waves

Generalisation of Hooke’s law: \( \sigma_{ij} = c_{ijkl} \varepsilon_{kl} \)

For isotropic medium: \( \sigma_{ij} = \lambda \delta_{ij} \varepsilon_{kk} + 2\mu \varepsilon_{ij} \)

Kronecker ‘delta’ \( \delta_{ij} = 1 \) (for \( i = j \)), 0 (for \( i \neq j \))

Einstein summation convention \( \varepsilon_{kk} = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33} = \Delta \)

(known as the dilatation)

The wave equation \( \rho \partial^2 u_i/\partial t^2 = \partial \sigma_{ij}/\partial x_j \) becomes

\[
\rho \partial^2 u_i/\partial t^2 = \lambda \delta_{ij} \partial^2 u_k/\partial x_j \partial x_k + \mu (\partial^2 u_i/\partial x_j \partial x_j + \partial^2 u_j/\partial x_j \partial x_i)
\]

Substit’n of trial plane-wave solution \( u_i = u_{i0} f(n_r - vt) = u_{i0} f(n_m x_m - vt) \)

\( \rightarrow \) system of 3 eqns. linear in \( u_{i0} \) for given \( n_m \)

\( \rightarrow \) 3 eigenvalues given by cubic in \( \rho v^2 \)

1 compressional mode \( \rho v_p^2 = \lambda + 2\mu = K + (4/3)G \)

2 orthogonal shear modes \( \rho v_s^2 = \mu = G \)
‘Geophysical’ thermodynamics: the internally consistent framework for understanding the Earth’s internal structure

First law of thermodynamics (conservation of energy embodying the equivalence of heat and work and their relationship with internal energy $E$)

$$dE = dQ - PdV; \text{ substitute for entropy } S \text{ defined by } dS = dQ/T, \text{ to get}$$

$$dE(S,V) = TdS - PdV$$

Similar expressions for the other thermodynamic potentials:

**Enthalpy** $H = E + PV$

$$dH(S,P) = TdS + VdP$$

**Helmholtz free energy** $F = -kT \ln Z = E - TS$

$$dF(V,T) = -PdV - SdT$$

**Gibbs free energy** $G = H - TS = E + PV - TS$

$$dG(P,T) = VdP - SdT$$

$Z$ is the partition function of statistical mechanics

*References: Stacey, Appendix E; Poirier, Ch. 1*
Useful thermodynamic identities

Tools for functional analysis:
For $Z = Z(X,Y)$,
\[
dZ = \left(\frac{\partial Z}{\partial X}\right)_Y dX + \left(\frac{\partial Z}{\partial Y}\right)_X dY,
\]
\[
\frac{\partial^2 Z}{\partial X \partial Y} = \frac{\partial^2 Z}{\partial Y \partial X}, \quad \&
\]
\[
\left(\frac{\partial Z}{\partial X}\right)_W = \left(\frac{\partial Z}{\partial X}\right)_Y + \left(\frac{\partial Z}{\partial Y}\right)_X \left(\frac{dY}{dX}\right)_W
\]
\[
\left(\frac{\partial Z}{\partial Y}\right)_X = \left(\frac{\partial Z}{\partial W}\right)_X / \left(\frac{\partial Y}{\partial W}\right)_X
\]

Applications in deriving thermodynamic identities:

$E(S,V)$: \( \left(\frac{\partial E}{\partial S}\right)_V = T \quad \left(\frac{\partial E}{\partial V}\right)_S = -P \quad \left(\frac{\partial T}{\partial V}\right)_S = -(\frac{\partial P}{\partial S})_V \)

$H(P,S)$: \( \left(\frac{\partial H}{\partial S}\right)_P = T \quad \left(\frac{\partial H}{\partial P}\right)_S = V \quad \left(\frac{\partial T}{\partial P}\right)_S = \left(\frac{\partial V}{\partial S}\right)_P \)

$F(V,T)$: \( \left(\frac{\partial F}{\partial V}\right)_T = -P \quad \left(\frac{\partial F}{\partial T}\right)_V = -S \quad \left(\frac{\partial P}{\partial T}\right)_V = \left(\frac{\partial S}{\partial V}\right)_T \)

$G(P,T)$: \( \left(\frac{\partial G}{\partial P}\right)_T = V \quad \left(\frac{\partial G}{\partial T}\right)_P = -S \quad \left(\frac{\partial V}{\partial T}\right)_P = -(\frac{\partial S}{\partial P})_T \)
Applications of thermodynamic identities

