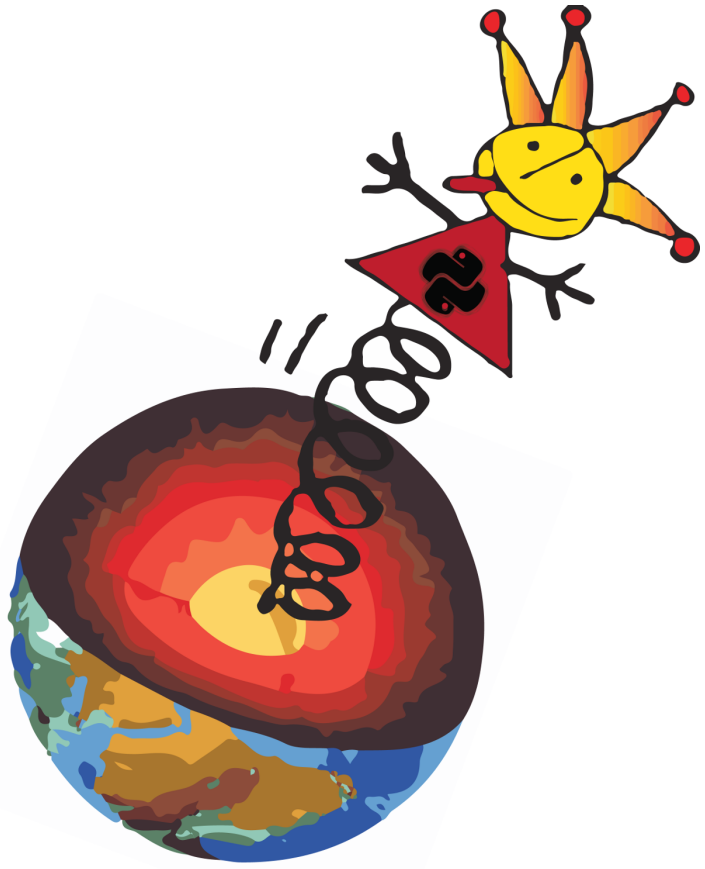
COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS (CIG)

BurnMan

a thermodynamics and thermoelasticity toolkit

User Manual

Version 0.8.0b3



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CHAPTER

ONE

BURNMAN

BurnMan is an open source mineral physics toolbox written in Python which determines the velocities of seismic waves in mineral assemblages at high pressure and temperature. It was designed to calculate seismic velocities in the lower mantle, but is equally suited to any part of the solid Earth (or indeed any of the terrestrial planets). BurnMan calculates the isotropic thermoelastic moduli by solving the equations-of-state for a mixture of minerals defined by the user. The user may select from an extensive list of minerals obtained from published databases. Alternatively, they can easily define their own minerals.

Features:

- a range of thermoelastic models, choice between second or third order accuracy
- a range of thermodynamic models for mineral endmembers
- consistent, comprehensive treatment of minerals with solid solutions
- form composites of arbitrary combination of Materials
- extensive Mineral database
- easy plotting and comparison of seismic profiles using matplotlib
- many examples highlighting different features of BurnMan
- different averaging schemes for seismic velocities in composite materials
- a catalogue of published geotherms
- extensible: all parts can be replaced by user-written modules if desired

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CHAPTER

TWO

OVERVIEW

2.1 Overall Structure

BurnMan is designed to be a general mineral physics and seismological toolkit which can enable a user to calculate (or fit) the physical and chemical properties of endmember minerals, fluids/melts, solid solutions, and composite assemblages. Such properties include:

- the thermodynamic free energies, allowing phase equilibrium calculations, endmember activities, chemical potentials and oxygen (and other) fugacities.
- entropy, enabling the user to calculate isentropes for a given assemblage.
- volume, to allow the user to create density profiles.
- seismic velocities, including Voigt-Reuss-Hill and Hashin-Strikman bounds and averages.

Data and functions are provided to allow the user to compare calculated isentropes and seismic velocity profiles to profiles computed for other compositions or constrained by seismology.

BurnMan is written in the Python language and is run from the command line. This allows the library to be incorporated into other projects. BurnMan makes extensive use of SciPy and NumPy, which are widely used Python libraries for scientific computation. Matplotlib is used to display results and produce publication quality figures. The computations are consistently formulated in terms of SI units.

The toolkit includes:

- the full codebase, including many equations of state and solution models
- popular datasets already coded into burnman-usable format
- a tutorial on the basic use of BurnMan
- a large collection of annotated examples
- an extensive suite of unit tests to ensure code functions as intended
- a series of benchmarks comparing BurnMan output with published data
- a directory containing user-contributed code from published papers

This software has been designed to allow the end-user a great deal of freedom to do whatever calculations they may wish. We have endeavoured to provide examples and benchmarks which cover the most popular uses of the software, some of which are included in the figure below. This list is certainly not exhaustive,

and we will definitely have missed interesting applications. As a result we will be very happy to accept contributions in form of corrections, examples, or new features.

CHAPTER

THREE

MATHEMATICAL BACKGROUND

Here is a bit of background on the methods used to calculate thermoelastic and thermodynamic properties in BurnMan. More detail can be found in the cited papers.

3.1 Endmember Properties

3.1.1 Calculating Thermoelastic Properties

To calculate the bulk (K) modulus, shear modulus (G) and density (ρ) of a material at a given pressure (P) and temperature (T), optionally defined by a geotherm) and determine the seismic velocities (V_S, V_P, V_Φ), one uses an Equation of State (EoS). Currently the following EoSs are supported in BurnMan:

- Birch-Murnaghan finite-strain EoS (excludes temperature effects, *[Poi91]*),
- Birch-Murnaghan finite-strain EoS with a Mie-Grüneisen-Debye thermal correction, as formulated by *[SLB05]*.
- Birch-Murnaghan finite-strain EoS with a Mie-Grüneisen-Debye thermal correction, as formulated by *[MBR+07]*.
- Modified Tait EoS (excludes temperature effects, *[HuangChow74]*),
- Modified Tait EoS with a pseudo-Einstein model for thermal corrections, as formulated by *[HollandPowell11]*.
- Compensated-Redlich-Kwong for fluids, as formulated by *[HP91]*.

To calculate these thermoelastic parameters, the EoS requires the user to input the pressure, temperature, and the phases and their molar fractions. These inputs and outputs are further discussed in *User input*.

Birch-Murnaghan (isothermal)

The Birch-Murnaghan equation is an isothermal Eulerian finite-strain EoS relating pressure and volume. The negative finite-strain (or compression) is defined as

$$f = \frac{1}{2}\left[\left(\frac{V}{V_0}\right)^{-2/3} - 1\right], \tag{3.1}$$

where V is the volume at a given pressure and V_0 is the volume at a reference state ($P = 10^5$ Pa , T = 300 K). The pressure and elastic moduli are derived from a third-order Taylor expansion of Helmholtz free energy in f and evaluating the appropriate volume and strain derivatives (e.g., *[Poi91]*). For an isotropic material one obtains for the pressure, isothermal bulk modulus, and shear modulus:

$$P = 3K_0 f \left(1 + 2f\right)^{5/2} \left[1 + \frac{3}{2}\left(K_0' - 4\right) f\right], \tag{3.2}$$

$$\begin{aligned} K_T = (1 + 2f)^{5/2} \Big[& K_0 + (3K_0K_0' - 5K_0)f \\ & + \frac{27}{2}(K_0K_0' - 4K_0)f^2 \Big], \end{aligned} \tag{3.3}$$

$$\begin{aligned} G = (1+2f)^{5/2} \Big[& G_0 + (3K_0G_0' - 5G_0)f \\ & + (6K_0G_0' - 24K_0 - 14G_0 + \frac{9}{2}K_0K_0')f^2 \Big]. \end{aligned} \tag{3.4}$$

Here K_0 and G_0 are the reference bulk modulus and shear modulus and K_0' and G_0' are the derivative of the respective moduli with respect to pressure.

BurnMan has the option to use the second-order expansion for shear modulus by dropping the f^2 terms in these equations (as is sometimes done for experimental fits or EoS modeling).

Modified Tait (isothermal)

The Modified Tait equation of state was developed by *[HuangChow74]*. It has the considerable benefit of allowing volume to be expressed as a function of pressure. It performs very well to pressures and temperatures relevant to the deep Earth *[HollandPowell11]*.

$$\begin{aligned} \frac{V_{P,T}}{V_{1bar,298K}} &= 1 - a(1 - (1 + bP)^{-c}), \\ a &= \frac{1 + K_0'}{1 + K_0' + K_0K_0''}, \\ b &= \frac{K_0'}{K_0} - \frac{K_0''}{1 + K_0'}, \\ c &= \frac{1 + K_0' + K_0K_0''}{K_0'^2 + K_0' - K_0K_0''} \end{aligned} \tag{3.5}$$

Mie-Grüneisen-Debye (thermal correction to Birch-Murnaghan)

The Debye model for the Helmholtz free energy can be written as follows *[MBR+07]*

$$\begin{aligned}
\mathcal{F} &= \frac{9nRT}{V}\frac{1}{x^3}\int_0^x \xi^2 \ln(1-e^{-\xi})d\xi, \\
x &= \theta/T, \\
\theta &= \theta_0 \exp\left(\frac{\gamma_0-\gamma}{q_0}\right), \\
\gamma &= \gamma_0\left(\frac{V}{V_0}\right)^{q_0}
\end{aligned}$$

where θ is the Debye temperature and γ is the Grüneisen parameter.

Using thermodynamic relations we can derive equations for the thermal pressure and bulk modulus

$$\begin{aligned}
P_{th}(V,T) &= -\frac{\partial \mathcal{F}(\mathcal{V},\mathcal{T})}{\partial V}, \\
&= \frac{3n\gamma RT}{V}D(x), \\
K_{th}(V,T) &= -V\frac{\partial P(V,T)}{\partial V}, \\
&= \frac{3n\gamma RT}{V}\gamma\left[(1-q_0-3\gamma)D(x)+3\gamma\frac{x}{e^x-1}\right], \\
D(x) &= \frac{3}{x^3}\int_0^x \frac{\xi^3}{e^\xi-1}d\xi
\end{aligned}$$

The thermal shear correction used in BurnMan was developed by *[HamaSuito98]*

$$G_{th}(V,T) = \frac{3}{5}\left[K_{th}(V,T) - 2\frac{3nRT}{V}\gamma D(x)\right]$$

The total pressure, bulk and shear moduli can be calculated from the following sums

$$\begin{aligned}
P(V,T) &= P_{\text{ref}}(V,T_0) + P_{th}(V,T) - P_{th}(V,T_0), \\
K(V,T) &= K_{\text{ref}}(V,T_0) + K_{th}(V,T) - K_{th}(V,T_0), \\
G(V,T) &= G_{\text{ref}}(V,T_0) + G_{th}(V,T) - G_{th}(V,T_0)
\end{aligned}$$

This equation of state is substantially the same as that in SLB2005 (see below). The primary differences are in the thermal correction to the shear modulus and in the volume dependences of the Debye temperature and the Gruneisen parameter.

HP2011 (thermal correction to Modified Tait)

The thermal pressure can be incorporated into the Modified Tait equation of state, replacing P with $P - (P_{\text{th}} - P_{\text{th0}})$ in Equation (3.5) *[HollandPowell11]*. Thermal pressure is calculated using a Mie-Grüneisen equation of state and an Einstein model for heat capacity, even though the Einstein model is not actually

used for the heat capacity when calculating the enthalpy and entropy (see following section).

$$
\begin{aligned}
P_{\text{th}} &= \frac{\alpha_0 K_0 E_{\text{th}}}{C_{V0}}, \\
E_{\text{th}} &= 3nR\Theta \left(0.5 + \frac{1}{\exp(\frac{\Theta}{T}) - 1} \right), \\
C_V &= 3nR \frac{(\frac{\Theta}{T})^2 \exp(\frac{\Theta}{T})}{(\exp(\frac{\Theta}{T}) - 1)^2}
\end{aligned}
$$

Θ is the Einstein temperature of the crystal in Kelvin, approximated for a substance i with n_i atoms in the unit formula and a molar entropy S_i using the empirical formula

$$
\Theta_i = \frac{10636}{S_i/n_i + 6.44}
$$

SLB2005 (for solids, thermal)

Thermal corrections for pressure, and isothermal bulk modulus and shear modulus are derived from the Mie-Grüneisen-Debye EoS with the quasi-harmonic approximation. Here we adopt the formalism of *[SLB05]* where these corrections are added to equations (3.2)–(3.4):

$$
\begin{aligned}
P_{th}(V,T) &= \frac{\gamma \Delta \mathcal{U}}{V}, \\
K_{th}(V,T) &= (\gamma + 1 - q)\frac{\gamma \Delta \mathcal{U}}{V} - \gamma^2 \frac{\Delta(C_V T)}{V}, \\
G_{th}(V,T) &= -\frac{\eta_S \Delta \mathcal{U}}{V}.
\end{aligned}
\tag{3.6}
$$

The Δ refers to the difference in the relevant quantity from the reference temperature (300 K). γ is the Grüneisen parameter, q is the logarithmic volume derivative of the Grüneisen parameter, η_S is the shear strain derivative of the Grüneisen parameter, C_V is the heat capacity at constant volume, and $\mathcal{U}$ is the internal energy at temperature T. C_V and $\mathcal{U}$ are calculated using the Debye model for vibrational energy of

a lattice. These quantities are calculated as follows:

$$
\begin{aligned}
C_V &= 9nR\left(\frac{T}{\theta}\right)^3 \int_0^{\frac{\theta}{T}} \frac{e^\tau \tau^4}{(e^\tau - 1)^2} d\tau, \\
\mathcal{U} &= 9nRT\left(\frac{T}{\theta}\right)^3 \int_0^{\frac{\theta}{T}} \frac{\tau^3}{(e^\tau - 1)} d\tau, \\
\gamma &= \frac{1}{6}\frac{\nu_0^2}{\nu^2}(2f+1)\left[a_{ii}^{(1)} + a_{iikk}^{(2)} f\right], \\
q &= \frac{1}{9\gamma}\left[18\gamma^2 - 6\gamma - \frac{1}{2}\frac{\nu_0^2}{\nu^2}(2f+1)^2 a_{iikk}^{(2)}\right], \\
\eta_S &= -\gamma - \frac{1}{2}\frac{\nu_0^2}{\nu^2}(2f+1)^2 a_S^{(2)}, \\
\frac{\nu^2}{\nu_0^2} &= 1 + a_{ii}^{(1)} f + \frac{1}{2} a_{iikk}^{(2)} f^2, \\
a_{ii}^{(1)} &= 6\gamma_0, \\
a_{iikk}^{(2)} &= -12\gamma_0 + 36\gamma_0^2 - 18 q_0 \gamma_0, \\
a_S^{(2)} &= -2\gamma_0 - 2\eta_{S0},
\end{aligned}
$$

where θ is the Debye temperature of the mineral, ν is the frequency of vibrational modes for the mineral, n is the number of atoms per formula unit (e.g. 2 for periclase, 5 for perovskite), and R is the gas constant. Under the approximation that the vibrational frequencies behave the same under strain, we may identify $\nu/\nu_0 = \theta/\theta_0$. The quantities γ_0, η_{S0} q_0, and θ_0 are the experimentally determined values for those parameters at the reference state.

Due to the fact that a planetary mantle is rarely isothermal along a geotherm, it is more appropriate to use the adiabatic bulk modulus K_S instead of K_T, which is calculated using

$$K_S = K_T(1 + \gamma\alpha T), \tag{3.7}$$

where α is the coefficient of thermal expansion:

$$\alpha = \frac{\gamma C_V V}{K_T}. \tag{3.8}$$

There is no difference between the isothermal and adiabatic shear moduli for an isotropic solid. All together this makes an eleven parameter EoS model, which is summarized in the Table below. For more details on the EoS, we refer readers to *[SLB05]*.

User Input	Symbol	Definition	Units
V_0	V_0	**Volume at P =** 10^5 Pa , T = 300 K	$m^3\ mol^{-1}$
K_0	K_0	Isothermal bulk modulus at *P=10^5* Pa, T = 300 K	Pa
Kprime_0	K'_0	Pressure derivative of K_0	
G_0	G_0	Shear modulus at P = 10^5 Pa, T = 300 K	Pa
Gprime_0	G'_0	Pressure derivative of G_0	
molar_mass	μ	mass per mole formula unit	$kg\ mol^{-1}$
n	n	number of atoms per formula unit	
Debye_0	θ_0	Debye Temperature	K
grueneisen_0	γ_0	Grüneisen parameter at P = 10^5 Pa, T = 300 K	
q0	q_0	Logarithmic volume derivative of the Grüneisen parameter	
eta_s_0	η_{S0}	Shear strain derivative of the Grüneisen parameter	

This equation of state is substantially the same as that of the Mie-Gruneisen-Debye (see above). The primary differences are in the thermal correction to the shear modulus and in the volume dependences of the Debye temperature and the Gruneisen parameter.

Compensated-Redlich-Kwong (for fluids, thermal)

The CORK equation of state *[HP91]* is a simple virial-type extension to the modified Redlich-Kwong (MRK) equation of state. It was designed to compensate for the tendency of the MRK equation of state to overestimate volumes at high pressures and accommodate the volume behaviour of coexisting gas and liquid phases along the saturation curve.

$$
\begin{aligned}
V &= \frac{RT}{P} + c_1 - \frac{c_0 R T^{0.5}}{(RT + c_1 P)(RT + 2c_1 P)} + c_2 P^{0.5} + c_3 P, \\
c_0 &= c_{0,0} T_c^{2.5}/P_c + c_{0,1} T_c^{1.5}/P_c T, \\
c_1 &= c_{1,0} T_c / P_c, \\
c_2 &= c_{2,0} T_c / P_c^{1.5} + c_{2,1}/P_c^{1.5} T, \\
c_3 &= c_{3,0} T_c / P_c^2 + c_{3,1}/P_c^2 T
\end{aligned}
$$

3.1.2 Calculating Thermodynamic Properties

So far, we have concentrated on the thermoelastic properties of minerals. There are, however, thermodynamic properties which depend on properties which do not affect the volume of the phase. These are the

internal energy, Helmholtz and Gibbs Free energies, entropy and heat capacities. These properties are related by the following expressions:

$$\mathcal{G} = \mathcal{E} - T\mathcal{S} + PV = \mathcal{H} - TS = \mathcal{F} + PV \tag{3.9}$$

where P is the pressure, T is the temperature and $\mathcal{E}$, $\mathcal{F}$, $\mathcal{H}$, $\mathcal{S}$ and V are the molar internal energy, Helmholtz free energy, enthalpy, entropy and volume respectively.

HP2011

$$\begin{aligned}
\mathcal{G}(P,T) &= \mathcal{H}_{\text{1 bar, T}} - T\mathcal{S}_{\text{1 bar, T}} + \int_{\text{1 bar}}^{P} V(P,T)\, dP, \\
\mathcal{H}_{\text{1 bar, T}} &= \Delta_f \mathcal{H}_{\text{1 bar, 298 K}} + \int_{298}^{T} C_P\, dT, \\
\mathcal{S}_{\text{1 bar, T}} &= \mathcal{S}_{\text{1 bar, 298 K}} + \int_{298}^{T} \frac{C_P}{T}\, dT, \\
\int_{\text{1 bar}}^{P} V(P,T)\, dP &= PV_0 \left(1 - a + \left(a\frac{(1-bP_{th})^{1-c} - (1+b(P-P_{th}))^{1-c}}{b(c-1)P}\right)\right)
\end{aligned} \tag{3.10}$$

The heat capacity at one bar is given by an empirical polynomial fit to experimental data

$$C_p = a + bT + cT^{-2} + dT^{-0.5}$$

The entropy at high pressure and temperature can be calculated by differentiating the expression for $\mathcal{G}$ with respect to temperature

$$\begin{aligned}
\mathcal{S}(P,T) &= S_{\text{1 bar, T}} + \frac{\partial \int V dP}{\partial T}, \\
\frac{\partial \int V dP}{\partial T} &= V_0 \alpha_0 K_0 a \frac{C_{V0}(T)}{C_{V0}(T_{\text{ref}})}((1+b(P-P_{th}))^{-c} - (1-bP_{th})^{-c})
\end{aligned}$$

Finally, the enthalpy at high pressure and temperature can be calculated

$$\mathcal{H}(P,T) = \mathcal{G}(P,T) + T\mathcal{S}(P,T)$$

SLB2005

The Debye model yields the Helmholtz free energy and entropy due to lattice vibrations

$$\begin{aligned}
\mathcal{G} &= \mathcal{F} + PV, \\
\mathcal{F} &= nRT\left(3\ln(1-e^{-\frac{\theta}{T}}) - \int_0^{\frac{\theta}{T}} \frac{\tau^3}{(e^\tau - 1)} d\tau\right), \\
\mathcal{S} &= nR\left(4\int_0^{\frac{\theta}{T}} \frac{\tau^3}{(e^\tau - 1)} d\tau - 3\ln(1-e^{-\frac{\theta}{T}})\right), \\
\mathcal{H} &= \mathcal{G} + T\mathcal{S}
\end{aligned}$$

3.1.3 Modifying Properties

There are a number of peculiarities of minerals which require modifications to the equations of state which are not contained within the thermodynamic frameworks listed above. Burnman currently includes implementations of the following:

- Linear excesses (useful for DQF modifications for *[HollandPowell11]*)
- Tricritical Landau model (two formulations)
- Bragg-Williams model
- Magnetic excesses

In all cases, the excess Gibbs free energy and first and second partial derivatives with respect to pressure and temperature are calculated. The thermodynamic properties of each phase are then modified in a consistent manner; specifically:

$$
\begin{aligned}
\mathcal{G} &= \mathcal{G}_o + \mathcal{G}_m, \\
\mathcal{S} &= \mathcal{S}_o - \frac{\partial \mathcal{G}}{\partial T}_m, \\
\mathcal{V} &= \mathcal{V}_o + \frac{\partial \mathcal{G}}{\partial P}_m, \\
K_T &= \mathcal{V} / \left(\frac{\mathcal{V}_o}{K_T o} - \frac{\partial^2 \mathcal{G}}{\partial P^2} \right)_m, \\
C_p &= C_p o - T \frac{\partial^2 \mathcal{G}}{\partial T^2}_m, \\
\alpha &= \left(\alpha_o \mathcal{V}_o + \frac{\partial^2 \mathcal{G}}{\partial P \partial T}_m \right) / \mathcal{V}, \\
\mathcal{H} &= \mathcal{G} + T\mathcal{S}, \\
\mathcal{F} &= \mathcal{G} - P\mathcal{V}, \\
C_v &= C_p - \mathcal{V} T \alpha^2 K_T, \\
\gamma &= \frac{\alpha K_T \mathcal{V}}{C_v}, \\
K_S &= K_T \frac{C_p}{C_v}
\end{aligned}
$$

Subscripts $_o$ and $_m$ indicate original properties and modifiers respectively. Importantly, this allows us to stack modifications such as multiple Landau transitions in a simple and straightforward manner.

In each of the following sections, $\mathcal{G}$ is the excess Gibbs free energy.

Linear excesses (linear)

$$\begin{aligned}
\mathcal{G} = \Delta\mathcal{E} - T\Delta\mathcal{S} + P\Delta\mathcal{V}, \\
\frac{\partial\mathcal{G}}{\partial T} = -\Delta\mathcal{S}, \\
\frac{\partial\mathcal{G}}{\partial P} = \Delta\mathcal{V}, \\
\frac{\partial^2\mathcal{G}}{\partial T^2} = 0, \\
\frac{\partial^2\mathcal{G}}{\partial P^2} = 0, \\
\frac{\partial^2\mathcal{G}}{\partial T\partial P} = 0
\end{aligned}$$

Tricritical Landau model (landau)

Applies a tricritical Landau correction to the properties of an endmember which undergoes a displacive phase transition. These transitions are not associated with an activation energy, and therefore they occur rapidly compared with seismic wave propagation. These minerals

This correction follows [Putnis1992], and is done relative to the completely *ordered* state (at 0 K). It therefore differs in implementation from both *[SLB11]* and *[HollandPowell11]*, who compute properties relative to the completely disordered state and standard states respectively. The current implementation is preferred, as the excess entropy (and heat capacity) terms are equal to zero at 0 K.

$$T_c = T_c0 + \frac{V_D P}{S_D}$$

If the temperature is above the critical temperature, Q (the order parameter) is equal to zero, and the Gibbs free energy is simply that of the disordered phase:

$$\begin{aligned}
\mathcal{G}_{\text{dis}} = -S_D \left((T - T_c) + \frac{T_{c0}}{3} \right), \\
\frac{\partial\mathcal{G}}{\partial P}_{\text{dis}} = V_D, \\
\frac{\partial\mathcal{G}}{\partial T}_{\text{dis}} = -S_D
\end{aligned}$$

If temperature is below the critical temperature, Q is between 0 and 1. The gibbs free energy can be described

thus:

$$
\begin{aligned}
Q^2 &= \sqrt{\left(1 - \frac{T}{T_c}\right)}, \\
\mathcal{G} &= S_D \left((T - T_c)Q^2 + \frac{T_{c0}Q^6}{3}\right) + \mathcal{G}_{\text{dis}}, \\
\frac{\partial \mathcal{G}}{\partial P} &= -V_D Q^2 \left(1 + \frac{T}{2T_c}\left(1. - \frac{T_{c0}}{T_c}\right)\right) + \frac{\partial \mathcal{G}}{\partial P}_{\text{dis}}, \\
\frac{\partial \mathcal{G}}{\partial T} &= S_D Q^2 \left(\frac{3}{2} - \frac{T_{c0}}{2T_c}\right) + \frac{\partial \mathcal{G}}{\partial T}_{\text{dis}}, \\
\frac{\partial^2 \mathcal{G}}{\partial P^2} &= V_D^2 \frac{T}{S_D T_c^2 Q^2}\left(\frac{T}{4T_c}\left(1. + \frac{T_{c0}}{T_c}\right) + Q^4\left(1. - \frac{T_{c0}}{Tc}\right) - 1\right), \\
\frac{\partial^2 \mathcal{G}}{\partial T^2} &= -\frac{S_D}{T_c Q^2}\left(\frac{3}{4} - \frac{T_{c0}}{4Tc}\right), \\
\frac{\partial^2 \mathcal{G}}{\partial P \partial T} &= \frac{V_D}{2TcQ^2}\left(1 + \left(\frac{T}{2Tc} - Q^4\right)\left(1 - \frac{T_{c0}}{Tc}\right)\right)
\end{aligned}
$$

Tricritical Landau model (landau_hp)

Applies a tricritical Landau correction similar to that described above. However, this implementation follows *[HollandPowell11]*, who compute properties relative to the standard state.

It is worth noting that the correction described by *[HollandPowell11]* has been incorrectly used throughout the geological literature, particularly in studies involving magnetite (which includes studies comparing oxygen fugacities to the FMQ buffer (due to an incorrect calculation of the properties of magnetite). Note that even if the implementation is correct, it still allows the order parameter Q to be greater than one, which is physically impossible.

We include this implementation in order to reproduce the dataset of *[HollandPowell11]*. If you are creating your own minerals, we recommend using the standard implementation.

$$T_c = T_c0 + \frac{V_D P}{S_D}$$

If the temperature is above the critical temperature, Q (the order parameter) is equal to zero. Otherwise

$$Q^2 = \sqrt{\left(\frac{T_c - T}{T_c0}\right)}$$

$$
\begin{aligned}
\mathcal{G} = Tc_0 S_D \left(Q_0^2 - \frac{Q_0^6}{3}\right) - S_D \left(TcQ^2 - Tc_0\frac{Q^6}{3}\right) - TS_D\left(Q_0^2 - Q^2\right) + PV_D Q_0^2, \\
\frac{\partial \mathcal{G}}{\partial P} = -V_D\left(Q^2 - Q_0^2\right), \\
\frac{\partial \mathcal{G}}{\partial T} = S_D\left(Q^2 - Q_0^2\right),
\end{aligned}
$$

The second derivatives of the Gibbs free energy are only non-zero if the order parameter exceeds zero. Then

$$\frac{\partial^2 \mathcal{G}}{\partial P^2} = -\frac{V_D^2}{2S_D T c_0 Q^2},$$
$$\frac{\partial^2 \mathcal{G}}{\partial T^2} = -\frac{S_D}{2T c_0 Q^2},$$
$$\frac{\partial^2 \mathcal{G}}{\partial P \partial T} = \frac{V_D}{2T c_0 Q^2}$$

Bragg-Williams model (bragg_williams)

The Bragg-Williams model is essentially a symmetric solid solution model between endmembers, with an excess configurational entropy term predicted on the basis of the specifics of order-disorder in the mineral, multiplied by some empirical factor. Expressions for the excess Gibbs free energy can be found in *[HP96]*.

Magnetic model (magnetic_chs)

This model approximates the excess energy due to magnetic ordering. It was originally described in *[CHS87]*. The expressions used by BurnMan can be found in *[Sun91]*.

3.2 Calculating Solid Solution Properties

Many minerals can exist over a range of compositions. The compositional domains of minerals with a common crystal structure are called solid solutions. Different elements substitute for one another within distinct crystallographic sites in the structure. For example, low pressure silicate garnets have two distinct sites on which mixing takes place; a dodecahedral site (3 per unit cell) and octahedral site (2 per unit cell). The chemical formula of many low pressure garnets exist within the solid solution:

$$[\mathrm{Mg,Fe,Mn,Ca}]_3[\mathrm{Al,Fe,Cr}]_2\mathrm{Si}_3\mathrm{O}_{12}$$

We typically calculate solid solution properties by appropriate differentiation of the Gibbs Free energy, where

$$\mathcal{G} = \sum_i n_i \left(\mathcal{G}_i + RT \ln \alpha_i\right)$$
$$\alpha_i = \gamma_i \alpha_{\text{ideal},i}$$

3.2.1 Implemented models

Ideal solid solutions

A solid solution is not simply a mechanical mixture of its constituent endmembers. Most fundamentally, the mixing of different elements on sites results in an excess configurational entropy

$$\mathcal{S}_{\text{conf}} = R \ln \prod_s (X_c^s)^\nu$$

where s is a site in the lattice M, c are the cations mixing on site s and ν is the number of s sites in the formula unit. Solid solutions where this configurational entropy is the only deviation from a mechanical mixture are termed *ideal*. From this expression, we can see that

$$\alpha_{\text{ideal},i} = \prod_s (X_c^s)^\nu$$

Symmetric solid solutions

Many minerals exhibit deviations from ideal solutions. These deviations arise as a result of interactions between ions with different physical and chemical characteristics. Regular solid solution models are designed to account for this, by allowing the addition of excess enthalpies, entropies and volumes to the solution model. These excess terms have the matrix form *[DPWH07]*

$$\mathcal{G}_{\text{excess}} = RT \ln \gamma = p^T W p$$

where p is a vector of molar fractions of each of the n endmembers and W is a strictly upper-triangular matrix of interaction terms between endmembers. Excesses within binary systems (i-j) have a quadratic form and a maximum of $W_{ij}/4$ half-way between the two endmembers.

Asymmetric solid solutions

Some solid solutions exhibit asymmetric excess terms. These can be accounted for with an asymmetric solid solution *[DPWH07]*

$$\mathcal{G}_{\text{excess}} = \alpha^T p(\phi^T W \phi)$$

α is a vector of "van Laar parameters" governing asymmetry in the excess properties.

$$\phi_i = \frac{\alpha_i p_i}{\sum_{k=1}^{n} \alpha_k p_k},$$
$$W_{ij} = \frac{2w_{ij}}{\alpha_i + \alpha_j} \text{for i<j}$$

The w_{ij} terms are a set of interaction terms between endmembers i and j. If all the α terms are equal to unity, a non-zero w yields an excess with a quadratic form and a maximum of $w/4$ half-way between the two endmembers.

Subregular solid solutions

An alternative way to create asymmetric solution models is to expand each binary term as a cubic expression *[HW89]*. In this case,

$$\mathcal{G}_{\text{excess}} = \sum_i p_i p_j^2 W_{ij} + p_j p_i^2 W_{ji}$$

Note the similarity with the symmetric solution model, the primary difference being that there are not two interaction terms for each binary.

3.2.2 Thermodynamic and thermoelastic properties

From the preceeding equations, we can define the thermodynamic potentials of solid solutions:

$$\mathcal{G}_{\rm SS} = \sum_i n_i \left(\mathcal{G}_i + RT \ln \alpha_i\right)$$
$$\mathcal{S}_{\rm SS} = \sum_i n_i \mathcal{S}_i + \mathcal{S}_{\rm conf} - \frac{\partial \mathcal{G}_{\rm excess}}{\partial T}$$
$$\mathcal{H}_{\rm SS} = \mathcal{G}_{\rm SS} + T\mathcal{S}_{\rm SS}$$
$$V_{\rm SS} = \sum_i n_i V_i + \frac{\partial \mathcal{G}_{\rm excess}}{\partial P}$$

We can also define the derivatives of volume with respect to pressure and temperature

$$\alpha_{P,\rm SS} = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P = \left(\frac{1}{V_{\rm SS}}\right)\left(\sum_i \left(n_i\, \alpha_i\, V_i\right)\right)$$
$$K_{T,\rm SS} = V\left(\frac{\partial P}{\partial V}\right)_T = V_{\rm SS}\left(\frac{1}{\sum_i \left(n_i \frac{V_i}{K_{Ti}}\right)} + \frac{\partial P}{\partial V_{\rm excess}}\right)$$

Making the approximation that the excess entropy has no temperature dependence

$$C_{P,\rm SS} = \sum_i n_i C_{Pi}$$
$$C_{V,\rm SS} = C_{P,\rm SS} - V_{\rm SS}\, T\, \alpha_{\rm SS}^2\, K_{T,\rm SS}$$
$$K_{S,\rm SS} = K_{T,\rm SS}\, \frac{C_{P,\rm SS}}{C_{V,\rm SS}}$$
$$\gamma_{\rm SS} = \frac{\alpha_{\rm SS}\, K_{T,\rm SS}\, V_{\rm SS}}{C_{V,\rm SS}}$$

3.2.3 Including order-disorder

Order-disorder can be treated trivially with solid solutions. The only difference between mixing between ordered and disordered endmembers is that disordered endmembers have a non-zero configurational entropy, which must be accounted for when calculating the excess entropy within a solid solution.

3.2.4 Including spin transitions

The regular solid solution formalism should provide an elegant way to model spin transitions in phases such as periclase and bridgmanite. High and low spin iron can be treated as different elements, providing distinct endmembers and an excess configurational entropy. Further excess terms can be added as necessary.

3.3 Calculating Multi-phase Composite Properties

3.3.1 Equilibrium composition

In any equilibrium problem at constant bulk composition with m endmembers, we have $m + 2$ unknowns, which are the compositions and amounts of the phases, and the pressure and temperature of the reaction. In order to solve such problems, a set of $m + 2$ equations is required.

Consider the m x n stoichiometric matrix $\mathbf{A}$ where the m rows correspond to the set of endmembers, and the n columns correspond to the elements contained within those compounds. We're interested in finding the set of independent reactions between the endmembers which do not change the bulk composition, i.e., the set of vectors contained within the left nullspace:

$$\mathcal{N}(\mathbf{A}^T) = \{\mathbf{y} \in \mathbb{R}^m \ : \ \mathbf{A}^T\mathbf{y} = 0\}$$

As will become clear later on, it is also useful to consider the set of vectors orthogonal to the left nullspace, which are known as the column space of A:

$$\mathcal{R}(\mathbf{A}) = \{\mathbf{y} \in \mathbb{R}^m \ : \ \mathbf{A}^T\mathbf{y} \neq 0\}$$

We can find the column space and left null space of $\mathbf{A}$ by singular value decomposition:

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$$

where $\mathbf{U}$ is an m x m matrix, $\mathbf{V}$ is an n x n matrix, and Σ is a m x n diagonal matrix where the diagonal entries are known as singular values. The left nullspace corresponds to the rows of U^T with singular values equal to zero.

Now that we have these m vectors, we can use them to set up an equilibrium relation. The equilibrium relation must hold for all the reactions described by the left nullspace. For each reaction, the equilibrium relation states that

$$0 = \sum_i n_i \left(\mathcal{G}_i + RT \ln \alpha_i\right)$$

For a pure phase, the activity α is equal to 1. A second requirement is that the bulk composition must not change. For this to be true, the compositional vector X must satisfy the following relationship

$$0 = \mathcal{R}(\mathbf{A}) \left(X - X_0\right)$$

where X_0 is any initial guess which satisfies the bulk composition. These two requirements yield m reactions. Two further equations are required to solve for the $m + 2$ unknowns, which may be constraints on the pressure, temperature or compositions of the phases.

3.3.2 Chemical potentials

3.3.3 Averaging schemes

Some of the properties of multiphase composites are simple arithmetic averages/sums of the properties of the individual phases. This is true, for example, of the Gibbs free energy and volume of aggregate materials:

$$\mathcal{G}_{\text{system}} = \sum_i n_i \mathcal{G}_i, \tag{3.11}$$

$$V = \sum_i n_i V_i, \tag{3.12}$$

$$\rho = \sum_i \nu_i \rho_i = \frac{1}{V} \sum_i n_i \mu_i \tag{3.13}$$

Unlike density and volume, the bulk and shear moduli of a multiphase rock are dependent on the shape, orientation and texture of the individual phases. We first define the volume fraction of the individual minerals in an assemblage:

$$\nu_i = n_i \frac{V_i}{V},$$

where V_i and n_i are the molar volume and the molar fractions of the i th individual phase. BurnMan allows several schemes for averaging the elastic moduli: the Voigt and Reuss bounds, the Hashin-Shtrikman bounds, the Voigt-Reuss-Hill average, and the Hashin-Shtrikman average *[WDOConnell76]*.

The Voigt average, assuming constant strain across all phases, is defined as

$$X_V = \sum_i \nu_i X_i, \tag{3.14}$$

where X_i is the bulk or shear modulus for the i th phase. The Reuss average, assuming constant stress across all phases, is defined as

$$X_R = \left(\sum_i \frac{\nu_i}{X_i} \right)^{-1}. \tag{3.15}$$

The Voigt-Reuss-Hill average is the arithmetic mean of Voigt and Reuss bounds:

$$X_{VRH} = \frac{1}{2} \left(X_V + X_R \right). \tag{3.16}$$

The Hashin-Shtrikman bounds make an additional assumption that the distribution of the phases is statistically isotropic and are usually much narrower than the Voigt and Reuss bounds *[WDOConnell76]*. This may be a poor assumption in regions of Earth with high anisotropy, such as the lowermost mantle, however these bounds are more physically motivated than the commonly-used Voigt-Reuss-Hill average. In most instances, the Voigt-Reuss-Hill average and the arithmetic mean of the Hashin-Shtrikman bounds are quite similar with the pure arithmetic mean (linear averaging) being well outside of both.

It is worth noting that each of the above bounding methods are derived from mechanical models of a linear elastic composite. It is thus only appropriate to apply them to elastic moduli, and not to other thermoelastic properties, such as wave speeds or density.

3.3.4 Computing seismic velocities

Once the moduli for the multiphase assemblage are computed, the compressional (P), shear (S) and bulk sound (Φ) velocities are then result from the equations:

$$V_P = \sqrt{\frac{K_S + \frac{4}{3}G}{\rho}}, \qquad V_S = \sqrt{\frac{G}{\rho}}, \qquad V_\Phi = \sqrt{\frac{K_S}{\rho}}. \tag{3.17}$$

To correctly compare to observed seismic velocities one needs to correct for the frequency sensitivity of attenuation. Moduli parameters are obtained from experiments that are done at high frequencies (MHz-GHz) compared to seismic frequencies (mHz-Hz). The frequency sensitivity of attenuation causes slightly lower velocities for seismic waves than they would be for high frequency waves. In BurnMan one can correct the calculated acoustic velocity values to those for long period seismic tomography *[MA81]*:

$$V_{S/P} = V_{S/P}^{\text{uncorr.}} \left(1 - \frac{1}{2}\cot(\frac{\beta\pi}{2})\frac{1}{Q_{S/P}}(\omega)\right).$$

Similar to *[MBR+07]*, we use a β value of 0.3, which falls in the range of values of 0.2 to 0.4 proposed for the lower mantle (e.g. *[KS90]*). The correction is implemented for Q values of PREM for the lower mantle. As Q_S is smaller than Q_P, the correction is more significant for S waves. In both cases, though, the correction is minor compared to, for example, uncertainties in the temperature (corrections) and mineral physical parameters. More involved models of relaxation mechanisms can be implemented, but lead to the inclusion of more poorly constrained parameters, *[MB07]*. While attenuation can be ignored in many applications *[TVV01]*, it might play a significant role in explaining strong variations in seismic velocities in the lowermost mantle *[DGD+12]*.

3.4 User input

3.4.1 Mineralogical composition

A number of pre-defined minerals are included in the mineral library and users can create their own. The library includes wrapper functions to include a transition from the high-spin mineral to the low-spin mineral *[LSMM13]* or to combine minerals for a given iron number.

Standard minerals – The 'standard' mineral format includes a list of parameters given in the above table. Each mineral includes a suggested EoS with which the mineral parameters are derived. For some minerals the parameters for the thermal corrections are not yet measured or calculated, and therefore the corrections can not be applied. An occasional mineral will not have a measured or calculated shear moduli, and therefore can only be used to compute densities and bulk sound velocities. The mineral library is subdivided by citation. BurnMan includes the option to produce a LaTeX; table of the mineral parameters used. BurnMan can be easily setup to incorporate uncertainties for these parameters.

Minerals with a spin transition – A standard mineral for the high spin and low spin must be defined separately. These minerals are "wrapped," so as to switch from the high spin to high spin mineral at a give pressure. While not realistic, for the sake of simplicity, the spin transitions are considered to be sharp at a given pressure.

Minerals depending on Fe partitioning – The wrapper function can partition iron, for example between ferropericlase, fp, and perovskite, pv. It requires the input of the iron mol fraction with regards to Mg, X_{fp} and X_{pv}, which then defines the chemistry of an Mg-Fe solid solution according to $(\text{Mg}_{1-X_{\text{Fe}}^{\text{fp}}}, \text{Fe}_{X_{\text{Fe}}^{\text{fp}}})\text{O}$ or $(\text{Mg}_{1-X_{\text{Fe}}^{\text{pv}}}, \text{Fe}_{X_{\text{Fe}}^{\text{pv}}})\text{SiO}_3$. The iron mol fractions can be set to be constant or varying with P and T as needed. Alternatively one can calculate the iron mol fraction from the distribution coefficient K_D defined as

$$K_D = \frac{X_{\text{Fe}}^{\text{pv}}/X_{\text{Mg}}^{\text{pv}}}{X_{\text{Fe}}^{\text{fp}}/X_{\text{Mg}}^{\text{fp}}}. \tag{3.18}$$

We adopt the formalism of *[NFR12]* choosing a reference distribution coefficient K_{D0} and standard state volume change (Δv^0) for the Fe-Mg exchange between perovskite and ferropericlase

$$K_D = K_{D0} \exp\left(\frac{(P_0 - P)\Delta v^0}{RT}\right), \tag{3.19}$$

where R is the gas constant and P_0 the reference pressure. As a default, we adopt the average Δv^0 of *[NFR12]* of $2 \cdot 10^{-7}\ m^3 mol^{-1}$ and suggest using their K_{D0} value of 0.5.

The multiphase mixture of these minerals can be built by the user in three ways:

1. Molar fractions of an arbitrary number of pre-defined minerals, for example mixing standard minerals mg_perovskite ($MgSiO_3$), fe_perovskite ($FeSiO_3$), periclase (MgO) and wüstite (FeO).

2. A two-phase mixture with constant or (P, T) varying Fe partitioning using the minerals that include Fe-dependency, for example mixing $(Mg, Fe)SiO_3$ and $(Mg, Fe)O$ with a pre-defined distribution coefficient.

3. Weight percents (wt%) of (Mg, Si, Fe) and distribution coefficient (includes (P,T)-dependent Fe partitioning). This calculation assumes that each element is completely oxidized into its corresponding oxide mineral (MgO, FeO, SiO_2) and then combined to form iron-bearing perovskite and ferropericlase taking into account some Fe partition coefficient.

3.4.2 Geotherm

Unlike the pressure, the temperature of the lower mantle is relatively unconstrained. As elsewhere, BurnMan provides a number of built-in geotherms, as well as the ability to use user-defined temperature-depth relationships. A geotherm in BurnMan is an object that returns temperature as a function of pressure. Alternatively, the user could ignore the geothermal and compute elastic velocities for a range of temperatures at any give pressure.

Currently, we include geotherms published by *[BS81]* and *[And82a]*. Alternatively one can use an adiabatic gradient defined by the thermoelastic properties of a given mineralogical model. For a homogeneous material, the adiabatic temperature profile is given by integrating the ordinary differential equation (ODE)

$$\left(\frac{\mathrm{d}T}{\mathrm{d}P}\right)_S = \frac{\gamma T}{K_S}. \tag{3.20}$$

This equation can be extended to multiphase composite using the first law of thermodynamics to arrive at

$$\left(\frac{\mathrm{d}T}{\mathrm{d}P}\right)_S = \frac{T\sum_i \frac{n_i C_{Pi}\gamma_i}{K_{Si}}}{\sum_i n_i C_{Pi}}, \tag{3.21}$$

where the subscripts correspond to the i th phase, C_P is the heat capacity at constant pressure of a phase, and the other symbols are as defined above. Integrating this ODE requires a choice in anchor temperature (T_0) at the top of the lower mantle (or including this as a parameter in an inversion). As the adiabatic geotherm is dependent on the thermoelastic parameters at high pressures and temperatures, it is dependent on the equation of state used.

3.4.3 Seismic Models

BurnMan allows for direct visual and quantitative comparison with seismic velocity models. Various ways of plotting can be found in the examples. Quantitative misfits between two profiles include an L2-norm and a chi-squared misfit, but user defined norms can be implemented. A seismic model in BurnMan is an object that provides pressure, density, and seismic velocities (V_P, V_Φ, V_S) as a function of depth.

To compare to seismically constrained profiles, BurnMan provides the 1D seismic velocity model PREM *[DA81]*. One can choose to evaluate $V_P, V_\Phi, V_S, \rho, K_S$ and/or G. The user can input their own seismic profile, an example of which is included using AK135 *[KEB95]*.

Besides standardized 1D radial profiles, one can also compare to regionalized average profiles for the lower mantle. This option accommodates the observation that the lowermost mantle can be clustered into two regions, a 'slow' region, which represents the so-called Large Low Shear Velocity Provinces, and 'fast' region, the continuous surrounding region where slabs might subduct *[LCDR12]*. This clustering as well as the averaging of the 1D model occurs over five tomographic S wave velocity models (SAW24B16: *[MegninR00]*; HMSL-S: *[HMSL08]*; S362ANI: *[KED08]*; GyPSuM: *[SFBG10]*; S40RTS: *[RDvHW11]*). The strongest deviations from PREM occur in the lowermost 1000 km. Using the 'fast' and 'slow' S wave velocity profiles is therefore most important when interpreting the lowermost mantle. Suggestion of compositional variation between these regions comes from seismology *[TRCT05][HW12]* as well as geochemistry *[DCT12][JCK+10]*. Based on thermo-chemical convection models, *[SDG11]* also show that averaging profiles in thermal boundary layers may cause problems for seismic interpretation.