**Thermal pressure**

\[
\left(\frac{\partial P}{\partial T}\right)_V = \left(\frac{\partial S}{\partial V}\right)_T = \alpha K_T \implies (dP_{th})_V = (\gamma/V) \ dE_{th}
\]

(Grüneisen parameter: \(\gamma = \alpha K_T V/C_V\))

**Isobaric & isochoric derivatives** (\(\partial Z[X,Y]/\partial X\)\(_W\) with \(X = T\), \(Y = V\) & \(W = P\):

\[
(\partial Z/\partial T)_P = (\partial Z/\partial T)_V + (\partial Z/\partial V)_T (\partial V/\partial T)_P = (\partial Z/\partial T)_V - \alpha K_T (\partial Z/\partial P)_T
\]

e.g., \(C_P= (\partial Q/\partial T)_P = T(\partial S/\partial T)_P = T(\partial S/\partial T)_V + V\alpha T(\partial S/\partial V)_T = C_V[1 + \alpha \gamma T]\)

**Isothermal & adiabatic derivatives** (\(\partial Z[X,Y]/\partial X\)_\(W\) with \(X = V\), \(Y = T\) & \(W = S\):

\[
(\partial Z/\partial V)_S = (\partial Z/\partial V)_T + (\partial Z/\partial T)_P (\partial T/\partial V)_S
\]

e.g., (\(\partial P/\partial V\)_\(S\) = (\(\partial P/\partial V\)_\(T\) + (\(\partial P/\partial T\)_\(V\)(\(\partial T/\partial V\))\)

hence \(K_S = K_T[1 + \alpha \gamma T]\)

**Adiabatic temperature gradient**

\[
(\partial T/\partial P)_S = (\partial V/\partial S)_P = (\partial V/\partial T)_P/(\partial S/\partial T)_P = \gamma T/K_S
\]

\[
(\partial \ln T/\partial \ln \rho)_S = -(\partial \ln T/\partial \ln V)_S = \gamma
\]

Stacey Appendix E, Poirier Ch. 1
Elasticity & interatomic forces

Volume per ion pair $V = 2r^3$

Internal energy $E = -C_0/r + D_0/r^n = -C(V/V_0)^{-1/3} + D (V/V_0)^{-n/3}$

$P = -dE/dV$ [strictly $-(\partial F/\partial V)_T$ with $F = E - TS$]

Bulk modulus $K_T = -V(\partial P/\partial V)_T$

Pressure derivative of $K_T' = (\partial K_T/\partial P)_T$

$\therefore K_0V_0 = (C/9)(n-1) \propto d^2E/dV^2 \sim $ constant for isostructural compounds & $K'_0 = (n+7)/3$
Interplanar forces & lattice vibrations

Sequence of identical parallel planes of atoms interacting with neighbours:

\[ \mathbf{F}_n = -K [u_n - u_{n-1}] + K [u_{n+1} - u_n] = M \frac{\partial^2 u_n}{\partial t^2} \]

Trial solution \( u_n = u_0 \sin(kx_n - \omega t) \) with \( x_n = na \)
Dispersion relation for lattice vibrations

Condition for solution: \( \omega = 2(K/M)^{1/2} |\sin(ka/2)| \)

Phase speed for longitudinal vibrations \( c = \frac{\omega}{k} \)

In general, group velocity \( u = \frac{d\omega}{dk} \neq c \rightarrow \text{dispersion} \)

Limit as \( k \rightarrow 0, u = c = a(K/M)^{1/2} \)
Lattice vibrations: acoustic & optic branches

\( p \) atoms per unit cell \( \rightarrow \) 3p modes of vibration

Acoustic modes: \( u_n \) and \( u_{n+1} \) in-phase as \( k \rightarrow 0 \)

Optic modes: \( u_n \) and \( u_{n+1} \) out-of-phase as \( k \rightarrow 0 \)
Quantisation & lattice vibrational energy

Periodic boundary conditions for crystal of length $L = Na$ require $k = m(2\pi/L)$ with $m = 0, \pm 1, \pm 2, \ldots, \pm N/2$.

Density of $(k, \omega)$ states in reciprocal $(k)$ space is $g(k) = 1/dk = L/2\pi = Na/2\pi$ such that $\int g(k) dk = N$.