We additionally apply cluster analysis to and provide models for P wave velocity based on two tomographic models (MIT-P08: *[LvdH08]*; GyPSuM: *[SMJM12]*). The clustering results correlate well with the fast and slow regions for S wave velocities; this could well be due to the fact that the initial model for the P wave velocity models is scaled from S wave tomographic velocity models. Additionally, the variations in P wave velocities are a lot smaller than for S waves. For this reason using these adapted models is most important when comparing the S wave velocities.

While interpreting lateral variations of seismic velocity in terms of composition and temperature is a major goal *[TDRY04][MCD+12]*, to determine the bulk composition the current challenge appears to be concurrently fitting absolute P and S wave velocities and incorporate the significant uncertainties in mineral physical parameters).

CHAPTER

FOUR

EXAMPLES

BurnMan comes with a small tutorial in the tutorial/ folder, and large collection of example programs under examples/. Below you can find a summary of the different examples. They are grouped into *Tutorial*, *Simple Examples*, and *More Advanced Examples*. We suggest starting with the tutorial before moving on to the simpler examples, especially if you are new to using BurnMan.

Finally, we also include the scripts that were used for all computations and figures in the 2014 BurnMan paper in the misc/ folder, see *Reproducing Cottaar, Heister, Rose and Unterborn (2014)*.

4.1 Tutorial

The tutorial for BurnMan currently consists of three separate units:

- `step 1`,
- `step 2`, and
- `step 3`.

4.1.1 CIDER 2014 BurnMan Tutorial — step 1

In this first part of the tutorial we will acquaint ourselves with a basic script for calculating the elastic properties of a mantle mineralogical model.

In general, there are three portions of this script:

1) Define a set of pressures and temperatures at which we want to calculate elastic properties

2) Setup a composite of minerals (or "rock") and calculate its elastic properties at those pressures and temperatures.

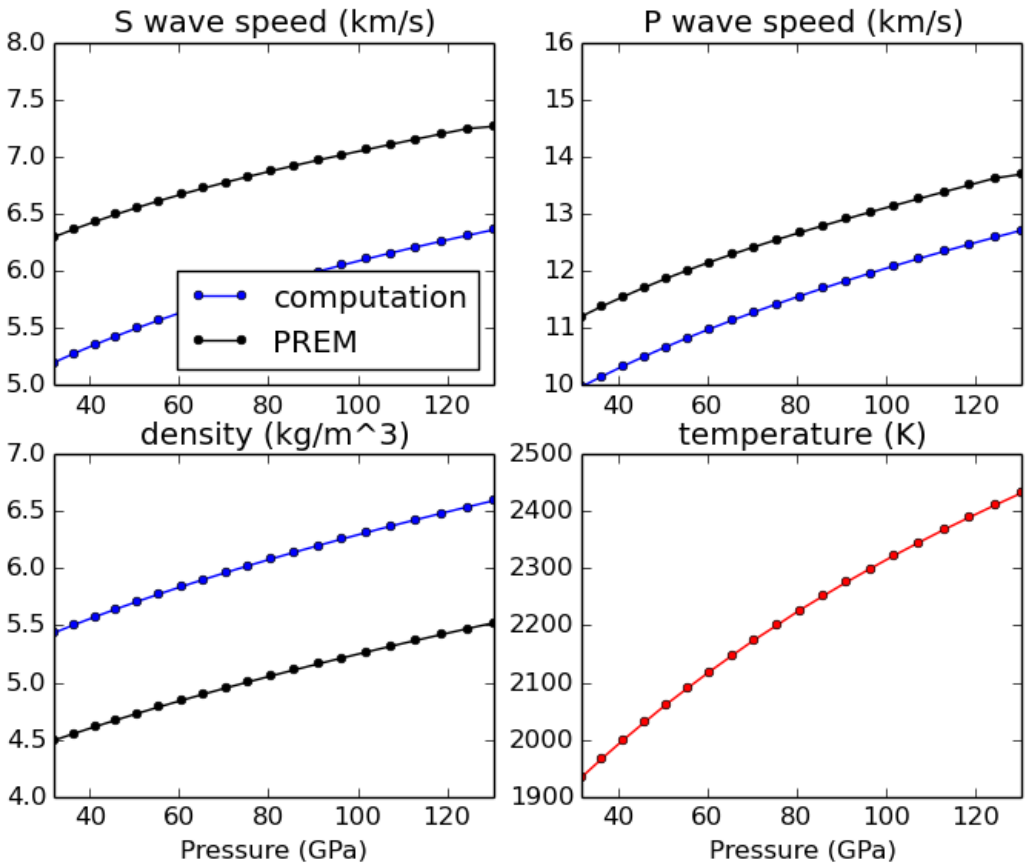
3) Plot those elastic properties, and compare them to a seismic model, in this case PREM

The script is basically already written, and should run as is by typing:

```
python step_1.py
```

on the command line. However, the mineral model for the rock is not very realistic, and you will want to change it to one that is more in accordance with what we think the bulk composition of Earth's lower mantle is.

When run (without putting in a more realistic composition), the program produces the following image:



Your goal in this tutorial is to improve this awful fit...

4.1.2 CIDER 2014 BurnMan Tutorial — step 2

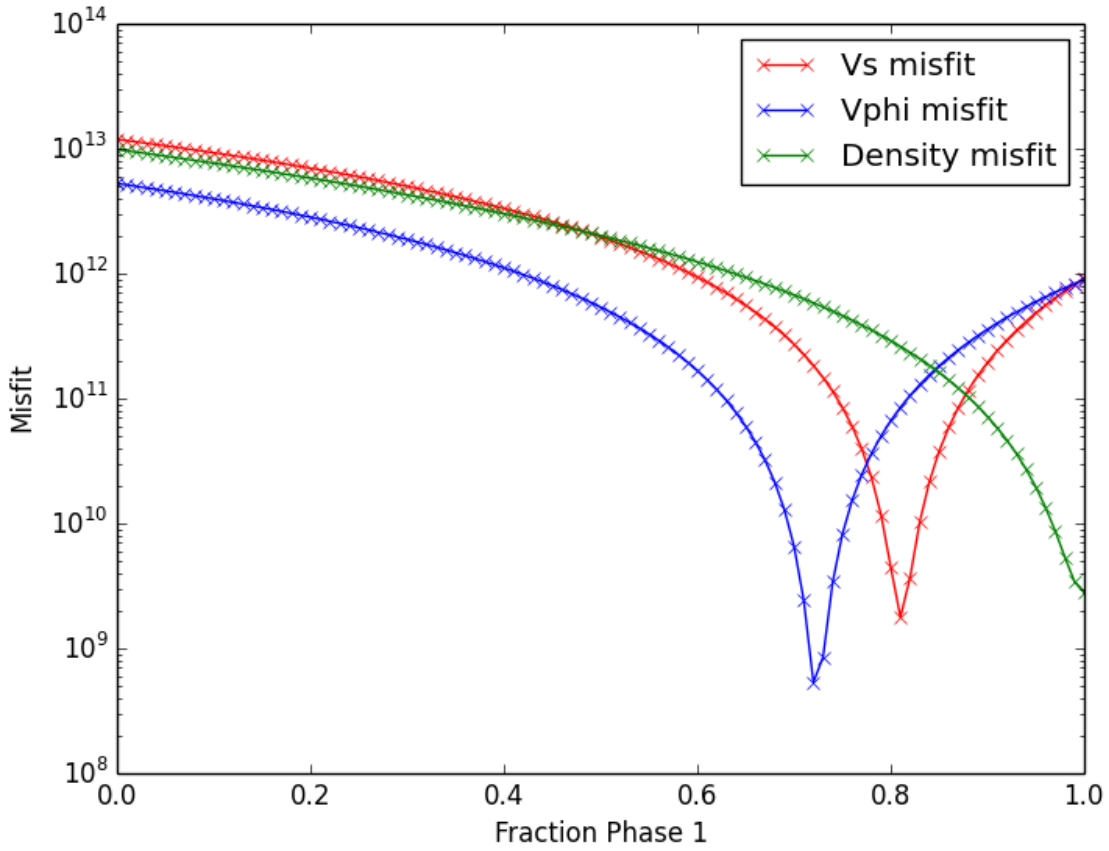
In this second part of the tutorial we try to get a closer fit to our 1D seismic reference model. In the simple Mg, Si, and O model that we used in step 1 there was one free parameter, namely phase_1_fraction, which goes between zero and one.

In this script we want to explore how good of a fit to PREM we can get by varying this fraction. We create a simple function that calculates a misfit between PREM and our mineral model as a function of phase_1_fraction, and then plot this misfit function to try to find a best model.

This script may be run by typing

```
python step_2.py
```

Without changing any input, the program should produce the following image showing the misfit as a function of perovskite content:



4.1.3 CIDER 2014 BurnMan Tutorial — step 3

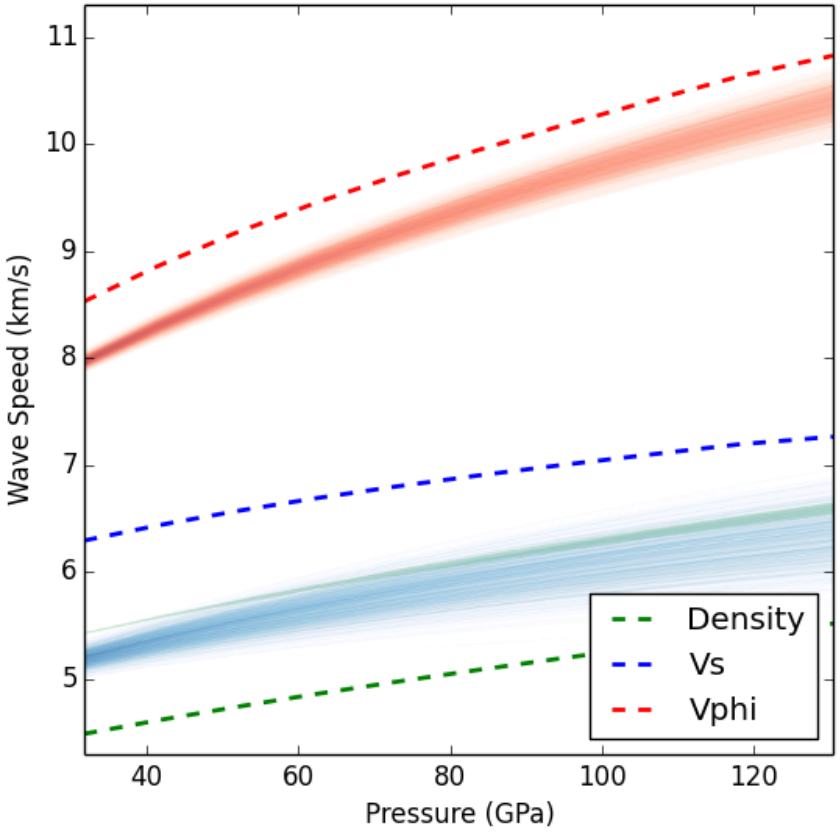
In the previous two steps of the tutorial we tried to find a very simple mineralogical model that best fit the 1D seismic model PREM. But we know that there is consideral uncertainty in many of the mineral physical parameters that control how the elastic properties of minerals change with pressure and temperature. In this step we explore how uncertainties in these parameters might affect the conclusions you draw.

The strategy here is to make many different "realizations" of the rock that you determined was the closest fit to PREM, where each realization has its mineral physical parameters perturbed by a small amount, hopefully related to the uncertainty in that parameter. In particular, we will look at how perturbations to K_0' and G_0' (the pressure derivatives of the bulk and shear modulus, respectively) change the calculated 1D seismic profiles.

This script may be run by typing

```
python step_3.py
```

After changing the standard deviations for K_0' and G_0' to 0.2, the following figure of velocities for 1000 realizations is produced:



4.2 Simple Examples

The following is a list of simple examples:

- *example_beginner*,
- *example_solid_solution*,
- *example_geotherms*,
- *example_seismic*,
- *example_composition*,
- *example_averaging*, and
- *example_chemical_potentials*.

4.2.1 example_beginner

This example script is intended for absolute beginners to BurnMan. We cover importing BurnMan modules, creating a composite material, and calculating its seismic properties at lower mantle pressures and

temperatures. Afterwards, we plot it against a 1D seismic model for visual comparison.

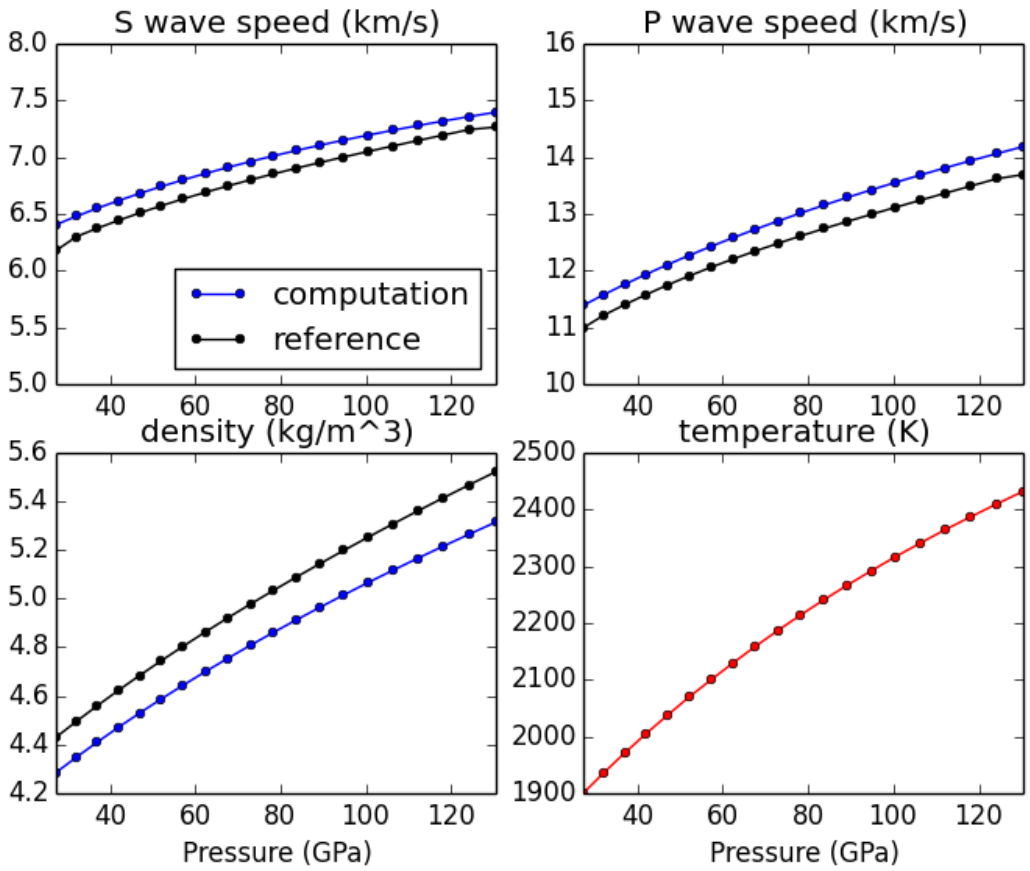
Uses:

- Mineral database
- *burnman.composite.Composite*
- *burnman.seismic.PREM*
- *burnman.geotherm.brown_shankland()*
- *burnman.material.Material.evaluate()*

Demonstrates:

- creating basic composites
- calculating thermoelastic properties
- seismic comparison

Resulting figure:



4.2.2 example_solid_solution

This example shows how to create different solid solution models and output thermodynamic and thermoelastic quantities.

There are four main types of solid solution currently implemented in BurnMan:

1. Ideal solid solutions
2. Symmmetric solid solutions
3. Asymmetric solid solutions
4. Subregular solid solutions

These solid solutions can potentially deal with:

- Disordered endmembers (more than one element on a crystallographic site)
- Site vacancies
- More than one valence/spin state of the same element on a site

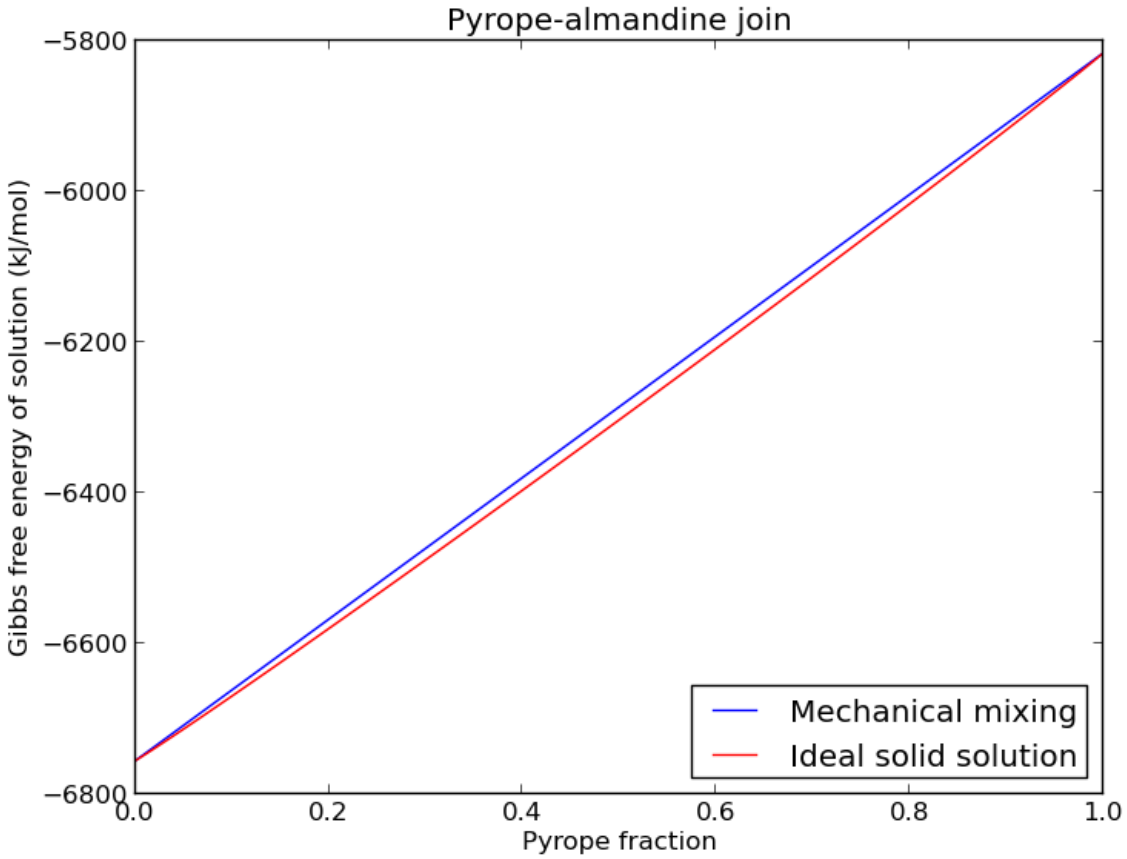
Uses:

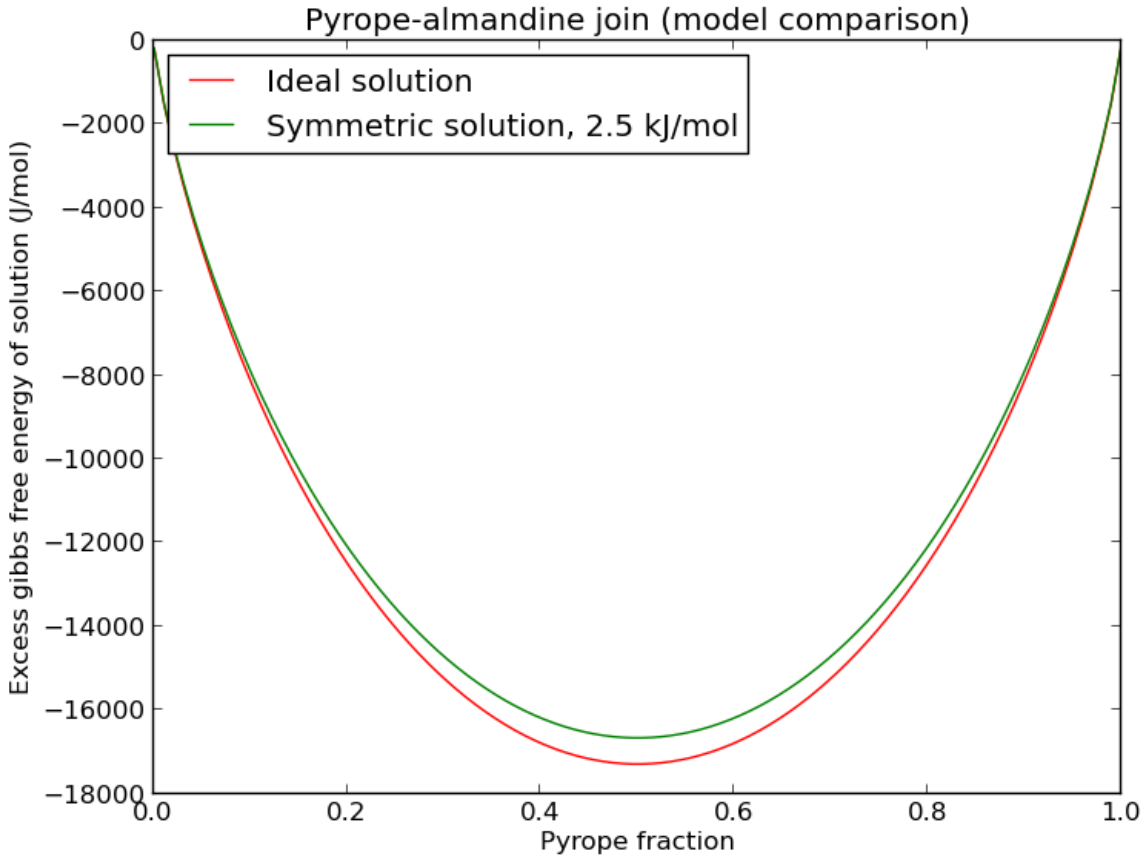
- Mineral database
- *burnman.solidsolution.SolidSolution*
- *burnman.solutionmodel.SolutionModel*

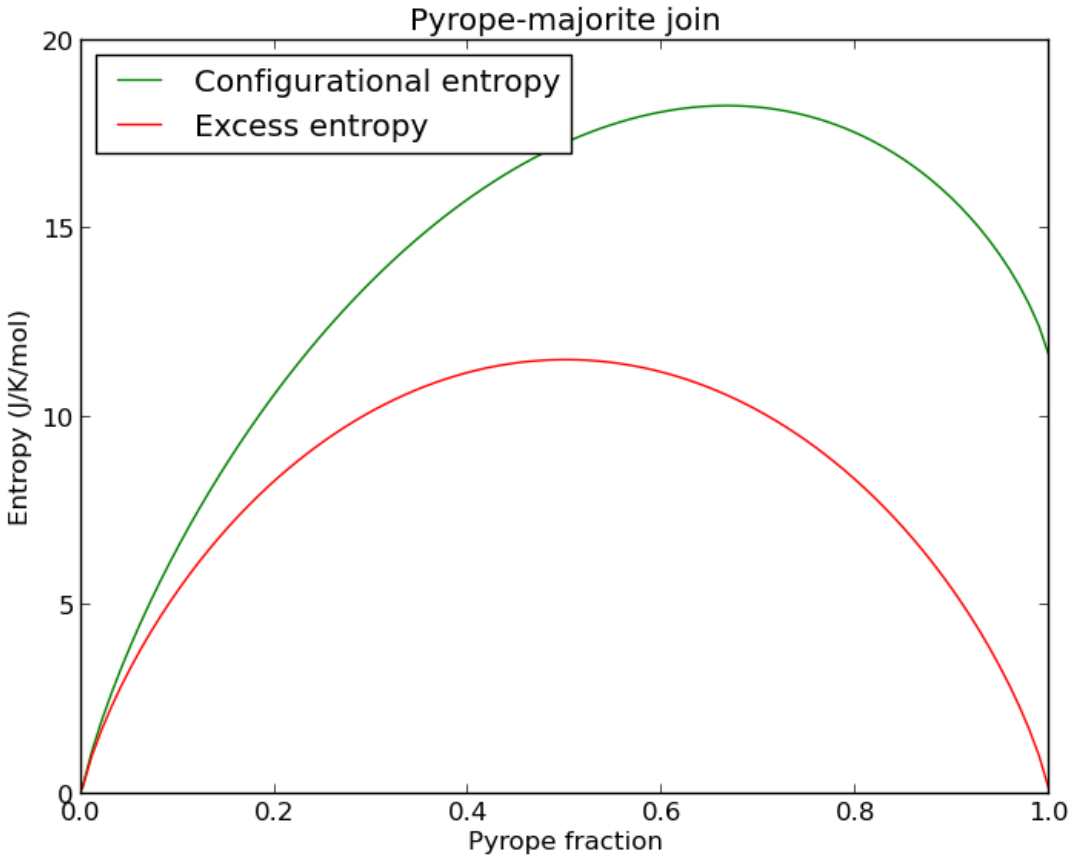
Demonstrates:

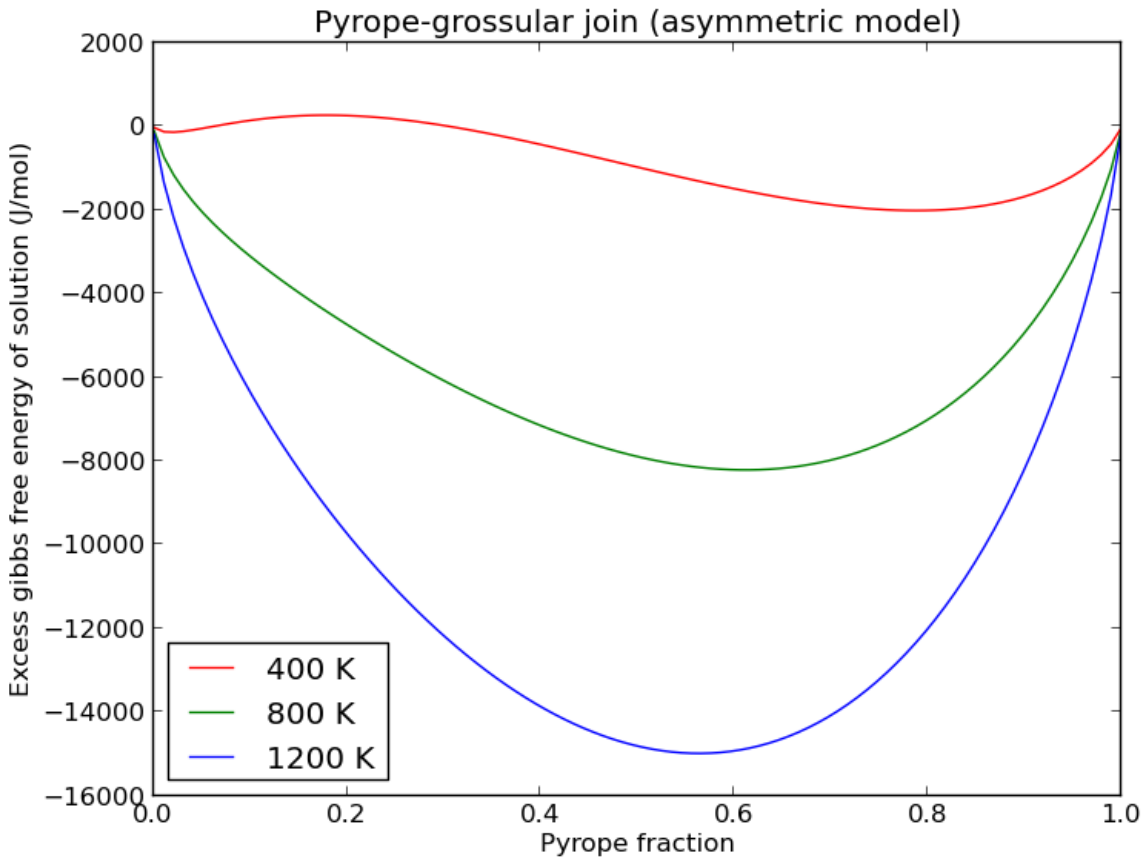
- Different ways to define a solid solution
- How to set composition and state
- How to output thermodynamic and thermoelastic properties

Resulting figures:


Pyrope-almandine join
Gibbs free energy of solution (kJ/mol)
−5800
−6000
−6200
−6400
−6600
−6800
0.0
0.2
0.4
0.6
0.8
1.0
Pyrope fraction
Mechanical mixing
Ideal solid solution


Pyrope-almandine join (model comparison)
Ideal solution
Symmetric solution, 2.5 kJ/mol
Excess gibbs free energy of solution (J/mol)
0
−2000
−4000
−6000
−8000
−10000
−12000
−14000
−16000
−18000
0.0
0.2
0.4
0.6
0.8
1.0
Pyrope fraction


Pyrope-majorite join
Configurational entropy
Excess entropy
Entropy (J/K/mol)
Pyrope fraction
0
5
10
15
20
0.0
0.2
0.4
0.6
0.8
1.0



4.2.3 example_geotherms

This example shows each of the geotherms currently possible with BurnMan. These are:

1. Brown and Shankland, 1981 *[BS81]*
2. Anderson, 1982 *[And82a]*
3. Watson and Baxter, 2007 *[WB07]*
4. linear extrapolation
5. Read in from file from user
6. Adiabatic from potential temperature and choice of mineral

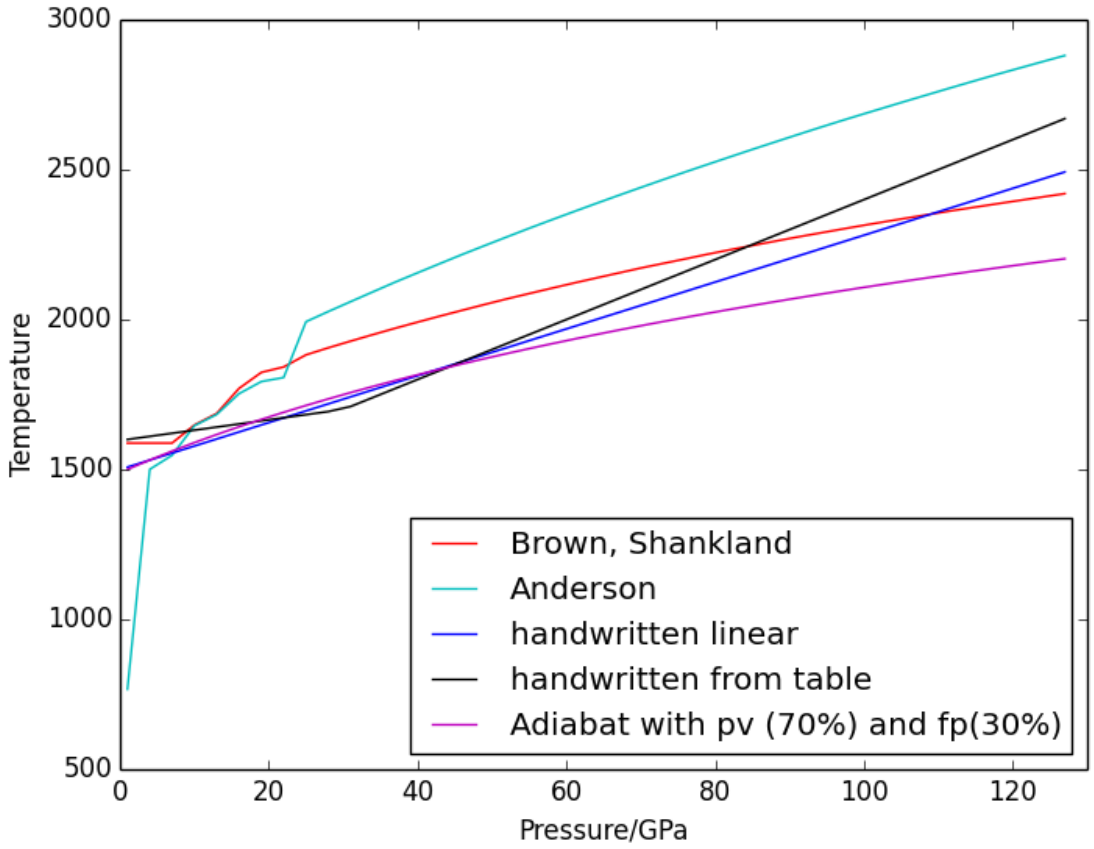
Uses:

- `burnman.geotherm.brown_shankland()`
- `burnman.geotherm.anderson()`
- input geotherm file *input_geotherm/example_geotherm.txt* (optional)
- `burnman.composite.Composite` for adiabat

Demonstrates:

- the available geotherms

Resulting figure:



4.2.4 example_seismic

Shows the various ways to input seismic models (V_s, V_p, V_ϕ, ρ) as a function of depth (or pressure) as well as different velocity model libraries available within Burnman:

1. PREM *[DA81]*
2. STW105 *[KED08]*
3. AK135 *[KEB95]*
4. IASP91 *[KE91]*

This example will first calculate or read in a seismic model and plot the model along the defined pressure range. The example also illustrates how to import a seismic model of your choice, here shown by importing AK135 *[KEB95]*.

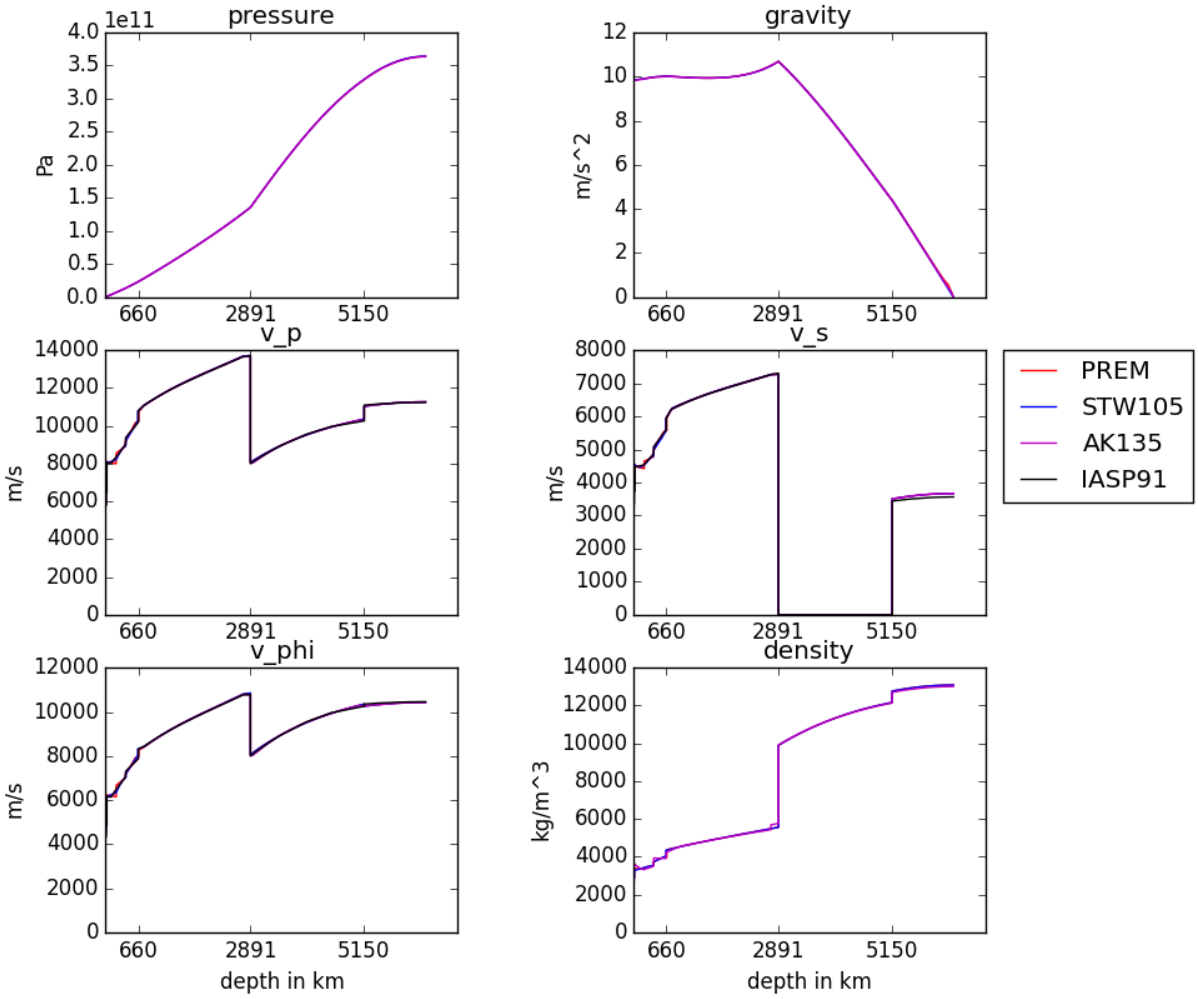
Uses:

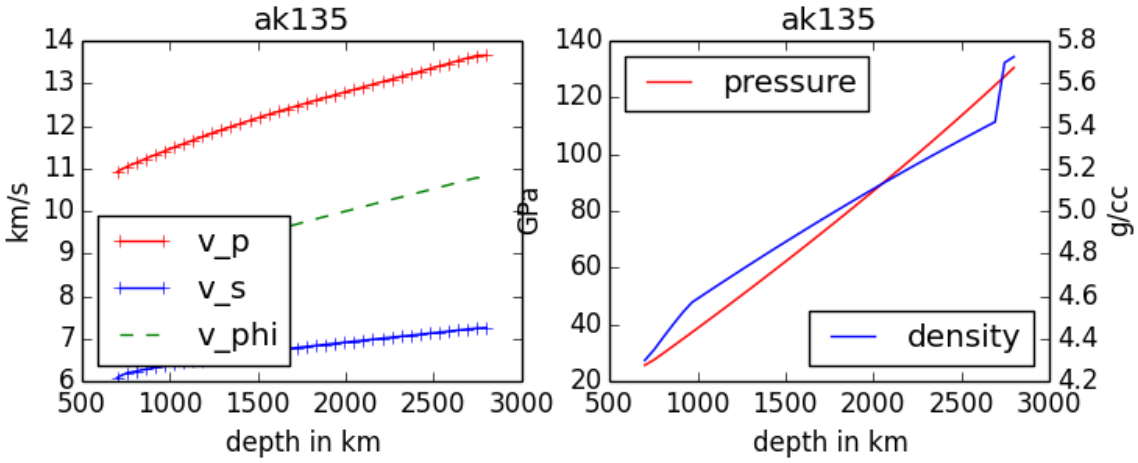
- Seismic

Demonstrates:

- Utilization of library seismic models within BurnMan
- Input of user-defined seismic models

Resulting figures:





4.2.5 example_composition

This example shows how to create different minerals, how to compute seismic velocities, and how to compare them to a seismic reference model.

There are many different ways in BurnMan to combine minerals into a composition. Here we present a couple of examples:

1. Two minerals mixed in simple mole fractions. Can be chosen from the BurnMan libraries or from user defined minerals (see example_user_input_material)
2. Example with three minerals
3. Using preset solid solutions
4. Defining your own solid solution

To turn a method of mineral creation "on" the first if statement above the method must be set to True, with all others set to False.

Note: These minerals can include a spin transition in (Mg,Fe)O, see example_spintransition.py for explanation of how to implement this

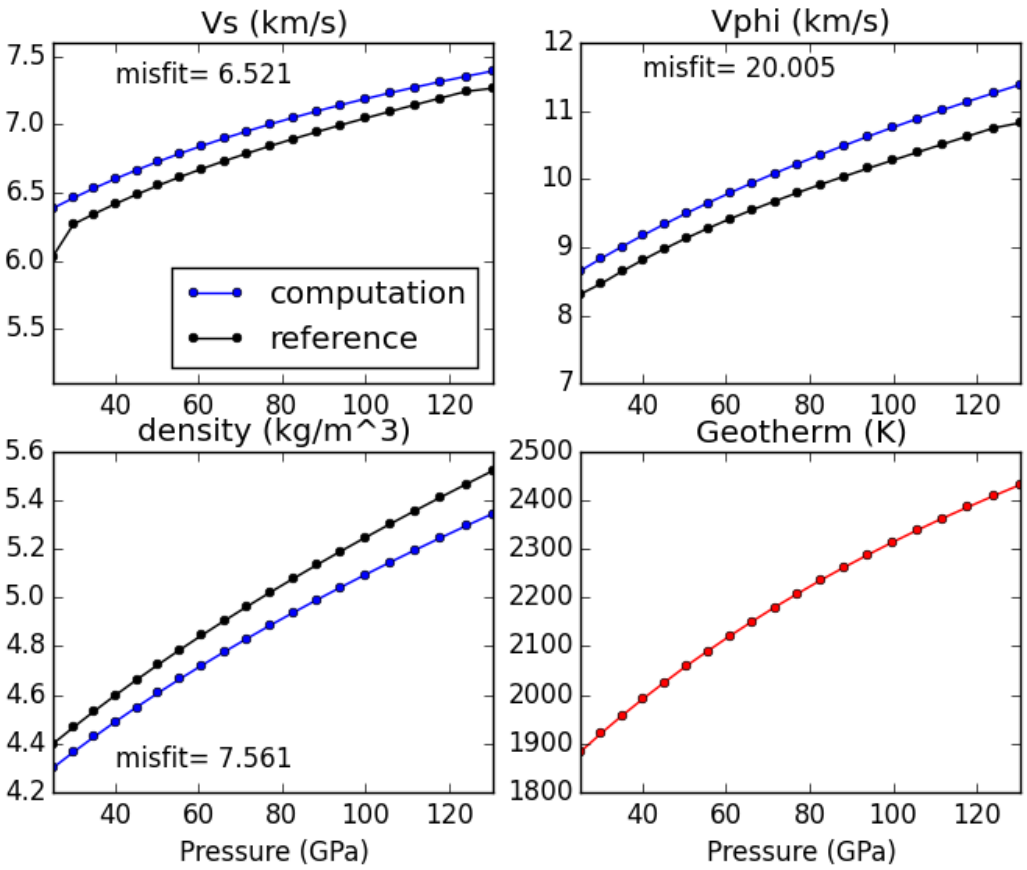
Uses:

- Mineral database
- *burnman.composite.Composite*
- *burnman.mineral.Mineral*
- *burnman.solidsolution.SolidSolution*

Demonstrates:

- Different ways to define a composite
- Using minerals and solid solutions
- Compare computations to seismic models

Resulting figure:



4.2.6 example_averaging

This example shows the effect of different averaging schemes. Currently four averaging schemes are available:

1. Voight-Reuss-Hill
2. Voight averaging

3. Reuss averaging
4. Hashin-Shtrikman averaging

See *[WDOConnell76]* Journal of Geophysics and Space Physics for explanations of each averaging scheme.

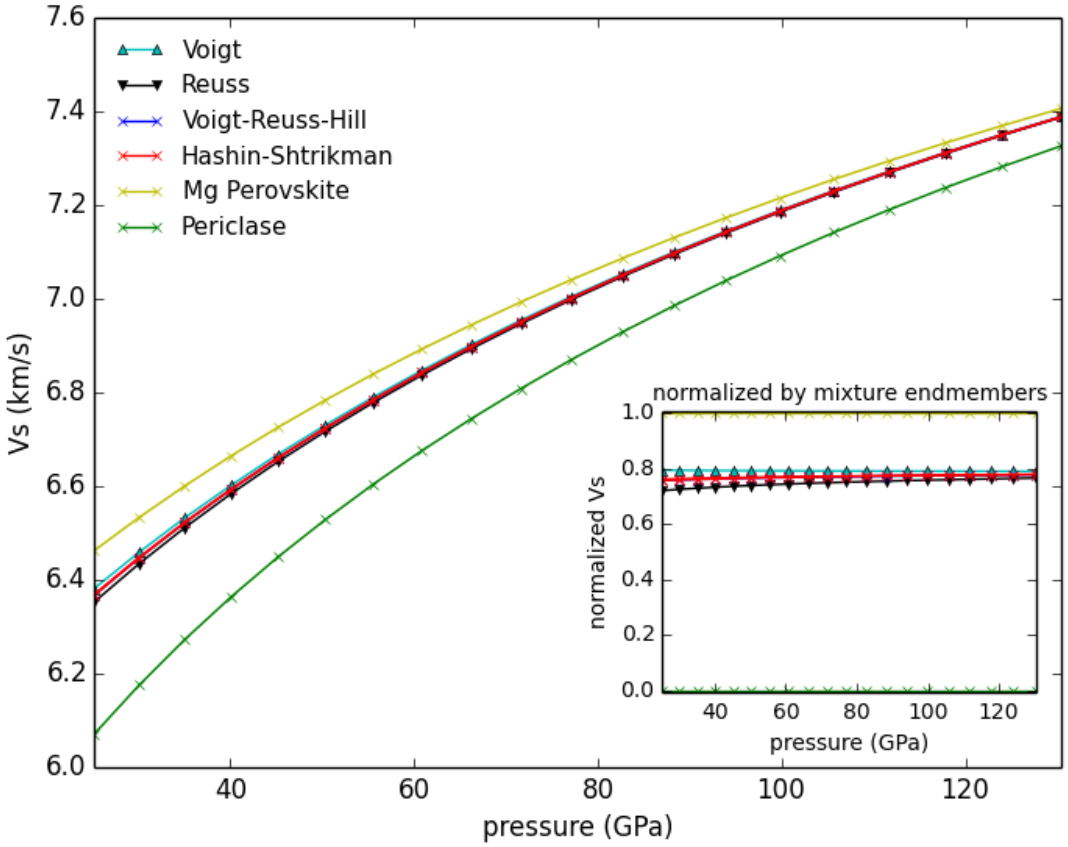
Specifically uses:

- `burnman.averaging_schemes.VoigtReussHill`
- `burnman.averaging_schemes.Voigt`
- `burnman.averaging_schemes.Reuss`
- `burnman.averaging_schemes.HashinShtrikmanUpper`
- `burnman.averaging_schemes.HashinShtrikmanLower`

Demonstrates:

- implemented averaging schemes

Resulting figure:



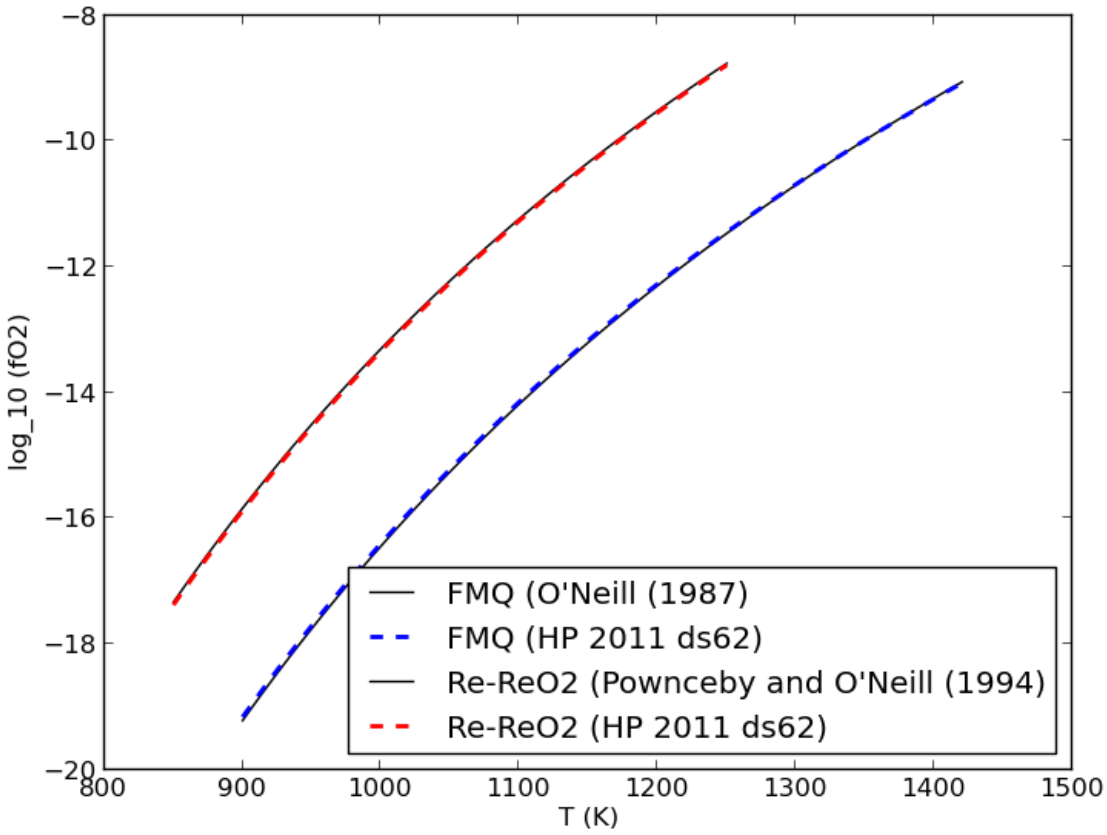
4.2.7 example_chemical_potentials

This example shows how to use the chemical potentials library of functions.