1st approx’n to crystal lattice: collection of independent harmonic oscillators of frequency $\nu$, energy quantum $h\nu$, & (equilibrium) phonon occupancy quantum number $p(\nu, T) = [\exp(h\nu/k_B T) - 1]^{-1} \sim k_B T/ h\nu$ @ high $T$ (Bose-Einstein statistics)

$E_{vib}(T) = \sum_{i=1,N} h\nu_i p(\nu_i, T) = \int p(\nu, T) h\nu g(\nu) d\nu$
The Debye model of lattice vibrations

Key assumptions: all modes acoustic & non-dispersive \((\omega = \nu_D k)\)
& uniformly distributed within spherical BZ of radius \(k_D\) to match actual BZ volume \(\Rightarrow\) density of states \(g(\nu) = \frac{9m\nu^2}{\nu_D^3}\)
Normalisation: \(\int (0, \nu_D) g(\nu)d\nu = 3m, m \text{ atoms per unit cell}\)

\[\omega \propto k \quad g(\omega) \propto \omega^2\]

\(g(\omega)\) for MgO vs. Debye model
Debye model: thermal energy & specific heat

\[ E_D(T) = \int p(\nu, T) \hbar \nu g_D(\nu) \, d\nu \]
\[ = (9nRT/x^3) \int_{(0,x)} \xi^3 \, d\xi / [\exp(\xi) - 1] \text{ (per mol)} \]

with \( n \) atoms per formula unit, \( x = \theta/T \)

& Debye temperature \( \theta = h\nu_D/k_B \)

\[ C_V(T) = (\partial Q/\partial T)_V = (\partial E/\partial T)_V \]
\[ \sim T^3 \text{ as } T \Rightarrow 0, \sim 3R \text{ for } T >> \theta_D \]
Anharmonicity & thermal expansion

Asymmetry of potential well results in time-averaged inter-atomic spacing greater than static equilibrium value, reduced inter-planar stiffness constants, $K$ & reduced vibrational frequencies $\nu \sim (K/M)^{1/2}$

Quasi-harmonic approximation: $\nu_i = \nu_i(V)$

with $\gamma_i = -\frac{d\ln\nu_i}{d\ln V} = -\frac{d\ln\theta_D}{d\ln V} = \gamma_D$
Finite strain & cohesive energy @ high pressure

\[ K_T = -V(\partial P/\partial V)_T = K_0, \text{ constant} \]
integrates to \( P = -K_0 \ln (V/V_0) \) but incompressibility must increase with \( P \):
e. g., \( K'_0 = (\partial K_T/\partial P)_{T0} = (n+7)/3 \)
for rocksalt lattice

Eulerian finite strain \( \varepsilon_{ij} = (1/2)(\partial u_i/\partial X_j +\partial u_j/\partial X_i) \)
- \( (1/2)\sum_k (\partial u_k/\partial X_i)(\partial u_k/\partial X_j) \) (Poirier, p. 60)

P \rightarrow isotropic compressional finite strain \( \varepsilon: V_0/V = \rho/\rho_0 = (1-2\varepsilon)^{3/2} \)

Taylor series expansion of Helmholz free energy \( F = E - TS \):
\[ F(V,T) = a_0 + a_1 f + a_2 f^2 + a_3 f^3 + \ldots \text{ with } a_i = a_i(T) \& f = -\varepsilon \]
3rd-order Eulerian finite strain isotherm $P(V)$

Now $P = - (\partial F/\partial V)_T = - (\partial F/\partial f)_T / (\partial V/\partial f)_T$

$K_T = - V(\partial P/\partial V)_T = - V(\partial P/\partial f)_T / (\partial V/\partial f)_T$

$K'_T = (\partial K_T/\partial P)_T = (\partial K_T/\partial V)_T / (\partial P/\partial V)_T$

$= (\partial K_T/\partial f)_T / [(\partial V/\partial f)_T (\partial P/\partial V)_T] = -(V/K_T)(\partial K_T/\partial f)_T / (\partial V/\partial f)_T$ etc.

Thus $P = (1/3V_0)(1 + 2f)^{5/2}(2a_2f + 3a_3f^2)$ (P = 0 for strain f = 0)

$K_T = (1/9V_0)(1 + 2f)^{5/2}[ 2a_2 + (14a_2+6a_3)f + 27a_3f^2]$

$K'_T = (1/3)[24a_2 + 6a_3 + (98a_2 + 96a_3)f + 243a_3f^2]/$

$[2a_2 + (14a_2+6a_3)f + 27a_3f^2]$

Initial conditions: $K_T = K_{T_0}$, $K'_T = K'_{T_0} \rightarrow$

$a_2 = 9K_{T_0}V_0/2$, $a_3 = (9K_{T_0}V_0/2)(K'_{T_0} - 4)$

Hence 3rd-order Eulerian (Birch-Murnaghan) isotherm

$P = 3K_{T_0} (1 + 2f)^{5/2} [f + (3/2)(K'_{T_0} - 4) f^2]$
Finite-strain P(V) principal isotherm + Debye model for E(T,V) with $\theta(V)$

Construct $F(V,T) = F_{BM}(V,0) + F_D(V,T)$

$F_D = E_D - TS_D$ with $S = -(\partial F/\partial T)_V \rightarrow F_D = T (\partial F_D/\partial T)_V = E_D$

$\therefore (\partial [F_D/T]/\partial T)_V = -E_D/T^2 & F_D = -T \int_{(0,T)} (E_D/T^2) \, dT = -T \int_{(0,T)} (E_D/T^2) \, dT$

$\int$ by parts $\Rightarrow$

$F_D = 9nRT(\theta/T)^{-3} \int_{(0,\theta/T)} \xi^2 \ln [1- \exp(-\xi)] \, d\xi$

$P(V,T) = -(\partial F/\partial V)_T = -(\partial F_{BM}/\partial V)_T - (\partial F_D/\partial V)_T$

$\therefore P(V,T) = P(V,0) + (\gamma_D/V) E_D(V,T)$

i.e., thermal pressure: $\delta P_{TH}(V,T) = (\gamma_D/V) \delta E_D(V,T)$

c.f. $\delta P_{TH} = (\gamma/V) \delta E_{TH}$ from $(\partial P/\partial T)_V = \alpha K_T = (\gamma/V)C_V$

$\Rightarrow \gamma = \gamma_D$
The thermal pressure

\[ P(V,T) = P(V,0) + P_{TH}(V,T) \]

with \( P_{TH}(V,T) = \left( \frac{\gamma D}{V} \right) E_D(V,T) \)
Mie-Grüneisen-Debye EoS: completeness

From $F(V,T) = F(V,T_0) + F_D(V,T)$

$$= a_2f^2 + a_3f^3 + 9nRT[\theta(f)/T]^{-3} \int_{(0,\theta(f)/T)} \xi^2 \ln [1 - \exp(-\xi)] d\xi$$

[with $\theta(f)$ specified by $\gamma_0 = -(d\ln \theta/d\ln V)_0$ & $q_0 = (d\ln \gamma/d\ln V)_0$]

we have it all:

$$P(V,T) = -(\partial F/\partial V)_T, \quad S(V,T) = -(\partial F/\partial T)_V$$

Hence $E = F + TS, \quad H = E + PV, \quad G = F + PV$

$$C_V = T(\partial S/\partial T)_V$$

$$K_T(V,T) = -V(\partial P/\partial V)_T, (\partial P/\partial T)_V = \alpha K_T(V,T) = (\gamma/V)C_V$$

$$\alpha, \gamma, K_S = K_T(1 + \alpha \gamma T), (\partial T/\partial P)_S = \gamma T/K_S \text{ etc.}$$

Extension to shear strain

(Stixrude & Lithgow-Bertelloni, Geophys. J. Int., 2005)
Modelling the seismic properties of the Earth’s interior

\[ P(V,T), K_T(V,T) \text{ & hence } K_S(V,T), G(V,T) \]

from internally consistent finite-strain expansions of both static and thermal parts of the Helmholtz free energy \( F \)

\[ \rightarrow \rho(z), V_P(z), V_S(z) \]

For each mineral need

\[ F_0, V_0, K_{T0}, K_{T0}', G_0, G_0', \theta_0, \gamma_0, q_0, \eta_{S0} \]

constrained by experimental data and/or ab initio quantum-mechanical calculations
Optimal finite-strain model constrained by diverse experimental data for MgO
Elastic behaviour: essential characteristics

Hookean elasticity:

(i) **Linearity**: stress $\sigma \propto$ strain $\epsilon$

(ii) **Instantaneity**: strain appears (disappears) instantaneously when stress is applied (removed)