Demonstrates:

- How to calculate chemical potentials
- How to compute fugacities and relative fugacities

Resulting figure:



4.3 More Advanced Examples

Advanced examples:

- *example_spintransition*,
- *example_user_input_material*,
- *example_optimize_pv*, and
- *example_compare_all_methods*.

4.3.1 example_spintransition

This example shows the different minerals that are implemented with a spin transition. Minerals with spin transition are implemented by defining two separate minerals (one for the low and one for the high spin state). Then a third dynamic mineral is created that switches between the two previously defined minerals by comparing the current pressure to the transition pressure.

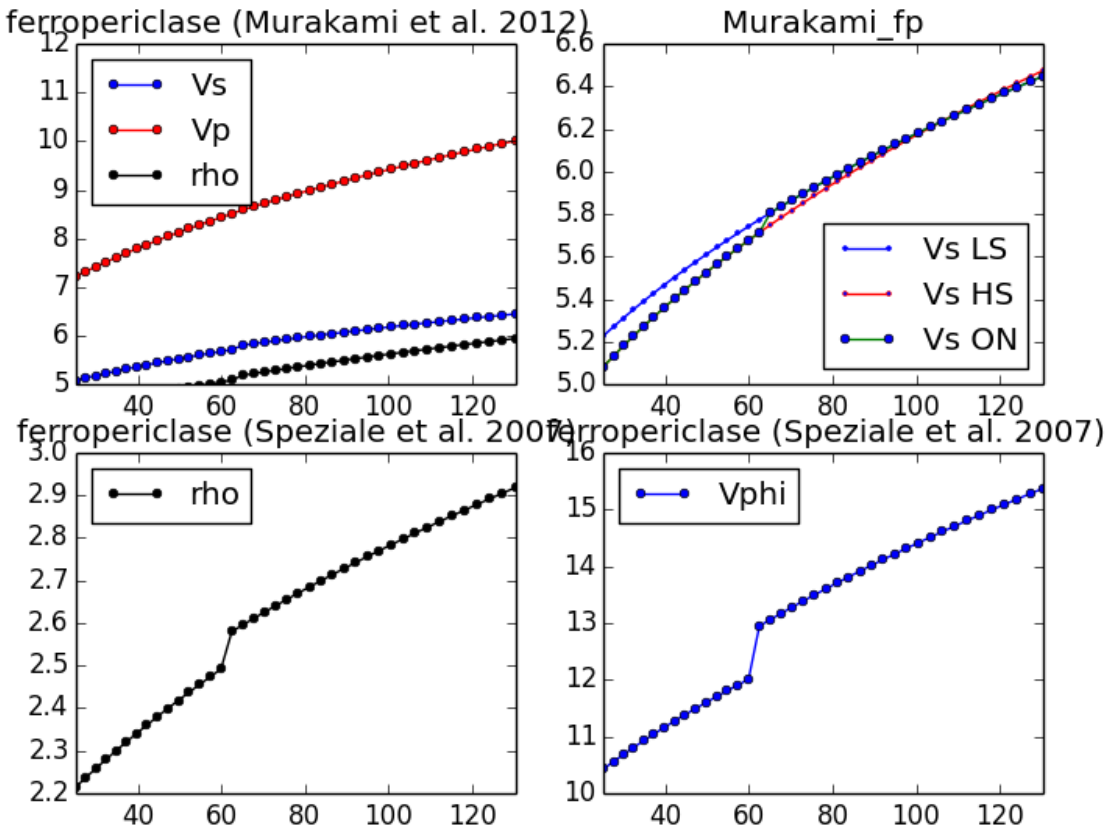
Specifically uses:

- *burnman.mineral_helpers.HelperSpinTransition()*
- *burnman.minerals.Murakami_etal_2012.fe_periclase()*
- *burnman.minerals.Murakami_etal_2012.fe_periclase_HS()*
- *burnman.minerals.Murakami_etal_2012.fe_periclase_LS()*

Demonstrates:

- implementation of spin transition in (Mg,Fe)O at user defined pressure

Resulting figure:



4.3.2 example_user_input_material

Shows user how to input a mineral of his/her choice without usint the library and which physical values need to be input for BurnMan to calculate V_P, V_Φ, V_S and density at depth.

Specifically uses:

- *burnman.mineral.Mineral*

Demonstrates:

- how to create your own minerals

4.3.3 example_optimize_pv

Vary the amount perovskite vs. ferropericlase and compute the error in the seismic data against PREM. For more extensive comments on this setup, see tutorial/step_2.py

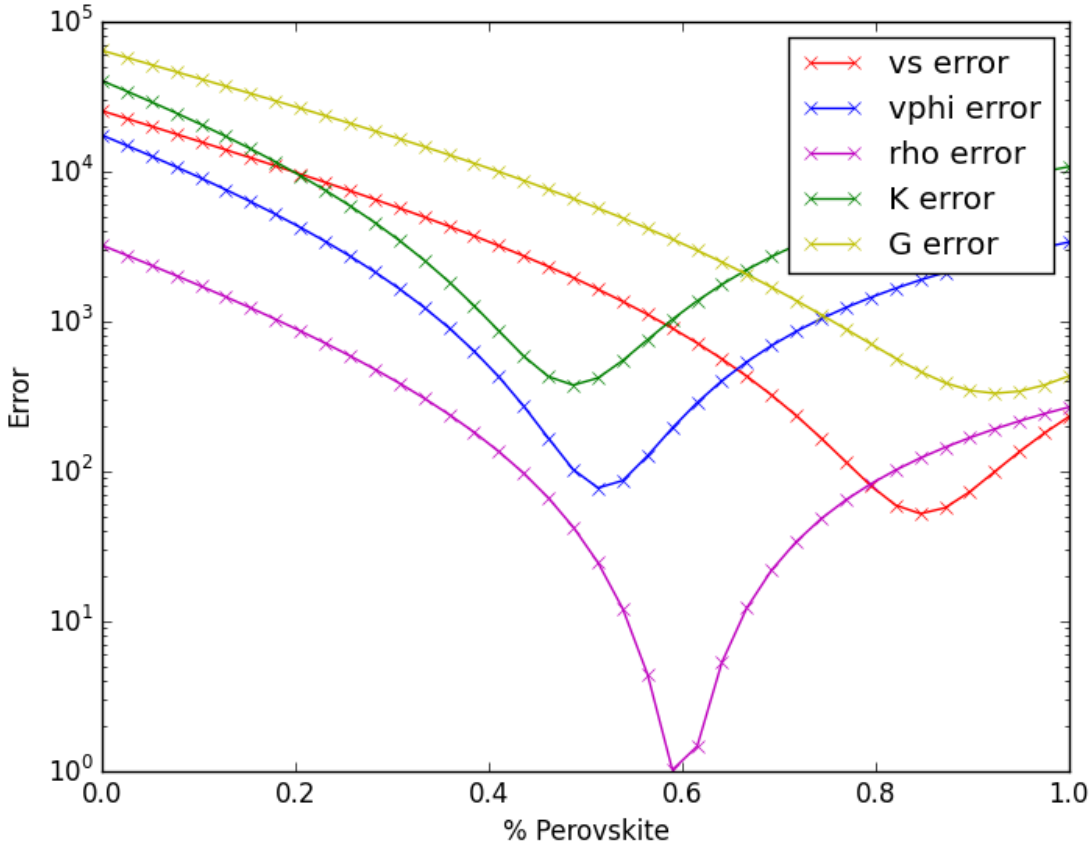
Uses:

- Mineral database
- *burnman.composite.Composite*
- *burnman.seismic.PREM*
- *burnman.geotherm.brown_shankland()*
- *burnman.material.Material.evaluate()*
- *burnman.main.compare_l2()*

Demonstrates:

- compare errors between models
- loops over models

Resulting figure:



4.3.4 example_build_planet

For Earth we have well-constrained one-dimensional density models. This allows us to calculate pressure as a funcion of depth. Furthermore, petrologic data and assumptions regarding the convective state of the planet allow us to estimate the temperature.

For planets other than Earth we have much less information, and in particular we know almost nothing about the pressure and temperature in the interior. Instead, we tend to have measurements of things like mass, radius, and moment-of-inertia. We would like to be able to make a model of the planet's interior that is consistent with those measurements.

However, there is a difficulty with this. In order to know the density of the planetary material, we need to know the pressure and temperature. In order to know the pressure, we need to know the gravity profile. And in order to the the gravity profile, we need to know the density. This is a nonlinear problem which requires us to iterate to find a self-consistent solution.

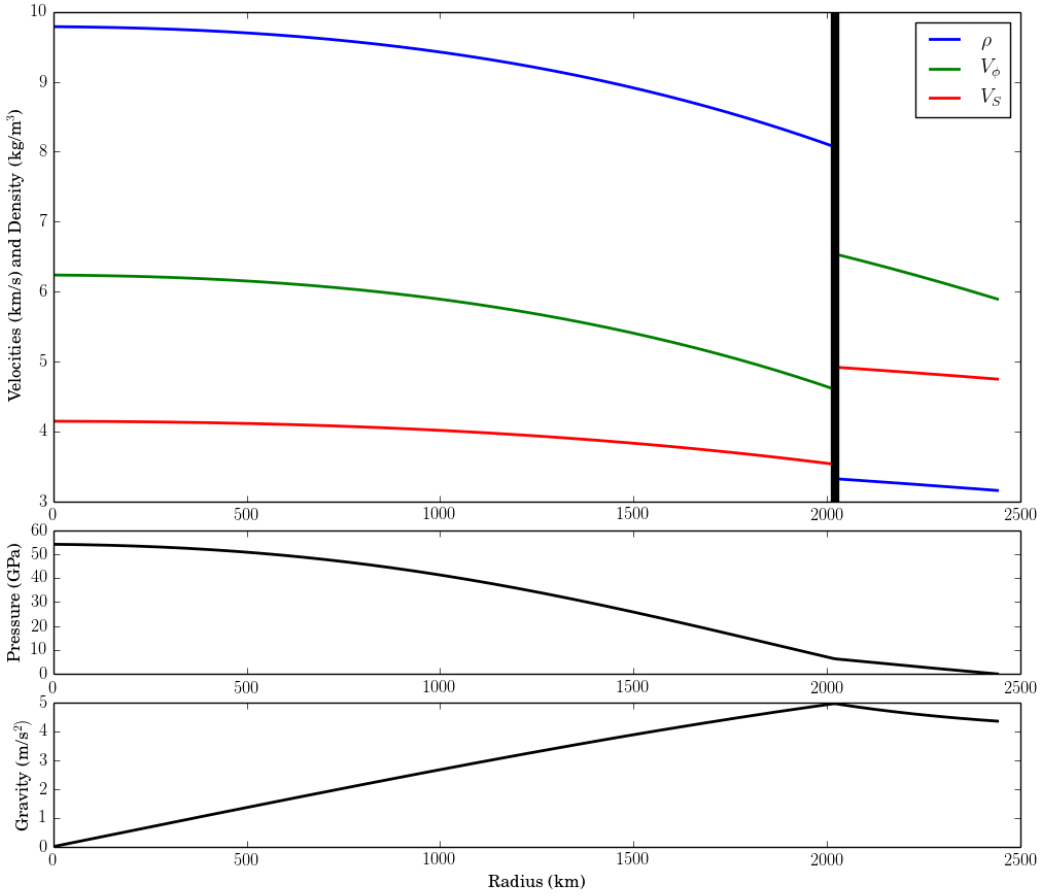
Here we show an example that does this, using the planet Mercury as motivation.

Uses:

- Mineral database
- `burnman.composite.Composite`

- *burnman.material.Material.evaluate()*

Resulting figure:



4.3.5 example_compare_all_methods

This example demonstrates how to call each of the individual calculation methodologies that exist within BurnMan. See below for current options. This example calculates seismic velocity profiles for the same set of minerals and a plot of V_s, V_ϕ and ρ is produce for the user to compare each of the different methods.

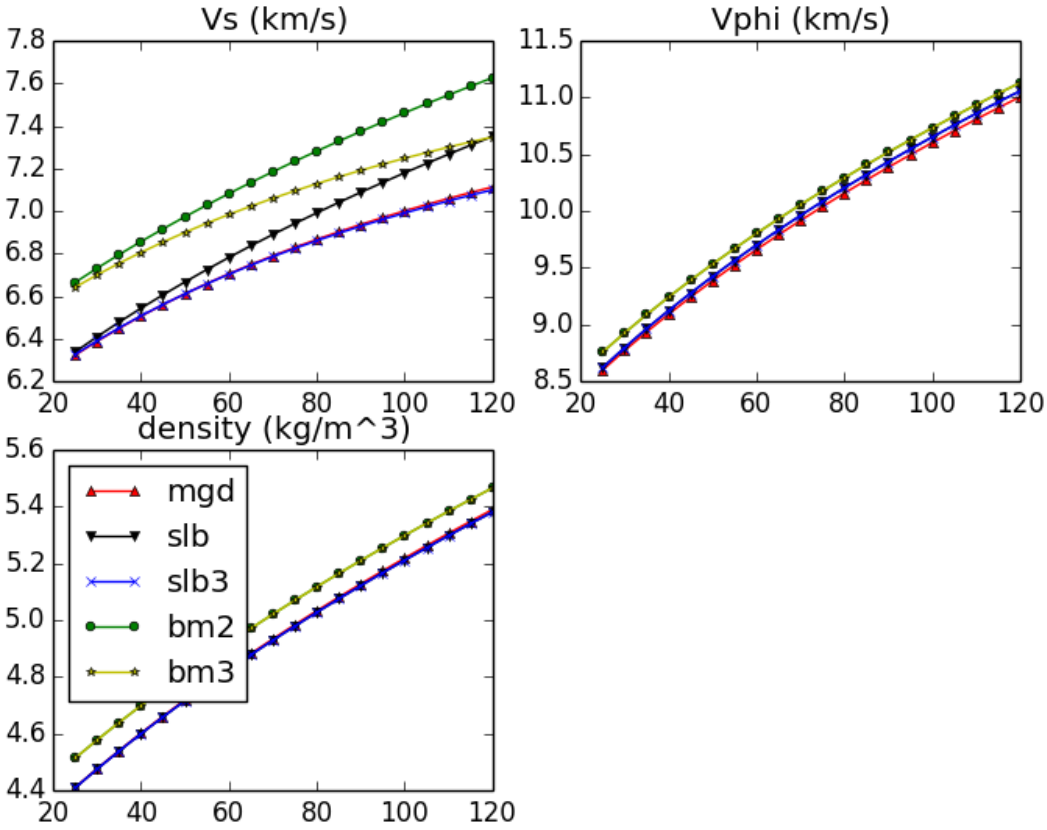
Specifically uses:

- Equations of state

Demonstrates:

- Each method for calculating velocity profiles currently included within BurnMan

Resulting figure:



4.4 Reproducing Cottaar, Heister, Rose and Unterborn (2014)

In this section we include the scripts that were used for all computations and figures in the 2014 BurnMan paper: Cottaar, Heister, Rose & Unterborn (2014) *[CHRU14]*

4.4.1 paper_averaging

This script reproduces *[CHRU14]*, Figure 2.

This example shows the effect of different averaging schemes. Currently four averaging schemes are available: 1. Voight-Reuss-Hill 2. Voight averaging 3. Reuss averaging 4. Hashin-Shtrikman averaging

See *[WDOConnell76]* for explanations of each averaging scheme.

requires: - geotherms - compute seismic velocities

teaches: - averaging

4.4.2 paper_benchmark

This script reproduces the benchmark in *[CHRU14]*, Figure 3.

4.4.3 paper_fit_data

This script reproduces *[CHRU14]* Figure 4.

This example demonstrates BurnMan's functionality to fit thermoelastic data to both 2nd and 3rd orders using the EoS of the user's choice at 300 K. User's must create a file with P, T and V_s. See input_minphys/ for example input files.

requires: - compute seismic velocities

teaches: - averaging

`misc.paper_fit_data.`**`calc_shear_velocities`**(*G_0*, *Gprime_0*, *mineral*, *pressures*)

`misc.paper_fit_data.`**`error`**(*guess*, *test_mineral*, *pressures*, *obs_vs*)

4.4.4 paper_incorrect_averaging

This script reproduces *[CHRU14]*, Figure 5. Attempt to reproduce Figure 6.12 from *[Mur13]*

4.4.5 paper_opt_pv

This script reproduces *[CHRU14]*, Figure 6. Vary the amount perovskite vs. ferropericlase and compute the error in the seismic data against PREM.

requires: - creating minerals - compute seismic velocities - geotherms - seismic models - seismic comparison

teaches: - compare errors between models - loops over models

4.4.6 paper_onefit

This script reproduces *[CHRU14]*, Figure 7. It shows an example for a best fit for a pyrolitic model within mineralogical error bars.

4.4.7 paper_uncertain

This script reproduces *[CHRU14]*, Figure 8. It shows the sensitivity of the velocities to various mineralogical parameters.

4.5 Misc or work in progress

4.5.1 example_compare_enstpyro

This example shows you how to create two materials from wt% determines the optimum mixing between the two to match the seismic model of your choice. Currently it compares two end member meteorite groups among the chondrites: carbonaceous and enstatite. Velocities are calculated for each set of minerals and plotted for comparison.

requires: - geotherms - seismic models - compute seismic velocities - creating minerals

teaches: - weight percent materials

4.5.2 example_parition_coef

This example shows how to vary the distribution coefficient of the perovskite/ferropericlase system. The user sets K_{d0} and BurnMan scales K_d as a function of P and T adopting the formalism of *[NFR12]*. Specifically we adopt equation 5 of *[NFR12]* with ΔV_0 = 0.2 cc/mol, and calculating the partition coefficient of Fe in each phase from stoichiometry.

This example will calculate mineral input parameters from Mg and Fe endmembers from Stixrude and Lithgow-bertelloni, 2005 with weighting determined by the calculated partition coefficients. Finally, output plots of X_{Fe} in pv and X_{Fe} in fp our output as well as the user's choice of geotherm

requires: - geotherms -input distribution coefficient K_{d0}

teaches: - creating varying proportions of Fe and its effect on seismic velocities

4.5.3 example_fit_data

This example demonstrates BurnMan's functionality to fit thermoelastic data to both 2nd and 3rd orders using the EoS of the user's choice at 300 K. User's must create a file with P, T and V_s. See input_minphys/ for example input files.

requires: - compute seismic velocities

teaches: - averaging

4.5.4 example_grid

This example shows how to evaluate seismic quantities on a P, T grid.

4.5.5 example_woutput

This example explains how to perform the basic i/o of BurnMan. A method of calculation is chosen, a composite mineral/material (see example_composition.py for explanation of this process) is created in the class "rock," finally a geotherm is created and seismic velocities calculated.

Post-calculation, the results are written to a simple text file to plot/manipulate at the user's whim.

requires: - creating minerals - compute seismic velocities - geotherms

teaches: - output computed seismic data to file

CHAPTER

FIVE

MAIN MODULE

burnman.main.**velocities_from_rock**(*rock*, *pressures*, *temperatures*, *averaging_scheme=<burnman.averaging_schemes.VoigtReussHill object>*)

This function is deprecated. Use *burnman.material.Material.evaluate()* instead.

A function that rolls several steps into one: given a rock and a list of pressures and temperatures, it calculates the elastic moduli of the individual phases using calculate_moduli(), averages them using average_moduli(), and calculates the seismic velocities using compute_velocities().

Parameters **rock** : burnman.Material

this is the rock for which you are calculating velocities

pressures: list of float

list of pressures you want to evaluate the rock at. $[Pa]$

temperatures: list of float

list of temperatures you want to evaluate the rock at. $[K]$

averaging_scheme: :class:'burnman.averaging_schemes.AveragingScheme'

Averaging scheme to use.

Returns **rho, V_p, V_s, V_phi, K, G** : lists of floats

Lists of density [kg/m^3], P-wave velocity [m/s], shear-wave velocity [m/s], bulk sound velocity [m/s], bulk modulus [Pa], and shear modulus [Pa] for each P,T point.

burnman.main.**compare_l2**(*depth*, *calc*, *obs*)

PUT IN TOOLS Computes the L2 norm for N profiles at a time (assumed to be linear between points).

$$mathdoesnotworkyet... \sum_{i=1}^{\infty} x_i$$

Parameters

- **depths** (*array of float*) – depths. $[m]$
- **calc** (*list of arrays of float*) – N arrays calculated values, e.g. [mat_vs,mat_vphi]

- **obs** (*list of arrays of float*) – N arrays of values (observed or calculated) to compare to , e.g. [seis_vs, seis_vphi]

Returns array of L2 norms of length N

Return type array of floats

burnman.main.**compare_chifactor**(*calc*, *obs*)

PUT IN TOOLS Computes the chi factor for N profiles at a time. Assumes a 1% a priori uncertainty on the seismic model.

Parameters

- **calc** (*list of arrays of float*) – N arrays calculated values, e.g. [mat_vs,mat_vphi]
- **obs** (*list of arrays of float*) – N arrays of values (observed or calculated) to compare to , e.g. [seis_vs, seis_vphi]

Returns error array of length N

Return type array of floats

burnman.main.**l2**(*x*, *funca*, *funcb*)

PUT IN TOOLS Computes the L2 norm for one profile(assumed to be linear between points).

Parameters

- **x** (*array of float*) – depths $[m]$.
- **funca** (*list of arrays of float*) – array calculated values
- **funcb** (*list of arrays of float*) – array of values (observed or calculated) to compare to

Returns L2 norm

Return type array of floats

burnman.main.**nrmse**(*x*, *funca*, *funcb*)

PUT IN TOOLS Normalized root mean square error for one profile :type x: array of float :param x: depths in m. :type funca: list of arrays of float :param funca: array calculated values :type funcb: list of arrays of float :param funcb: array of values (observed or calculated) to compare to

Returns RMS error

Return type array of floats

burnman.main.**chi_factor**(*calc*, *obs*)

PUT IN TOOLS χ factor for one profile assuming 1% uncertainty on the reference model (obs) :type calc: list of arrays of float :param calc: array calculated values :type obs: list of arrays of float :param obs: array of reference values to compare to

Returns χ factor

Return type array of floats

CHAPTER

SIX

MATERIALS

Burnman operates on materials (type *Material*) most prominently in form of minerals (*Mineral*) and composites (*Composite*).

6.1 Material Base Class

class burnman.material.**Material**

Bases: object

Base class for all materials. The main functionality is unroll() which returns a list of objects of type *Mineral* and their molar fractions. This class is available as burnman.Material.