(iii) **Recoverability**: strain is fully recovered when stress is removed

**No dissipation**: time-varying stress and strain in phase

**No dispersion**: wave speeds are frequency independent
Beyond elasticity: **anelastic** behaviour

Relax requirement of instantaneity $\rightarrow$ **anelasticity**

Stress-induced diffusion of defects or redistribution of fluid occurs with characteristic timescale $\tau$, typically thermally activated and contributes well-defined, delayed component of strain

More strain for the same stress $\rightarrow$

lower (relaxed) modulus $= \text{stress/strain}$
Strain energy dissipation

Delayed anelastic strain $\rightarrow$ phase lag between stress

$\sigma(t) = \sigma_0 \sin \omega t$ & resulting strain $\epsilon(t) = \epsilon_0 \sin(\omega t - \delta)$

**Energy dissipated per cycle**

$\Delta E = \int_{(0,2\pi)} \sigma \ d\epsilon = \omega \sigma_0 \epsilon_0 \int_{(0,2\pi)} \sin \omega t \cos(\omega t - \delta) \ dt$

Using $\cos(\omega t - \delta) = \cos \omega t \cos \delta + \sin \omega t \sin \delta$ &

$\sin 2\omega t = 2\sin \omega t \cos \omega t$ and $\cos 2\omega t = 1 - 2\sin^2 \omega t$ obtain

$\Delta E = (\sigma_0 \epsilon_0 / 2) \int_{(0,2\pi)} [\sin 2\omega t \cos \delta + (1 - \cos 2\omega t) \sin \delta] \ d(\omega t) = \pi \sigma_0 \epsilon_0 \sin \delta$

**Maximum energy stored**

$E_{\text{max}} = \int_{(0,\pi/2)} \sigma \ d\epsilon_{\text{in phase}} = \sigma_0 \epsilon_0 \cos \delta \int_{(0,\pi/2)} \sin \omega t \ d(\sin \omega t)$

$= (\sigma_0 \epsilon_0 \cos \delta) / 2$

**Quality factor Q**

$Q = 2\pi E_{\text{max}} / \Delta E = 1 / \tan \delta$ or $Q^{-1} = \tan \delta$
Complementary experimental techniques probe a wide range of frequencies (c.f. mHz - Hz of teleseismic waves)
Elastic wavespeeds: ultrasonic methods

Mode-specific piezoelectric or ferroelectric transducers
Generate & detect elastic waves

Simple pulse transmission (time-of-flight) & interferometric methods
Ultrasonic wave-propagation methods: representative results

MgSiO$_3$ perovskite
Li & Zhang
*PEPI* (2005)

Data fitted to $F(f,T)$ model $\Rightarrow$

$V_0, K_0, K'_0, G_0, G'_0, \theta_0, \gamma_0, q_0, \eta_{S0}$
Jackson & Kung, *PEPI*, 2008

Silicate perovskite analogue ScAlO$_3$
**Opto-acoustic methods: Brillouin scattering**

\[ V_i = \Delta \omega \lambda / 2 \sin(\theta/2) \ (i = P, S) \]

from Doppler shift \( \Delta \omega \)

Application in diamond-anvil apparatus

\( \Rightarrow \) G(P) to 100 GPa for MgSiO\(_3\) perovskite

\( \Rightarrow \) improved constraints on G'

Murakami et al., *EPSL* (2007)
Forced-oscillation method for laboratory study of anelasticity at seismic frequencies

Implementation within internally heated gas apparatus (Jackson & Paterson, *PAGEOPH*, 1993):

- P = 200 MPa, T to 1300°C
- Oscillation periods 1-1000 s
- Shear strains < $10^{-5}$

Specimen & reference assemblies & T profile

Underlying principle

Specimen encapsulation
Seismic-frequency forced-oscillation data for dry melt-free polycrystalline olivine

Jackson, Fitz Gerald, Faul & Tan, JGR, 2002
Modelling elasticity with interatomic potentials

$K$ (quartz) = 39.7 GPa

c.f. 39.3 GPa (measured)


Putnis (1992)
Quantum chemistry: H atom to crystals

**Schrödinger equation:** \((-\frac{\hbar^2}{2m}) \nabla^2 \psi + V\psi = E\psi\)

**Hydrogen atom**
Analytical solution: s, p, d, ... orbitals
Energy levels consistent with observed line spectrum

**Multi-electron atoms**
Electron-electron interaction: no analytic solutions
Aufbau and Pauli exclusion principles: self-consistent field atomic orbitals (a.o.)