The user needs to call set_method() (once in the beginning) and set_state() before querying the material with unroll() or density().

Attributes

pressure
temperature

name

Human-readable name of this material.

By default this will return the name of the class, but it can be set to an arbitrary string. Overriden in Mineral.

set_method(*method*)

Set the averaging method. See Averaging Schemes for details.

Notes

Needs to be implemented in derived classes.

to_string()

Returns a human-readable name of this material. The default implementation will return the

name of the class, which is a reasonable default.

Returns **name** : string

Name of this material.

debug_print(*indent=''*)
Print a human-readable representation of this Material.

print_minerals_of_current_state()
Print a human-readable representation of this Material at the current P, T as a list of minerals. This requires set_state() has been called before.

set_state(*pressure*, *temperature*)
Set the material to the given pressure and temperature.

Parameters **pressure** : float

The desired pressure in [Pa].

temperature : float

The desired temperature in [K].

reset()
Resets all cached material properties.

It is typically not required for the user to call this function.

unroll()
Unroll this material into a list of `burnman.Mineral` and their molar fractions. All averaging schemes then operate on this list of minerals. Note that the return value of this function may depend on the current state (temperature, pressure).

Returns **fractions** : list of float

List of molar fractions, should sum to 1.0.

minerals : list of `burnman.Mineral`

List of minerals.

Notes

Needs to be implemented in derived classes.

evaluate(*vars_list*, *pressures*, *temperatures*)
Returns an array of material properties requested through a list of strings at given pressure and temperature conditions. At the end it resets the set_state to the original values. The user needs to call set_method() before.

Parameters **vars_list** : list of strings

Variables to be returned for given conditions

pressure : array of float

Array of pressures in [Pa].

temperature : float

Array of temperatures in [K].

Returns **output** : array of array of float

Array returning all variables at given pressure/temperature values. output[i][j] is property vars_list[j] and temperatures[i] and pressures[i].

pressure

Returns current pressure that was set with *set_state()*.

Returns **pressure** : float

Pressure in [Pa].

Notes

•Aliased with *P()*.

temperature

Returns current temperature that was set with *set_state()*.

Returns **temperature** : float

Temperature in [K].

Notes

•Aliased with *T()*.

internal_energy

Returns the internal energy of the mineral.

Returns **internal_energy** : float

The internal energy in [J].

Notes

•Needs to be implemented in derived classes.

•Aliased with *energy()*.

molar_gibbs

Returns the Gibbs free energy of the mineral.

Returns **molar_gibbs** : float

Gibbs free energy in [J].

Notes

- Needs to be implemented in derived classes.
- Aliased with *gibbs()*.

molar_helmholtz

Returns the Helmholtz free energy of the mineral.

Returns **molar_helmholtz** : float

Helmholtz free energy in [J].

Notes

- Needs to be implemented in derived classes.
- Aliased with *helmholtz()*.

molar_mass

Returns molar mass of the mineral.

Returns **molar_mass** : float

Molar mass in [kg/mol].

Notes

- Needs to be implemented in derived classes.

molar_volume

Returns molar volume of the mineral.

Returns **molar_volume** : float

Molar volume in [m^3/mol].

Notes

- Needs to be implemented in derived classes.
- Aliased with *V()*.

density

Returns the density of this material.

Returns **density** : float

The density of this material in [kg/m^3].

Notes

- Needs to be implemented in derived classes.
- Aliased with *rho()*.

molar_entropy
Returns entropy of the mineral.

Returns **entropy** : float

Entropy in [J].

Notes

- Needs to be implemented in derived classes.
- Aliased with *S()*.

molar_enthalpy
Returns enthalpy of the mineral.

Returns **enthalpy** : float

Enthalpy in [J].

Notes

- Needs to be implemented in derived classes.
- Aliased with *H()*.

isothermal_bulk_modulus
Returns isothermal bulk modulus of the material.

Returns **isothermal_bulk_modulus** : float

Bulk modulus in [Pa].

Notes

- Needs to be implemented in derived classes.
- Aliased with *K_T()*.

adiabatic_bulk_modulus
Returns the adiabatic bulk modulus of the mineral.

Returns **adiabatic_bulk_modulus** : float

Adiabatic bulk modulus in [Pa].

Notes

- Needs to be implemented in derived classes.
- Aliased with *K_S()*.

isothermal_compressibility

Returns isothermal compressibility of the mineral (or inverse isothermal bulk modulus).

Returns **(K_T)^-1** : float

Compressibility in [1/Pa].

Notes

- Needs to be implemented in derived classes.
- Aliased with *beta_T()*.

adiabatic_compressibility

Returns adiabatic compressibility of the mineral (or inverse adiabatic bulk modulus).

Returns **adiabatic_compressibility** : float

adiabatic compressibility in [1/Pa].

Notes

- Needs to be implemented in derived classes.
- Aliased with *beta_S()*.

shear_modulus

Returns shear modulus of the mineral.

Returns **shear_modulus** : float

Shear modulus in [Pa].

Notes

- Needs to be implemented in derived classes.
- Aliased with `beta_G()`.

p_wave_velocity

Returns P wave speed of the mineral.

Returns **p_wave_velocity** : float

P wave speed in [m/s].

Notes

- Needs to be implemented in derived classes.
- Aliased with `v_p()`.

bulk_sound_velocity

Returns bulk sound speed of the mineral.

Returns bulk sound velocity: float

Sound velocity in [m/s].

Notes

- Needs to be implemented in derived classes.
- Aliased with `v_phi()`.

shear_wave_velocity

Returns shear wave speed of the mineral.

Returns **shear_wave_velocity** : float

Wave speed in [m/s].

Notes

- Needs to be implemented in derived classes.
- Aliased with `v_s()`.

grueneisen_parameter

Returns the grueneisen parameter of the mineral.

Returns **gr** : float

Grueneisen parameters [unitless].

Notes

- Needs to be implemented in derived classes.
- Aliased with `gr()`.

thermal_expansivity

Returns thermal expansion coefficient of the mineral.

Returns **alpha** : float

Thermal expansivity in [1/K].

Notes

- Needs to be implemented in derived classes.
- Aliased with *alpha()*.

heat_capacity_v
Returns heat capacity at constant volume of the mineral.

Returns **heat_capacity_v** : float

Heat capacity in [J/K/mol].

Notes

- Needs to be implemented in derived classes.
- Aliased with *C_v()*.

heat_capacity_p
Returns heat capacity at constant pressure of the mineral.

Returns **heat_capacity_p** : float

Heat capacity in [J/K/mol].

Notes

- Needs to be implemented in derived classes.
- Aliased with *C_p()*.

P
Alias for *pressure()*

T
Alias for *temperature()*

energy
Alias for *internal_energy()*

helmholtz
Alias for *molar_helmholtz()*

gibbs
Alias for *molar_gibbs()*

V
Alias for *molar_volume()*

rho
Alias for *density()*

S
Alias for *molar_entropy()*

H
Alias for *molar_enthalpy()*

K_T
Alias for *isothermal_bulk_modulus()*

K_S
Alias for *adiabatic_bulk_modulus()*

beta_T
Alias for *isothermal_compressibility()*

beta_S
Alias for *adiabatic_compressibility()*

G
Alias for *shear_modulus()*

v_p
Alias for *p_wave_velocity()*

v_phi
Alias for *bulk_sound_velocity()*

v_s
Alias for *shear_wave_velocity()*

gr
Alias for *grueneisen_parameter()*

alpha
Alias for *thermal_expansivity()*

C_v
Alias for *heat_capacity_v()*

C_p
Alias for *heat_capacity_p()*

6.2 Minerals

6.2.1 Endmembers

class burnman.mineral.**Mineral**
Bases: *burnman.material.Material*

This is the base class for all minerals. States of the mineral can only be queried after setting the pressure and temperature using set_state(). The method for computing properties of the material is set using set_method(). This is done during initialisation if the param 'equation_of_state' has been defined. The method can be overridden later by the user.

This class is available as `burnman.Mineral`.

If deriving from this class, set the properties in self.params to the desired values. For more complicated materials you can overwrite set_state(), change the params and then call set_state() from this class.

All the material parameters are expected to be in plain SI units. This means that the elastic moduli should be in Pascals and NOT Gigapascals, and the Debye temperature should be in K not C. Additionally, the reference volume should be in m^3/(mol molecule) and not in unit cell volume and 'n' should be the number of atoms per molecule. Frequently in the literature the reference volume is given in Angstrom^3 per unit cell. To convert this to m^3/(mol of molecule) you should multiply by 10^(-30) * N_a / Z, where N_a is Avogadro's number and Z is the number of formula units per unit cell. You can look up Z in many places, including www.mindat.org

name
Human-readable name of this material.

By default this will return the name of the class, but it can be set to an arbitrary string. Overriden in Mineral.

set_method(*equation_of_state*)
Set the equation of state to be used for this mineral. Takes a string corresponding to any of the predefined equations of state: 'bm2', 'bm3', 'mgd2', 'mgd3', 'slb2', 'slb3', 'mt', 'hp_tmt', or 'cork'. Alternatively, you can pass a user defined class which derives from the equation_of_state base class. After calling set_method(), any existing derived properties (e.g., elastic parameters or thermodynamic potentials) will be out of date, so set_state() will need to be called again.

to_string()
Returns the name of the mineral class

debug_print(*indent=''*)

unroll()

set_state(**args*)
(copied from set_state):

Set the material to the given pressure and temperature.

Parameters **pressure** : float

The desired pressure in [Pa].

temperature : float

The desired temperature in [K].

molar_gibbs
Returns the Gibbs free energy of the mineral.

Returns **molar_gibbs** : float

Gibbs free energy in [J].

Notes

- Needs to be implemented in derived classes.
- Aliased with *gibbs()*.

molar_volume

Returns molar volume of the mineral.

Returns **molar_volume** : float

Molar volume in [m^3/mol].

Notes

- Needs to be implemented in derived classes.
- Aliased with *V()*.

molar_entropy

Returns entropy of the mineral.

Returns **entropy** : float

Entropy in [J].

Notes

- Needs to be implemented in derived classes.
- Aliased with *S()*.

isothermal_bulk_modulus

Returns isothermal bulk modulus of the material.

Returns **isothermal_bulk_modulus** : float

Bulk modulus in [Pa].

Notes

- Needs to be implemented in derived classes.
- Aliased with *K_T()*.

heat_capacity_p

Returns heat capacity at constant pressure of the mineral.

Returns **heat_capacity_p** : float

Heat capacity in [J/K/mol].

Notes

- Needs to be implemented in derived classes.
- Aliased with *C_p()*.

thermal_expansivity

Returns thermal expansion coefficient of the mineral.

Returns **alpha** : float

Thermal expansivity in [1/K].

Notes

- Needs to be implemented in derived classes.
- Aliased with *alpha()*.

shear_modulus

Returns shear modulus of the mineral.

Returns **shear_modulus** : float

Shear modulus in [Pa].

Notes

- Needs to be implemented in derived classes.
- Aliased with `beta_G()`.

molar_mass

Returns molar mass of the mineral.

Returns **molar_mass** : float

Molar mass in [kg/mol].

Notes

- Needs to be implemented in derived classes.

density

Returns the density of this material.

Returns **density** : float

The density of this material in [kg/m^3].

Notes

- Needs to be implemented in derived classes.
- Aliased with *rho()*.

internal_energy
Returns the internal energy of the mineral.

Returns **internal_energy** : float

The internal energy in [J].

Notes

- Needs to be implemented in derived classes.
- Aliased with *energy()*.

molar_helmholtz
Returns the Helmholtz free energy of the mineral.

Returns **molar_helmholtz** : float

Helmholtz free energy in [J].

Notes

- Needs to be implemented in derived classes.
- Aliased with *helmholtz()*.

molar_enthalpy
Returns enthalpy of the mineral.

Returns **enthalpy** : float

Enthalpy in [J].

Notes

- Needs to be implemented in derived classes.
- Aliased with *H()*.

adiabatic_bulk_modulus
Returns the adiabatic bulk modulus of the mineral.

Returns **adiabatic_bulk_modulus** : float

Adiabatic bulk modulus in [Pa].

Notes

- Needs to be implemented in derived classes.
- Aliased with *K_S()*.

isothermal_compressibility

Returns isothermal compressibility of the mineral (or inverse isothermal bulk modulus).

Returns **(K_T)^-1** : float

Compressibility in [1/Pa].

Notes

- Needs to be implemented in derived classes.
- Aliased with *beta_T()*.

adiabatic_compressibility

Returns adiabatic compressibility of the mineral (or inverse adiabatic bulk modulus).

Returns **adiabatic_compressibility** : float

adiabatic compressibility in [1/Pa].

Notes

- Needs to be implemented in derived classes.
- Aliased with *beta_S()*.

p_wave_velocity

Returns P wave speed of the mineral.

Returns **p_wave_velocity** : float

P wave speed in [m/s].

Notes

- Needs to be implemented in derived classes.
- Aliased with *v_p()*.

bulk_sound_velocity

Returns bulk sound speed of the mineral.

Returns bulk sound velocity: float

Sound velocity in [m/s].

Notes

- Needs to be implemented in derived classes.
- Aliased with *v_phi()*.

shear_wave_velocity
Returns shear wave speed of the mineral.

Returns **shear_wave_velocity** : float

Wave speed in [m/s].

Notes

- Needs to be implemented in derived classes.
- Aliased with *v_s()*.

grueneisen_parameter
Returns the grueneisen parameter of the mineral.

Returns **gr** : float

Grueneisen parameters [unitless].

Notes

- Needs to be implemented in derived classes.
- Aliased with *gr()*.

heat_capacity_v
Returns heat capacity at constant volume of the mineral.

Returns **heat_capacity_v** : float

Heat capacity in [J/K/mol].

Notes

- Needs to be implemented in derived classes.
- Aliased with *C_v()*.

C_p
Alias for *heat_capacity_p()*

C_v
Alias for *heat_capacity_v()*

G
Alias for *shear_modulus()*

H
Alias for *molar_enthalpy()*

K_S
Alias for *adiabatic_bulk_modulus()*

K_T
Alias for *isothermal_bulk_modulus()*

P
Alias for *pressure()*

S
Alias for *molar_entropy()*

T
Alias for *temperature()*

V
Alias for *molar_volume()*

alpha
Alias for *thermal_expansivity()*

beta_S
Alias for *adiabatic_compressibility()*

beta_T
Alias for *isothermal_compressibility()*

energy
Alias for *internal_energy()*

evaluate(*vars_list*, *pressures*, *temperatures*)
Returns an array of material properties requested through a list of strings at given pressure and temperature conditions. At the end it resets the set_state to the original values. The user needs to call set_method() before.

Parameters **vars_list** : list of strings

Variables to be returned for given conditions

pressure : array of float

Array of pressures in [Pa].

temperature : float

Array of temperatures in [K].

Returns **output** : array of array of float

Array returning all variables at given pressure/temperature values. output[i][j] is property vars_list[j] and temperatures[i] and pressures[i].

gibbs
Alias for *molar_gibbs()*

gr
Alias for *grueneisen_parameter()*

helmholtz
Alias for *molar_helmholtz()*

pressure
Returns current pressure that was set with *set_state()*.

Returns pressure : float

Pressure in [Pa].

Notes

•Aliased with *P()*.

print_minerals_of_current_state()
Print a human-readable representation of this Material at the current P, T as a list of minerals. This requires set_state() has been called before.

reset()
Resets all cached material properties.

It is typically not required for the user to call this function.

rho
Alias for *density()*

temperature
Returns current temperature that was set with *set_state()*.

Returns temperature : float

Temperature in [K].

Notes

•Aliased with *T()*.

v_p
Alias for *p_wave_velocity()*

v_phi
Alias for *bulk_sound_velocity()*

v_s
Alias for *shear_wave_velocity()*

6.2.2 Solid solutions

class burnman.solidsolution.**SolidSolution**(*molar_fractions=None*)

Bases: *burnman.mineral.Mineral*

This is the base class for all solid solutions. Site occupancies, endmember activities and the constant and pressure and temperature dependencies of the excess properties can be queried after using set_composition() States of the solid solution can only be queried after setting the pressure, temperature and composition using set_state().

This class is available as burnman.SolidSolution. It uses an instance of burnman.SolutionModel to calculate interaction terms between endmembers.

All the solid solution parameters are expected to be in SI units. This means that the interaction parameters should be in J/mol, with the T and P derivatives in J/K/mol and m^3/mol.

get_endmembers()

set_composition(*molar_fractions*)

Set the composition for this solid solution.

Parameters molar_fractions: list of float

molar abundance for each endmember, needs to sum to one.

set_method(*method*)

set_state(*pressure*, *temperature*)

activities

Returns a list of endmember activities [unitless]

activity_coefficients

Returns a list of endmember activity coefficients (gamma = activity / ideal activity) [unitless]

internal_energy

Returns internal energy of the mineral [J] Aliased with self.energy

excess_partial_gibbs

Returns excess partial gibbs free energy [J] Property specific to solid solutions.

partial_gibbs

Returns excess partial gibbs free energy [J] Property specific to solid solutions.

excess_gibbs

Returns excess gibbs free energy [J] Property specific to solid solutions.

molar_gibbs

Returns Gibbs free energy of the solid solution [J] Aliased with self.gibbs

molar_helmholtz

Returns Helmholtz free energy of the solid solution [J] Aliased with self.helmholtz

molar_mass

Returns molar mass of the solid solution [kg/mol]

excess_volume
Returns excess volume of the solid solution [m^3/mol] Specific property for solid solutions

molar_volume
Returns molar volume of the solid solution [m^3/mol] Aliased with self.V

density
Returns density of the solid solution [kg/m^3] Aliased with self.rho

excess_entropy
Returns excess entropy [J] Property specific to solid solutions.

molar_entropy
Returns entropy of the solid solution [J] Aliased with self.S

excess_enthalpy
Returns excess enthalpy [J] Property specific to solid solutions.

molar_enthalpy
Returns enthalpy of the solid solution [J] Aliased with self.H

isothermal_bulk_modulus
Returns isothermal bulk modulus of the solid solution [Pa] Aliased with self.K_T

adiabatic_bulk_modulus
Returns adiabatic bulk modulus of the solid solution [Pa] Aliased with self.K_S

isothermal_compressibility
Returns isothermal compressibility of the solid solution (or inverse isothermal bulk modulus) [1/Pa] Aliased with self.K_T

adiabatic_compressibility
Returns adiabatic compressibility of the solid solution (or inverse adiabatic bulk modulus) [1/Pa] Aliased with self.K_S

shear_modulus
Returns shear modulus of the solid solution [Pa] Aliased with self.G

p_wave_velocity
Returns P wave speed of the solid solution [m/s] Aliased with self.v_p

bulk_sound_velocity
Returns bulk sound speed of the solid solution [m/s] Aliased with self.v_phi

shear_wave_velocity
Returns shear wave speed of the solid solution [m/s] Aliased with self.v_s

C_p
Alias for *heat_capacity_p()*

C_v
Alias for *heat_capacity_v()*

G
Alias for *shear_modulus()*

H
Alias for *molar_enthalpy()*

K_S
Alias for *adiabatic_bulk_modulus()*

K_T
Alias for *isothermal_bulk_modulus()*

P
Alias for *pressure()*

S
Alias for *molar_entropy()*

T
Alias for *temperature()*

V
Alias for *molar_volume()*

alpha
Alias for *thermal_expansivity()*

beta_S
Alias for *adiabatic_compressibility()*

beta_T
Alias for *isothermal_compressibility()*

debug_print(*indent=''*)

energy
Alias for *internal_energy()*

evaluate(*vars_list*, *pressures*, *temperatures*)
Returns an array of material properties requested through a list of strings at given pressure and temperature conditions. At the end it resets the set_state to the original values. The user needs to call set_method() before.

Parameters **vars_list** : list of strings

Variables to be returned for given conditions

pressure : array of float

Array of pressures in [Pa].

temperature : float

Array of temperatures in [K].

Returns **output** : array of array of float

Array returning all variables at given pressure/temperature values. output[i][j] is property vars_list[j] and temperatures[i] and pressures[i].

gibbs
Alias for *molar_gibbs()*

gr
Alias for *grueneisen_parameter()*

grueneisen_parameter
Returns grueneisen parameter of the solid solution [unitless] Aliased with self.gr

helmholtz
Alias for *molar_helmholtz()*

name
Human-readable name of this material.

By default this will return the name of the class, but it can be set to an arbitrary string. Overriden in Mineral.

pressure
Returns current pressure that was set with *set_state()*.

Returns **pressure** : float

Pressure in [Pa].

Notes

•Aliased with *P()*.

print_minerals_of_current_state()
Print a human-readable representation of this Material at the current P, T as a list of minerals. This requires set_state() has been called before.

reset()
Resets all cached material properties.

It is typically not required for the user to call this function.

rho
Alias for *density()*

temperature
Returns current temperature that was set with *set_state()*.

Returns **temperature** : float

Temperature in [K].

Notes

•Aliased with *T()*.

to_string()
Returns the name of the mineral class

unroll()

v_p
Alias for *p_wave_velocity()*

v_phi
Alias for *bulk_sound_velocity()*

v_s
Alias for *shear_wave_velocity()*

thermal_expansivity
Returns thermal expansion coefficient (alpha) of the solid solution [1/K] Aliased with self.alpha

heat_capacity_v
Returns heat capacity at constant volume of the solid solution [J/K/mol] Aliased with self.C_v

heat_capacity_p
Returns heat capacity at constant pressure of the solid solution [J/K/mol] Aliased with self.C_p

6.2.3 Mineral helpers

class burnman.mineral_helpers.**HelperSpinTransition**(*transition_pressure*, *ls_mat*, *hs_mat*)

Bases: *burnman.composite.Composite*

Helper class that makes a mineral that switches between two materials (for low and high spin) based on some transition pressure [Pa]

debug_print(*indent=''*)

set_state(*pressure*, *temperature*)

C_p
Alias for *heat_capacity_p()*

C_v
Alias for *heat_capacity_v()*

G
Alias for *shear_modulus()*

H
Alias for *molar_enthalpy()*

K_S
Alias for *adiabatic_bulk_modulus()*

K_T
Alias for *isothermal_bulk_modulus()*

P
Alias for *pressure()*

S
Alias for *molar_entropy()*

T
Alias for *temperature()*

V
Alias for *molar_volume()*

adiabatic_bulk_modulus
Returns adiabatic bulk modulus of the mineral [Pa] Aliased with self.K_S

adiabatic_compressibility
Returns isothermal compressibility of the composite (or inverse isothermal bulk modulus) [1/Pa] Aliased with self.beta_S

alpha
Alias for *thermal_expansivity()*

beta_S
Alias for *adiabatic_compressibility()*

beta_T
Alias for *isothermal_compressibility()*

bulk_sound_velocity
Returns bulk sound speed of the composite [m/s] Aliased with self.v_phi

density
Compute the density of the composite based on the molar volumes and masses Aliased with self.rho

energy
Alias for *internal_energy()*

evaluate(*vars_list*, *pressures*, *temperatures*)
Returns an array of material properties requested through a list of strings at given pressure and temperature conditions. At the end it resets the set_state to the original values. The user needs to call set_method() before.

Parameters **vars_list** : list of strings

Variables to be returned for given conditions

pressure : array of float

Array of pressures in [Pa].

temperature : float

Array of temperatures in [K].