**Small molecules**
Molecular orbitals as linear combinations of a.o. - coefficients chosen to minimise total energy; high e\(^{-}\) density between atoms = chemical bonding

**Crystalline solids**
**Zero K** Density functional theory: ground-state energy a unique function of the spatial distribution of electron density;

**High-T** Quasi-harmonic approach – lattice vibrational frequencies \(\nu(V)\); anharmonic ab initio molecular dynamics.

1998 Nobel prize in chemistry to Kohn & Pople
Seismic properties: ab initio constraints

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\(\Delta E = (1/2)C \varepsilon^2\)

\textit{MgSiO}_3\textit{ perovskite: single-crystal elastic constants (GPa)}

Oganov et al. (2001)
Single-crystal elastic anisotropy: olivine

triangular clusters of edge-sharing MO$_6$ octahedra capped by SiO$_4$ tetrahedra form stiff columns $\Rightarrow$ high $V_p$ along [100]


Polyhedral structure of olivine (Putnis, 1992)

Mainprice (2007)
*Treatise on Geophysics*
Bulk Earth composition & pressure-induced phase transformations

Pyrolite model upper-mantle composition = magma (basalt) + residue (harzburgite) Green & Ringwood (1960’s)

Crystal structures of high-pressure minerals

(Mg,Fe)SiO$_3$ perovskite

(Mg,Fe)O magnesiowüstite

CaSiO$_3$ perovskite
Gross Earth seismological models

Fowler Fig. 8.1

Fowler Fig. 8.3

Inversion of traveltime versus angular distance & free-oscillation data for spherically averaged structure
Lateral variations of seismic wave speeds in the Australasian upper mantle

Surface-wave tomographic model of Fishwick et al., *EPSL*, 2005

$V_S$ variations (%) at 200 km depth
Optimal geotherms and $V_s(z)$ profiles for contrasting tectonic provinces

Lab-based model inclusive of anelastic relaxation (Faul & Jackson, *EPSL*, 2005)
$V_\phi = \left( \frac{K_s}{\rho} \right)^{1/2} = \left[ V_P^2 - \frac{4}{3} V_S^2 \right]^{1/2}$

Composition, elasticity & temperature of the lower mantle

Lower-mantle mineralogy for pyrolite composition

G’ & dG/dT from ultrasonics: pyrolite & 1600 K adiabat OK (Li & Zhang, PEPI, 2005)

Lower mantle: new developments

Post-perovskite \( \text{CaIrO}_3 \) phase of \( \text{MgSiO}_3 \) @ \( P > 120 \) GPa, \( T \sim 2500 \) K
Murakami et al., *Science*, 2004

Pressure-induced spin-pairing in Fe

\( \text{Fe}^{2+} \):
\( 3s^23p^63d^64s^0 \)

d-orbital degeneracy removed by the octahedral crystal field (Brown et al., *Chemistry*, 1991)

\( \delta \rho/\rho \sim 1\% \)
Earth’s core: composition & temperature

Preferred hexagonal close-packed structure for pure Fe under inner-core conditions

Core is significantly less dense & somewhat more compressible than pure Fe

Fowler Fig. 8.12b
Ab initio calculation of equations-of-state \( V(P, T) \) & Gibb’s free energies \( G(P, T) \) for both solid and liquid phases → melting temperature \( T_m \) and element partitioning

Can match densities of inner and outer core with thermodynamic equilibrium at inner-outer core boundary:

\[ P = 330 \text{ GPa}, T_m = 5600 \text{ K} \]

Inner core: 8 mol% S/Si & 0.3% O
Outer core: 10 mol% S/Si & 8% O

Alfè et al., EPSL, 2002
Stable crystal structure for the inner core?

- Hexagonal close-packed symmetric 12-coordination
- Body-centred cubic split 8-6 coordination with larger interstices

Part I: Elasticity, equations-of-state & interpretation of seismological models

Tensor stress & strain
Constitutive law & elastic waves
Elasticity & interatomic forces
Geophysical thermodynamics
Lattice vibrations & thermal energy
Anharmonicity & thermal expansion
Finite strain & cohesive energy @ high pressure
Mie-Grüneisen equation-of-state & thermal pressure
Anelasticity & seismic wave attenuation
Interpretation of seismological models

The End
Next: Part II  Heat transport & geodynamics