Returns **output** : array of array of float

Array returning all variables at given pressure/temperature values. output[i][j] is property vars_list[j] and temperatures[i] and pressures[i].

gibbs
Alias for *molar_gibbs()*

gr
Alias for *grueneisen_parameter()*

grueneisen_parameter
Returns grueneisen parameter of the composite [unitless] Aliased with self.gr

heat_capacity_p
Returns heat capacity at constant pressure of the composite [J/K/mol] Aliased with self.C_p

heat_capacity_v
Returns heat capacity at constant volume of the composite [J/K/mol] Aliased with self.C_v

helmholtz
Alias for *molar_helmholtz()*

internal_energy
Returns internal energy of the mineral [J] Aliased with self.energy

isothermal_bulk_modulus
Returns isothermal bulk modulus of the composite [Pa] Aliased with self.K_T

isothermal_compressibility
Returns isothermal compressibility of the composite (or inverse isothermal bulk modulus) [1/Pa] Aliased with self.beta_T

molar_enthalpy
Returns enthalpy of the mineral [J] Aliased with self.H

molar_entropy
Returns enthalpy of the mineral [J] Aliased with self.S

molar_gibbs
Returns Gibbs free energy of the composite [J] Aliased with self.gibbs

molar_helmholtz
Returns Helmholtz free energy of the mineral [J] Aliased with self.helmholtz

molar_mass
Returns molar mass of the composite [kg/mol]

molar_volume
Returns molar volume of the composite [m^3/mol] Aliased with self.V

name
Human-readable name of this material.

By default this will return the name of the class, but it can be set to an arbitrary string. Overriden in Mineral.

p_wave_velocity
Returns P wave speed of the composite [m/s] Aliased with self.v_p

pressure
Returns current pressure that was set with *set_state()*.

Returns **pressure** : float

Pressure in [Pa].

Notes

•Aliased with *P()*.

print_minerals_of_current_state()
Print a human-readable representation of this Material at the current P, T as a list of minerals. This requires set_state() has been called before.

reset()
Resets all cached material properties.

It is typically not required for the user to call this function.

rho
Alias for *density()*

set_averaging_scheme(*averaging_scheme*)
Set the averaging scheme for the moduli in the composite. Default is set to VoigtReussHill, when Composite is initialized.

set_fractions(*fractions*, *fraction_type='molar'*)
Change the fractions of the phases of this Composite.

Parameters **fractions: list of floats**

molar or mass fraction for each phase.

fraction_type: 'molar' or 'mass'

specify whether molar or mass fractions are specified.

set_method(*method*)
set the same equation of state method for all the phases in the composite

shear_modulus
Returns shear modulus of the mineral [Pa] Aliased with self.G

shear_wave_velocity
Returns shear wave speed of the composite [m/s] Aliased with self.v_s

temperature
Returns current temperature that was set with *set_state()*.

Returns **temperature** : float

Temperature in [K].

Notes

•Aliased with *T()*.

thermal_expansivity
Returns thermal expansion coefficient of the composite [1/K] Aliased with self.alpha

to_string()
return the name of the composite

unroll()

v_p
Alias for *p_wave_velocity()*

v_phi
Alias for *bulk_sound_velocity()*

v_s
Alias for *shear_wave_velocity()*

6.3 Composites

class burnman.composite.**Composite**(*phases*, *fractions=None*, *fraction_type='molar'*)
Bases: *burnman.material.Material*

Base class for a composite material. The static phases can be minerals or materials, meaning composite can be nested arbitrarily.

The fractions of the phases can be input as either 'molar' or 'mass' during instantiation, and modified (or initialised) after this point by using set_fractions.

This class is available as burnman.Composite.

set_fractions(*fractions*, *fraction_type='molar'*)
Change the fractions of the phases of this Composite.

Parameters fractions: list of floats

molar or mass fraction for each phase.

fraction_type: 'molar' or 'mass'

specify whether molar or mass fractions are specified.

set_method(*method*)
set the same equation of state method for all the phases in the composite

set_averaging_scheme(*averaging_scheme*)
Set the averaging scheme for the moduli in the composite. Default is set to VoigtReussHill, when Composite is initialized.

set_state(*pressure*, *temperature*)
Update the material to the given pressure [Pa] and temperature [K].

debug_print(*indent=''*)

unroll()

to_string()
return the name of the composite

internal_energy
Returns internal energy of the mineral [J] Aliased with self.energy

molar_gibbs
Returns Gibbs free energy of the composite [J] Aliased with self.gibbs

molar_helmholtz
Returns Helmholtz free energy of the mineral [J] Aliased with self.helmholtz

molar_volume
Returns molar volume of the composite [m^3/mol] Aliased with self.V

molar_mass
Returns molar mass of the composite [kg/mol]

density
Compute the density of the composite based on the molar volumes and masses Aliased with self.rho

molar_entropy
Returns enthalpy of the mineral [J] Aliased with self.S

molar_enthalpy
Returns enthalpy of the mineral [J] Aliased with self.H

isothermal_bulk_modulus
Returns isothermal bulk modulus of the composite [Pa] Aliased with self.K_T

adiabatic_bulk_modulus
Returns adiabatic bulk modulus of the mineral [Pa] Aliased with self.K_S

isothermal_compressibility
Returns isothermal compressibility of the composite (or inverse isothermal bulk modulus) [1/Pa] Aliased with self.beta_T

adiabatic_compressibility
Returns isothermal compressibility of the composite (or inverse isothermal bulk modulus) [1/Pa] Aliased with self.beta_S

shear_modulus
Returns shear modulus of the mineral [Pa] Aliased with self.G

p_wave_velocity
Returns P wave speed of the composite [m/s] Aliased with self.v_p

bulk_sound_velocity
Returns bulk sound speed of the composite [m/s] Aliased with self.v_phi

shear_wave_velocity
Returns shear wave speed of the composite [m/s] Aliased with self.v_s

grueneisen_parameter
Returns grueneisen parameter of the composite [unitless] Aliased with self.gr

thermal_expansivity
Returns thermal expansion coefficient of the composite [1/K] Aliased with self.alpha

heat_capacity_v
Returns heat capacity at constant volume of the composite [J/K/mol] Aliased with self.C_v

heat_capacity_p
Returns heat capacity at constant pressure of the composite [J/K/mol] Aliased with self.C_p

C_p
Alias for *heat_capacity_p()*

C_v
Alias for *heat_capacity_v()*

G
Alias for *shear_modulus()*

H
Alias for *molar_enthalpy()*

K_S
Alias for *adiabatic_bulk_modulus()*

K_T
Alias for *isothermal_bulk_modulus()*

P
Alias for *pressure()*

S
Alias for *molar_entropy()*

T
Alias for *temperature()*

V
Alias for *molar_volume()*

alpha
Alias for *thermal_expansivity()*

beta_S
Alias for *adiabatic_compressibility()*

beta_T
Alias for *isothermal_compressibility()*

energy
Alias for *internal_energy()*

evaluate(*vars_list*, *pressures*, *temperatures*)
Returns an array of material properties requested through a list of strings at given pressure and temperature conditions. At the end it resets the set_state to the original values. The user needs to call set_method() before.

Parameters **vars_list** : list of strings

Variables to be returned for given conditions

pressure : array of float

Array of pressures in [Pa].

temperature : float

Array of temperatures in [K].

Returns **output** : array of array of float

Array returning all variables at given pressure/temperature values. output[i][j] is property vars_list[j] and temperatures[i] and pressures[i].

gibbs
Alias for *molar_gibbs()*

gr
Alias for *grueneisen_parameter()*

helmholtz
Alias for *molar_helmholtz()*

name
Human-readable name of this material.

By default this will return the name of the class, but it can be set to an arbitrary string. Overriden in Mineral.

pressure
Returns current pressure that was set with *set_state()*.

Returns **pressure** : float

Pressure in [Pa].

Notes

•Aliased with *P()*.

print_minerals_of_current_state()
Print a human-readable representation of this Material at the current P, T as a list of minerals. This requires set_state() has been called before.

reset()
Resets all cached material properties.

It is typically not required for the user to call this function.

rho
Alias for *density()*

temperature
Returns current temperature that was set with *set_state()*.

Returns **temperature** : float

Temperature in [K].

Notes

- Aliased with *T()*.

v_p
Alias for *p_wave_velocity()*

v_phi
Alias for *bulk_sound_velocity()*

v_s
Alias for *shear_wave_velocity()*

CHAPTER

SEVEN

EQUATIONS OF STATE

7.1 Base class

class burnman.eos.**EquationOfState**

Bases: object

This class defines the interface for an equation of state that a mineral uses to determine its properties at a given P, T. In order define a new equation of state, you should define these functions.

All functions should accept and return values in SI units.

In general these functions are functions of pressure, temperature, and volume, as well as a "params" object, which is a Python dictionary that stores the material parameters of the mineral, such as reference volume, Debye temperature, reference moduli, etc.

The functions for volume and density are just functions of temperature, pressure, and "params"; after all, it does not make sense for them to be functions of volume or density.

volume(*pressure*, *temperature*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. $[Pa]$

temperature : float

Temperature at which to evaluate the equation of state. $[K]$

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **volume** : float

Molar volume of the mineral. $[m^3]$

pressure(*temperature*, *volume*, *params*)

Parameters **volume** : float

Molar volume at which to evaluate the equation of state. [m^3]

temperature : float

Temperature at which to evaluate the equation of state. [K]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns pressure : float

Pressure of the mineral, including cold and thermal parts. [m^3]

density(*volume*, *params*)

Calculate the density of the mineral $[kg/m^3]$. The params object must include a "molar_mass" field.

Parameters volume : float

Molar volume of the mineral. For consistency this should be calculated

using :func:'volume'. :math:'[m^3]'

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns density : float

Density of the mineral. $[kg/m^3]$

grueneisen_parameter(*pressure*, *temperature*, *volume*, *params*)

Parameters pressure : float

Pressure at which to evaluate the equation of state. $[Pa]$

temperature : float

Temperature at which to evaluate the equation of state. $[K]$

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. $[m^3]$

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns gamma : float

Grueneisen parameter of the mineral. $[unitless]$

isothermal_bulk_modulus(*pressure*, *temperature*, *volume*, *params*)

Parameters pressure : float

Pressure at which to evaluate the equation of state. $[Pa]$

temperature : float

Temperature at which to evaluate the equation of state. $[K]$

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. $[m^3]$

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns K_T : float

Isothermal bulk modulus of the mineral. $[Pa]$

adiabatic_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)

Parameters pressure : float

Pressure at which to evaluate the equation of state. $[Pa]$

temperature : float

Temperature at which to evaluate the equation of state. $[K]$

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. $[m^3]$

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns K_S : float

Adiabatic bulk modulus of the mineral. $[Pa]$

shear_modulus (*pressure*, *temperature*, *volume*, *params*)

Parameters pressure : float

Pressure at which to evaluate the equation of state. $[Pa]$

temperature : float

Temperature at which to evaluate the equation of state. $[K]$

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. $[m^3]$

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns G : float

Shear modulus of the mineral. $[Pa]$

heat_capacity_v (*pressure*, *temperature*, *volume*, *params*)

Parameters pressure : float

Pressure at which to evaluate the equation of state. $[Pa]$

temperature : float

Temperature at which to evaluate the equation of state. $[K]$

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. $[m^3]$

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns C_V : float

Heat capacity at constant volume of the mineral. $[J/K/mol]$

heat_capacity_p (*pressure*, *temperature*, *volume*, *params*)

Parameters pressure : float

Pressure at which to evaluate the equation of state. $[Pa]$

temperature : float

Temperature at which to evaluate the equation of state. $[K]$

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. $[m^3]$

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns C_P : float

Heat capacity at constant pressure of the mineral. $[J/K/mol]$

thermal_expansivity (*pressure*, *temperature*, *volume*, *params*)

Parameters pressure : float

Pressure at which to evaluate the equation of state. $[Pa]$

temperature : float

Temperature at which to evaluate the equation of state. $[K]$

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. $[m^3]$

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns alpha : float

Thermal expansivity of the mineral. $[1/K]$

gibbs_free_energy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **G** : float

Gibbs free energy of the mineral

helmholtz_free_energy (*pressure*, *temperature*, *volume*, *params*)

Parameters **temperature** : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **F** : float

Helmholtz free energy of the mineral

entropy (*pressure*, *temperature*, *volume*, *params*)

Returns the entropy at the pressure and temperature of the mineral [J/K/mol]

enthalpy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **H** : float

Enthalpy of the mineral

internal_energy(*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **U** : float

Internal energy of the mineral

validate_parameters(*params*)

The params object is just a dictionary associating mineral physics parameters for the equation of state. Different equation of states can have different parameters, and the parameters may have ranges of validity. The intent of this function is twofold. First, it can check for the existence of the parameters that the equation of state needs, and second, it can check whether the parameters have reasonable values. Unreasonable values will frequently be due to unit issues (e.g., supplying bulk moduli in GPa instead of Pa). In the base class this function does nothing, and an equation of state is not required to implement it. This function will not return anything, though it may raise warnings or errors.

Parameters **params** : dictionary

Dictionary containing material parameters required by the equation of state.

7.2 Birch-Murnaghan

class `burnman.eos.birch_murnaghan.`**BirchMurnaghanBase**

Bases: `burnman.eos.equation_of_state.EquationOfState`

Base class for the isothermal Birch Murnaghan equation of state. This is third order in strain, and has no temperature dependence. However, the shear modulus is sometimes fit to a second order function, so if this is the case, you should use that. For more see `burnman.birch_murnaghan.BM2` and `burnman.birch_murnaghan.BM3`.

volume(*pressure*, *temperature*, *params*)

Returns volume $[m^3]$ as a function of pressure $[Pa]$.

pressure(*temperature*, *volume*, *params*)

isothermal_bulk_modulus(*pressure*, *temperature*, *volume*, *params*)

Returns isothermal bulk modulus K_T $[Pa]$ as a function of pressure $[Pa]$, temperature $[K]$ and volume $[m^3]$.

adiabatic_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns adiabatic bulk modulus K_s of the mineral. $[Pa]$.

shear_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns shear modulus G of the mineral. $[Pa]$

heat_capacity_v (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return a very large number. $[J/K/mol]$

heat_capacity_p (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return a very large number. $[J/K/mol]$

thermal_expansivity (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return zero. $[1/K]$

grueneisen_parameter (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return zero. $[unitless]$

validate_parameters (*params*)
Check for existence and validity of the parameters

density (*volume*, *params*)
Calculate the density of the mineral $[kg/m^3]$. The params object must include a "molar_mass" field.

Parameters **volume** : float

Molar volume of the mineral. For consistency this should be calculated

using :func:'volume'. :math:'[m^3]'

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **density** : float

Density of the mineral. $[kg/m^3]$

enthalpy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **H** : float

Enthalpy of the mineral

entropy(*pressure*, *temperature*, *volume*, *params*)

Returns the entropy at the pressure and temperature of the mineral [J/K/mol]

gibbs_free_energy(*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **G** : float

Gibbs free energy of the mineral

helmholtz_free_energy(*pressure*, *temperature*, *volume*, *params*)

Parameters **temperature** : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **F** : float

Helmholtz free energy of the mineral

internal_energy(*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **U** : float

Internal energy of the mineral

class burnman.eos.**BM2**

Bases: *burnman.eos.birch_murnaghan.BirchMurnaghanBase*

Third order Birch Murnaghan isothermal equation of state. This uses the third order expansion for shear modulus.

adiabatic_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)

Returns adiabatic bulk modulus K_s of the mineral. $[Pa]$.

density (*volume*, *params*)

Calculate the density of the mineral $[kg/m^3]$. The params object must include a "molar_mass" field.

Parameters **volume** : float

Molar volume of the mineral. For consistency this should be calculated

using :func:'volume'. :math:'[m^3]'

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **density** : float

Density of the mineral. $[kg/m^3]$

enthalpy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **H** : float

Enthalpy of the mineral

entropy (*pressure*, *temperature*, *volume*, *params*)

Returns the entropy at the pressure and temperature of the mineral [J/K/mol]

gibbs_free_energy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns G : float

Gibbs free energy of the mineral

gruneneisen_parameter(*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return zero. $[unitless]$

heat_capacity_p(*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return a very large number. $[J/K/mol]$

heat_capacity_v(*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return a very large number. $[J/K/mol]$

helmholtz_free_energy(*pressure*, *temperature*, *volume*, *params*)

Parameters temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns F : float

Helmholtz free energy of the mineral

internal_energy(*pressure*, *temperature*, *volume*, *params*)

Parameters pressure : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **U** : float

Internal energy of the mineral

isothermal_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns isothermal bulk modulus K_T $[Pa]$ as a function of pressure $[Pa]$, temperature $[K]$ and volume $[m^3]$.

pressure (*temperature*, *volume*, *params*)

shear_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns shear modulus G of the mineral. $[Pa]$

thermal_expansivity (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return zero. $[1/K]$

validate_parameters (*params*)
Check for existence and validity of the parameters

volume (*pressure*, *temperature*, *params*)
Returns volume $[m^3]$ as a function of pressure $[Pa]$.

class burnman.eos.**BM3**
Bases: *burnman.eos.birch_murnaghan.BirchMurnaghanBase*

Third order Birch Murnaghan isothermal equation of state. This uses the third order expansion for shear modulus.

adiabatic_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns adiabatic bulk modulus K_s of the mineral. $[Pa]$.

density (*volume*, *params*)
Calculate the density of the mineral $[kg/m^3]$. The params object must include a "molar_mass" field.

Parameters **volume** : float

Molar volume of the mineral. For consistency this should be calculated

using :func:'volume'. :math:'[m^3]'

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **density** : float

Density of the mineral. $[kg/m^3]$

enthalpy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns H : float

Enthalpy of the mineral

entropy (*pressure*, *temperature*, *volume*, *params*)
Returns the entropy at the pressure and temperature of the mineral [J/K/mol]

gibbs_free_energy (*pressure*, *temperature*, *volume*, *params*)

Parameters pressure : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns G : float

Gibbs free energy of the mineral

gruneisen_parameter (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return zero. $[unitless]$

heat_capacity_p (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return a very large number. $[J/K/mol]$

heat_capacity_v (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return a very large number. $[J/K/mol]$

helmholtz_free_energy (*pressure*, *temperature*, *volume*, *params*)

Parameters temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns F : float

Helmholtz free energy of the mineral

internal_energy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **U** : float

Internal energy of the mineral

isothermal_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns isothermal bulk modulus K_T $[Pa]$ as a function of pressure $[Pa]$, temperature $[K]$ and volume $[m^3]$.

pressure (*temperature*, *volume*, *params*)

shear_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns shear modulus G of the mineral. $[Pa]$

thermal_expansivity (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return zero. $[1/K]$

validate_parameters (*params*)
Check for existence and validity of the parameters

volume (*pressure*, *temperature*, *params*)
Returns volume $[m^3]$ as a function of pressure $[Pa]$.

7.3 Stixrude and Lithgow-Bertelloni Formulation

class `burnman.eos.slb.`**SLBBase**
Bases: `burnman.eos.equation_of_state.EquationOfState`

Base class for the finite strain-Mie-Grueneiesen-Debye equation of state detailed in *[SLB05]*. For the most part the equations are all third order in strain, but see further the `burnman.slb.SLB2` and `burnman.slb.SLB3` classes.

volume_dependent_q (*x*, *params*)
Finite strain approximation for q, the isotropic volume strain derivative of the grueneisen parameter.

volume (*pressure*, *temperature*, *params*)
Returns molar volume. $[m^3]$

pressure (*temperature*, *volume*, *params*)
Returns the pressure of the mineral at a given temperature and volume [Pa]

grueneisen_parameter (*pressure*, *temperature*, *volume*, *params*)
Returns grueneisen parameter $[unitless]$

isothermal_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns isothermal bulk modulus $[Pa]$

adiabatic_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns adiabatic bulk modulus. $[Pa]$

shear_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns shear modulus. $[Pa]$

heat_capacity_v (*pressure*, *temperature*, *volume*, *params*)
Returns heat capacity at constant volume. $[J/K/mol]$

heat_capacity_p (*pressure*, *temperature*, *volume*, *params*)
Returns heat capacity at constant pressure. $[J/K/mol]$

thermal_expansivity (*pressure*, *temperature*, *volume*, *params*)
Returns thermal expansivity. $[1/K]$

gibbs_free_energy (*pressure*, *temperature*, *volume*, *params*)
Returns the Gibbs free energy at the pressure and temperature of the mineral [J/mol]

internal_energy (*pressure*, *temperature*, *volume*, *params*)
Returns the internal energy at the pressure and temperature of the mineral [J/mol]

entropy (*pressure*, *temperature*, *volume*, *params*)
Returns the entropy at the pressure and temperature of the mineral [J/K/mol]

enthalpy (*pressure*, *temperature*, *volume*, *params*)
Returns the enthalpy at the pressure and temperature of the mineral [J/mol]

helmholtz_free_energy (*pressure*, *temperature*, *volume*, *params*)
Returns the Helmholtz free energy at the pressure and temperature of the mineral [J/mol]

validate_parameters (*params*)
Check for existence and validity of the parameters

density (*volume*, *params*)
Calculate the density of the mineral $[kg/m^3]$. The params object must include a "molar_mass" field.

Parameters **volume** : float

Molar volume of the mineral. For consistency this should be calculated

using :func:'volume'. :math:'[m^3]'

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **density** : float

Density of the mineral. $[kg/m^3]$

class burnman.eos.**SLB2**

Bases: *burnman.eos.slb.SLBBase*

SLB equation of state with second order finite strain expansion for the shear modulus. In general, this should not be used, but sometimes shear modulus data is fit to a second order equation of state. In that case, you should use this. The moral is, be careful!

adiabatic_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)

Returns adiabatic bulk modulus. $[Pa]$

density (*volume*, *params*)

Calculate the density of the mineral $[kg/m^3]$. The params object must include a "molar_mass" field.

Parameters **volume** : float

Molar volume of the mineral. For consistency this should be calculated

using :func:'volume'. :math:'[m^3]'

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **density** : float

Density of the mineral. $[kg/m^3]$

enthalpy (*pressure*, *temperature*, *volume*, *params*)

Returns the enthalpy at the pressure and temperature of the mineral [J/mol]

entropy (*pressure*, *temperature*, *volume*, *params*)

Returns the entropy at the pressure and temperature of the mineral [J/K/mol]

gibbs_free_energy (*pressure*, *temperature*, *volume*, *params*)

Returns the Gibbs free energy at the pressure and temperature of the mineral [J/mol]

grueneisen_parameter (*pressure*, *temperature*, *volume*, *params*)

Returns grueneisen parameter $[unitless]$

heat_capacity_p (*pressure*, *temperature*, *volume*, *params*)

Returns heat capacity at constant pressure. $[J/K/mol]$

heat_capacity_v (*pressure*, *temperature*, *volume*, *params*)

Returns heat capacity at constant volume. $[J/K/mol]$

helmholtz_free_energy (*pressure*, *temperature*, *volume*, *params*)

Returns the Helmholtz free energy at the pressure and temperature of the mineral [J/mol]

internal_energy (*pressure*, *temperature*, *volume*, *params*)

Returns the internal energy at the pressure and temperature of the mineral [J/mol]

isothermal_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)

Returns isothermal bulk modulus $[Pa]$

pressure (*temperature*, *volume*, *params*)
Returns the pressure of the mineral at a given temperature and volume [Pa]

shear_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns shear modulus. $[Pa]$

thermal_expansivity (*pressure*, *temperature*, *volume*, *params*)
Returns thermal expansivity. $[1/K]$

validate_parameters (*params*)
Check for existence and validity of the parameters

volume (*pressure*, *temperature*, *params*)
Returns molar volume. $[m^3]$

volume_dependent_q (*x*, *params*)
Finite strain approximation for q, the isotropic volume strain derivative of the grueneisen parameter.

class burnman.eos.**SLB3**
Bases: *burnman.eos.slb.SLBBase*

SLB equation of state with third order finite strain expansion for the shear modulus (this should be preferred, as it is more thermodynamically consistent.)

adiabatic_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns adiabatic bulk modulus. $[Pa]$

density (*volume*, *params*)
Calculate the density of the mineral $[kg/m^3]$. The params object must include a "molar_mass" field.

Parameters **volume** : float

Molar volume of the mineral. For consistency this should be calculated

using :func:'volume'. :math:'[m^3]'

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **density** : float

Density of the mineral. $[kg/m^3]$

enthalpy (*pressure*, *temperature*, *volume*, *params*)
Returns the enthalpy at the pressure and temperature of the mineral [J/mol]

entropy (*pressure*, *temperature*, *volume*, *params*)
Returns the entropy at the pressure and temperature of the mineral [J/K/mol]

gibbs_free_energy (*pressure*, *temperature*, *volume*, *params*)
Returns the Gibbs free energy at the pressure and temperature of the mineral [J/mol]

grueneisen_parameter (*pressure*, *temperature*, *volume*, *params*)
Returns grueneisen parameter $[unitless]$

heat_capacity_p (*pressure*, *temperature*, *volume*, *params*)
Returns heat capacity at constant pressure. $[J/K/mol]$

heat_capacity_v (*pressure*, *temperature*, *volume*, *params*)
Returns heat capacity at constant volume. $[J/K/mol]$

helmholtz_free_energy (*pressure*, *temperature*, *volume*, *params*)
Returns the Helmholtz free energy at the pressure and temperature of the mineral [J/mol]

internal_energy (*pressure*, *temperature*, *volume*, *params*)
Returns the internal energy at the pressure and temperature of the mineral [J/mol]

isothermal_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns isothermal bulk modulus $[Pa]$

pressure (*temperature*, *volume*, *params*)
Returns the pressure of the mineral at a given temperature and volume [Pa]

shear_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns shear modulus. $[Pa]$

thermal_expansivity (*pressure*, *temperature*, *volume*, *params*)
Returns thermal expansivity. $[1/K]$

validate_parameters (*params*)
Check for existence and validity of the parameters

volume (*pressure*, *temperature*, *params*)
Returns molar volume. $[m^3]$

volume_dependent_q (*x*, *params*)
Finite strain approximation for q, the isotropic volume strain derivative of the grueneisen parameter.

7.4 Mie-Grüneisen-Debye

class burnman.eos.mie_grueneisen_debye.**MGDBase**
Bases: burnman.eos.equation_of_state.EquationOfState

Base class for a generic finite-strain Mie-Grueneisen-Debye equation of state. References for this can be found in many places, such as Shim, Duffy and Kenichi (2002) and Jackson and Rigden (1996). Here we mostly follow the appendices of Matas et al (2007). Of particular note is the thermal correction to the shear modulus, which was developed by Hama and Suito (1998).

grueneisen_parameter (*pressure*, *temperature*, *volume*, *params*)
Returns grueneisen parameter [unitless] as a function of pressure, temperature, and volume (EQ B6)

volume (*pressure*, *temperature*, *params*)
Returns volume [m^3] as a function of pressure [Pa] and temperature [K] EQ B7

isothermal_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns isothermal bulk modulus [Pa] as a function of pressure [Pa], temperature [K], and volume [m^3]. EQ B8

shear_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns shear modulus [Pa] as a function of pressure [Pa], temperature [K], and volume [m^3]. EQ B11

heat_capacity_v (*pressure*, *temperature*, *volume*, *params*)
Returns heat capacity at constant volume at the pressure, temperature, and volume [J/K/mol]

thermal_expansivity (*pressure*, *temperature*, *volume*, *params*)
Returns thermal expansivity at the pressure, temperature, and volume [1/K]

heat_capacity_p (*pressure*, *temperature*, *volume*, *params*)
Returns heat capacity at constant pressure at the pressure, temperature, and volume [J/K/mol]

adiabatic_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns adiabatic bulk modulus [Pa] as a function of pressure [Pa], temperature [K], and volume [m^3]. EQ D6

pressure (*temperature*, *volume*, *params*)
Returns pressure [Pa] as a function of temperature [K] and volume[m^3] EQ B7

validate_parameters (*params*)
Check for existence and validity of the parameters

density (*volume*, *params*)
Calculate the density of the mineral $[kg/m^3]$. The params object must include a "molar_mass" field.

Parameters **volume** : float

Molar volume of the mineral. For consistency this should be calculated

using :func:'volume'. :math:'[m^3]'

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **density** : float

Density of the mineral. $[kg/m^3]$

enthalpy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **H** : float

Enthalpy of the mineral

entropy (*pressure*, *temperature*, *volume*, *params*)

Returns the entropy at the pressure and temperature of the mineral [J/K/mol]

gibbs_free_energy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **G** : float

Gibbs free energy of the mineral

helmholtz_free_energy (*pressure*, *temperature*, *volume*, *params*)

Parameters **temperature** : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **F** : float

Helmholtz free energy of the mineral

internal_energy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **U** : float

Internal energy of the mineral

class `burnman.eos.`**MGD2**

Bases: *burnman.eos.mie_grueneisen_debye.MGDBase*

MGD equation of state with second order finite strain expansion for the shear modulus. In general, this should not be used, but sometimes shear modulus data is fit to a second order equation of state. In that case, you should use this. The moral is, be careful!

adiabatic_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)

Returns adiabatic bulk modulus [Pa] as a function of pressure [Pa], temperature [K], and volume [m^3]. EQ D6

density (*volume*, *params*)

Calculate the density of the mineral $[kg/m^3]$. The params object must include a "molar_mass" field.

Parameters **volume** : float

Molar volume of the mineral. For consistency this should be calculated

using :func:'volume'. :math:'[m^3]'

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **density** : float

Density of the mineral. $[kg/m^3]$

enthalpy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **H** : float

Enthalpy of the mineral

entropy (*pressure*, *temperature*, *volume*, *params*)

Returns the entropy at the pressure and temperature of the mineral [J/K/mol]

gibbs_free_energy(*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **G** : float

Gibbs free energy of the mineral

grueneisen_parameter(*pressure*, *temperature*, *volume*, *params*)

Returns grueneisen parameter [unitless] as a function of pressure, temperature, and volume (EQ B6)

heat_capacity_p(*pressure*, *temperature*, *volume*, *params*)

Returns heat capacity at constant pressure at the pressure, temperature, and volume [J/K/mol]

heat_capacity_v(*pressure*, *temperature*, *volume*, *params*)

Returns heat capacity at constant volume at the pressure, temperature, and volume [J/K/mol]

helmholtz_free_energy(*pressure*, *temperature*, *volume*, *params*)

Parameters **temperature** : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **F** : float

Helmholtz free energy of the mineral

internal_energy(*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns U : float

Internal energy of the mineral

isothermal_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns isothermal bulk modulus [Pa] as a function of pressure [Pa], temperature [K], and volume [m^3]. EQ B8

pressure (*temperature*, *volume*, *params*)
Returns pressure [Pa] as a function of temperature [K] and volume[m^3] EQ B7

shear_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns shear modulus [Pa] as a function of pressure [Pa], temperature [K], and volume [m^3]. EQ B11

thermal_expansivity (*pressure*, *temperature*, *volume*, *params*)
Returns thermal expansivity at the pressure, temperature, and volume [1/K]

validate_parameters (*params*)
Check for existence and validity of the parameters

volume (*pressure*, *temperature*, *params*)
Returns volume [m^3] as a function of pressure [Pa] and temperature [K] EQ B7

class burnman.eos.**MGD3**
Bases: *burnman.eos.mie_grueneisen_debye.MGDBase*

MGD equation of state with third order finite strain expansion for the shear modulus (this should be preferred, as it is more thermodynamically consistent.

adiabatic_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns adiabatic bulk modulus [Pa] as a function of pressure [Pa], temperature [K], and volume [m^3]. EQ D6

density (*volume*, *params*)
Calculate the density of the mineral $[kg/m^3]$. The params object must include a "molar_mass" field.

Parameters volume : float

Molar volume of the mineral. For consistency this should be calculated

using :func:'volume'. :math:'[m^3]'

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns density : float

Density of the mineral. $[kg/m^3]$

enthalpy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **H** : float

Enthalpy of the mineral

entropy (*pressure*, *temperature*, *volume*, *params*)

Returns the entropy at the pressure and temperature of the mineral [J/K/mol]

gibbs_free_energy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **G** : float

Gibbs free energy of the mineral

grueneisen_parameter (*pressure*, *temperature*, *volume*, *params*)

Returns grueneisen parameter [unitless] as a function of pressure, temperature, and volume (EQ B6)

heat_capacity_p (*pressure*, *temperature*, *volume*, *params*)

Returns heat capacity at constant pressure at the pressure, temperature, and volume [J/K/mol]

heat_capacity_v (*pressure*, *temperature*, *volume*, *params*)

Returns heat capacity at constant volume at the pressure, temperature, and volume [J/K/mol]

helmholtz_free_energy (*pressure*, *temperature*, *volume*, *params*)

Parameters **temperature** : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns F : float

Helmholtz free energy of the mineral

internal_energy (*pressure*, *temperature*, *volume*, *params*)

Parameters pressure : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns U : float

Internal energy of the mineral

isothermal_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns isothermal bulk modulus [Pa] as a function of pressure [Pa], temperature [K], and volume [m^3]. EQ B8

pressure (*temperature*, *volume*, *params*)
Returns pressure [Pa] as a function of temperature [K] and volume[m^3] EQ B7

shear_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns shear modulus [Pa] as a function of pressure [Pa], temperature [K], and volume [m^3]. EQ B11

thermal_expansivity (*pressure*, *temperature*, *volume*, *params*)
Returns thermal expansivity at the pressure, temperature, and volume [1/K]

validate_parameters (*params*)
Check for existence and validity of the parameters

volume (*pressure*, *temperature*, *params*)
Returns volume [m^3] as a function of pressure [Pa] and temperature [K] EQ B7

7.5 Modified Tait

class burnman.eos.**MT**

Bases: burnman.eos.equation_of_state.EquationOfState

Base class for a generic modified Tait equation of state. References for this can be found in Huang and Chow (1974) and Holland and Powell (2011; followed here).

An instance "m" of a Mineral can be assigned this equation of state with the command m.set_method('mt') (or by initialising the class with the param equation_of_state = 'mt').

volume (*pressure*, *temperature*, *params*)
Returns volume $[m^3]$ as a function of pressure $[Pa]$.

pressure (*temperature*, *volume*, *params*)
Returns pressure [Pa] as a function of temperature [K] and volume[m^3]

isothermal_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns isothermal bulk modulus K_T of the mineral. $[Pa]$.

adiabatic_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return a very large number. $[Pa]$

shear_modulus (*pressure*, *temperature*, *volume*, *params*)
Not implemented in the Modified Tait EoS. $[Pa]$ Returns 0. Could potentially apply a fixed Poissons ratio as a rough estimate.

heat_capacity_v (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return a very large number. $[J/K/mol]$

heat_capacity_p (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return a very large number. $[J/K/mol]$

thermal_expansivity (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return zero. $[1/K]$

grueneisen_parameter (*pressure*, *temperature*, *volume*, *params*)
Since this equation of state does not contain temperature effects, simply return zero. $[unitless]$

validate_parameters (*params*)
Check for existence and validity of the parameters

density (*volume*, *params*)
Calculate the density of the mineral $[kg/m^3]$. The params object must include a "molar_mass" field.

Parameters **volume** : float

Molar volume of the mineral. For consistency this should be calculated

using :func:'volume'. :math:'[m^3]'

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns density : float

Density of the mineral. $[kg/m^3]$

enthalpy(*pressure*, *temperature*, *volume*, *params*)

Parameters pressure : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns H : float

Enthalpy of the mineral

entropy(*pressure*, *temperature*, *volume*, *params*)

Returns the entropy at the pressure and temperature of the mineral [J/K/mol]

gibbs_free_energy(*pressure*, *temperature*, *volume*, *params*)

Parameters pressure : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns G : float

Gibbs free energy of the mineral

helmholtz_free_energy(*pressure*, *temperature*, *volume*, *params*)

Parameters temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **F** : float

Helmholtz free energy of the mineral

internal_energy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **U** : float

Internal energy of the mineral

7.6 Cork

class burnman.eos.**CORK**

Bases: burnman.eos.equation_of_state.EquationOfState

Base class for a generic modified Tait equation of state. References for this can be found in Huang and Chow (1974) and Holland and Powell (2011; followed here).

grueneisen_parameter (*pressure*, *temperature*, *volume*, *params*)

Returns grueneisen parameter [unitless] as a function of pressure, temperature, and volume.

volume (*pressure*, *temperature*, *params*)

Returns volume [m^3] as a function of pressure [Pa] and temperature [K] Eq. 7 in Holland and Powell, 1991

isothermal_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)

Returns isothermal bulk modulus [Pa] as a function of pressure [Pa], temperature [K], and volume [m^3]. EQ 13+2

shear_modulus (*pressure*, *temperature*, *volume*, *params*)

Not implemented. Returns 0. Could potentially apply a fixed Poissons ratio as a rough estimate.

heat_capacity_v (*pressure*, *temperature*, *volume*, *params*)

Returns heat capacity at constant volume at the pressure, temperature, and volume [J/K/mol].

thermal_expansivity (*pressure*, *temperature*, *volume*, *params*)
Returns thermal expansivity at the pressure, temperature, and volume [1/K] Replace -Pth in EQ 13+1 with P-Pth for non-ambient temperature

heat_capacity_p0 (*temperature*, *params*)
Returns heat capacity at ambient pressure as a function of temperature [J/K/mol] Cp = a + bT + cT^-2 + dT^-0.5 in Holland and Powell, 2011

heat_capacity_p (*pressure*, *temperature*, *volume*, *params*)
Returns heat capacity at constant pressure at the pressure, temperature, and volume [J/K/mol]

adiabatic_bulk_modulus (*pressure*, *temperature*, *volume*, *params*)
Returns adiabatic bulk modulus [Pa] as a function of pressure [Pa], temperature [K], and volume [m^3].

gibbs_free_energy (*pressure*, *temperature*, *volume*, *params*)
Returns the gibbs free energy [J/mol] as a function of pressure [Pa] and temperature [K].

pressure (*temperature*, *volume*, *params*)
Returns pressure [Pa] as a function of temperature [K] and volume[m^3]

validate_parameters (*params*)
Check for existence and validity of the parameters

density (*volume*, *params*)
Calculate the density of the mineral $[kg/m^3]$. The params object must include a "molar_mass" field.

Parameters **volume** : float

Molar volume of the mineral. For consistency this should be calculated

using :func:'volume'. :math:'[m^3]'

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **density** : float

Density of the mineral. $[kg/m^3]$

enthalpy (*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **H** : float

Enthalpy of the mineral

entropy(*pressure*, *temperature*, *volume*, *params*)

Returns the entropy at the pressure and temperature of the mineral [J/K/mol]

helmholtz_free_energy(*pressure*, *temperature*, *volume*, *params*)

Parameters **temperature** : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **F** : float

Helmholtz free energy of the mineral

internal_energy(*pressure*, *temperature*, *volume*, *params*)

Parameters **pressure** : float

Pressure at which to evaluate the equation of state. [Pa]

temperature : float

Temperature at which to evaluate the equation of state. [K]

volume : float

Molar volume of the mineral. For consistency this should be calculated using `volume()`. [m^3]

params : dictionary

Dictionary containing material parameters required by the equation of state.

Returns **U** : float

Internal energy of the mineral

CHAPTER

EIGHT

AVERAGING SCHEMES

Given a set of mineral physics parameters and an equation of state we can calculate the density, bulk, and shear modulus for a given phase. However, as soon as we have a composite material (e.g., a rock), the determination of elastic properties become more complicated. The bulk and shear modulus of a rock are dependent on the specific geometry of the grains in the rock, so there is no general formula for its averaged elastic properties. Instead, we must choose from a number of averaging schemes if we want a single value, or use bounding methods to get a range of possible values. The module `burnman.averaging_schemes` provides a number of different average and bounding schemes for determining a composite rock's physical parameters.

8.1 Base class

class `burnman.averaging_schemes.`**`AveragingScheme`**

Bases: `object`

Base class defining an interface for determining average elastic properties of a rock. Given a list of volume fractions for the different mineral phases in a rock, as well as their bulk and shear moduli, an averaging will give back a single scalar values for the averages. New averaging schemes should define the functions average_bulk_moduli and average_shear_moduli, as specified here.

`average_bulk_moduli` (*volumes*, *bulk_moduli*, *shear_moduli*)

Average the bulk moduli K for a composite. This defines the interface for this method, and is not implemented in the base class.

Parameters **volumes** : list of floats

List of the volume of each phase in the composite. $[m^3]$

bulk_moduli : list of floats

List of bulk moduli of each phase in the composite. $[Pa]$

shear_moduli : list of floats

List of shear moduli of each phase in the composite. $[Pa]$

Returns **K** : float

The average bulk modulus K. $[Pa]$

average_shear_moduli(*volumes*, *bulk_moduli*, *shear_moduli*)
Average the shear moduli G for a composite. This defines the interface for this method, and is not implemented in the base class.

Parameters **volumes** : list of floats

List of the volume of each phase in the composite. $[m^3]$

bulk_moduli : list of floats

List of bulk moduli of each phase in the composite. $[Pa]$

shear_moduli : list of floats

List of shear moduli of each phase in the composite. $[Pa]$

Returns **G** : float

The average shear modulus G. $[Pa]$

average_density(*volumes*, *densities*)
Average the densities of a composite, given a list of volume fractions and densitites. This is implemented in the base class, as how to calculate it is not dependent on the geometry of the rock. The formula for density is given by

$$\rho = \frac{\Sigma_i \rho_i V_i}{\Sigma_i V_i}$$

Parameters **volumes** : list of floats

List of the volume of each phase in the composite. $[m^3]$

densities : list of floats

List of densities of each phase in the composite. $[kg/m^3]$

Returns **rho** : float

Density ρ. $[kg/m^3]$

average_thermal_expansivity(*volumes*, *alphas*)
thermal expansion coefficient of the mineral α. $[1/K]$

average_heat_capacity_v(*fractions*, *c_v*)
Averages the heat capacities at constant volume C_V by molar fractions as in eqn. (16) in *[IS92]*.

Parameters **fractions** : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_v : list of floats

List of heat capacities at constant volume C_V of each phase in the composite. $[J/K/mol]$

Returns **c_v** : float

heat capacity at constant volume of the composite C_V. $[J/K/mol]$

average_heat_capacity_p (*fractions*, *c_p*)

Averages the heat capacities at constant pressure C_P by molar fractions.

Parameters **fractions** : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_p : list of floats

List of heat capacities at constant pressure C_P of each phase in the composite. $[J/K/mol]$

Returns **c_p** : float

heat capacity at constant pressure C_P of the composite. $[J/K/mol]$

8.2 Voigt bound

class burnman.averaging_schemes.**Voigt**

Bases: *burnman.averaging_schemes.AveragingScheme*

Class for computing the Voigt (iso-strain) bound for elastic properties. This derives from burnman.averaging_schemes.averaging_scheme, and implements the burnman.averaging_schemes.averaging_scheme.average_bulk_moduli() and burnman.averaging_schemes.averaging_scheme.average_shear_moduli() functions.

average_bulk_moduli (*volumes*, *bulk_moduli*, *shear_moduli*)

Average the bulk moduli of a composite K with the Voigt (iso-strain) bound, given by:

$$K_V = \Sigma_i V_i K_i$$

Parameters **volumes** : list of floats

List of the volume of each phase in the composite. $[m^3]$

bulk_moduli : list of floats

List of bulk moduli K of each phase in the composite. $[Pa]$

shear_moduli : list of floats

List of shear moduli G of each phase in the composite. Not used in this average. $[Pa]$

Returns **K** : float

The Voigt average bulk modulus K_V. $[Pa]$

average_shear_moduli (*volumes*, *bulk_moduli*, *shear_moduli*)

Average the shear moduli of a composite with the Voigt (iso-strain) bound, given by:

$$G_V = \Sigma_i V_i G_i$$

Parameters **volumes** : list of floats

List of the volume of each phase in the composite. $[m^3]$

bulk_moduli : list of floats

List of bulk moduli K of each phase in the composite. Not used in this average. $[Pa]$

shear_moduli : list of floats

List of shear moduli G of each phase in the composite. $[Pa]$

Returns G : float

The Voigt average shear modulus G_V. $[Pa]$

average_density (*volumes*, *densities*)

Average the densities of a composite, given a list of volume fractions and densitites. This is implemented in the base class, as how to calculate it is not dependent on the geometry of the rock. The formula for density is given by

$$\rho = \frac{\Sigma_i \rho_i V_i}{\Sigma_i V_i}$$

Parameters volumes : list of floats

List of the volume of each phase in the composite. $[m^3]$

densities : list of floats

List of densities of each phase in the composite. $[kg/m^3]$

Returns rho : float

Density ρ. $[kg/m^3]$

average_heat_capacity_p (*fractions*, *c_p*)

Averages the heat capacities at constant pressure C_P by molar fractions.

Parameters fractions : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_p : list of floats

List of heat capacities at constant pressure C_P of each phase in the composite. $[J/K/mol]$

Returns c_p : float

heat capacity at constant pressure C_P of the composite. $[J/K/mol]$

average_heat_capacity_v (*fractions*, *c_v*)

Averages the heat capacities at constant volume C_V by molar fractions as in eqn. (16) in *[IS92]*.

Parameters fractions : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_v : list of floats

List of heat capacities at constant volume C_V of each phase in the composite. $[J/K/mol]$

Returns **c_v** : float

heat capacity at constant volume of the composite C_V. $[J/K/mol]$

average_thermal_expansivity (*volumes*, *alphas*)
thermal expansion coefficient of the mineral α. $[1/K]$

8.3 Reuss bound

class burnman.averaging_schemes.**Reuss**
Bases: *burnman.averaging_schemes.AveragingScheme*

Class for computing the Reuss (iso-stress) bound for elastic properties. This derives from burnman.averaging_schemes.averaging_scheme, and implements the burnman.averaging_schemes.averaging_scheme.average_bulk_moduli() and burnman.averaging_schemes.averaging_scheme.average_shear_moduli() functions.

average_bulk_moduli (*volumes*, *bulk_moduli*, *shear_moduli*)
Average the bulk moduli of a composite with the Reuss (iso-stress) bound, given by:

$$K_R = \left(\Sigma_i \frac{V_i}{K_i} \right)^{-1}$$

Parameters **volumes** : list of floats

List of the volume of each phase in the composite. $[m^3]$

bulk_moduli : list of floats

List of bulk moduli K of each phase in the composite. $[Pa]$

shear_moduli : list of floats

List of shear moduli G of each phase in the composite. Not used in this average. $[Pa]$

Returns **K** : float

The Reuss average bulk modulus K_R. $[Pa]$

average_shear_moduli (*volumes*, *bulk_moduli*, *shear_moduli*)
Average the shear moduli of a composite with the Reuss (iso-stress) bound, given by:

$$G_R = \left(\Sigma_i \frac{V_i}{G_i} \right)^{-1}$$

Parameters **volumes** : list of floats

List of the volume of each phase in the composite. $[m^3]$

bulk_moduli : list of floats

List of bulk moduli K of each phase in the composite. Not used in this average. $[Pa]$

shear_moduli : list of floats

List of shear moduli G of each phase in the composite. $[Pa]$

Returns G : float

The Reuss average shear modulus G_R. $[Pa]$

average_density (*volumes*, *densities*)

Average the densities of a composite, given a list of volume fractions and densitites. This is implemented in the base class, as how to calculate it is not dependent on the geometry of the rock. The formula for density is given by

$$\rho = \frac{\Sigma_i \rho_i V_i}{\Sigma_i V_i}$$

Parameters volumes : list of floats

List of the volume of each phase in the composite. $[m^3]$

densities : list of floats

List of densities of each phase in the composite. $[kg/m^3]$

Returns rho : float

Density ρ. $[kg/m^3]$

average_heat_capacity_p (*fractions*, *c_p*)

Averages the heat capacities at constant pressure C_P by molar fractions.

Parameters fractions : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_p : list of floats

List of heat capacities at constant pressure C_P of each phase in the composite. $[J/K/mol]$

Returns c_p : float

heat capacity at constant pressure C_P of the composite. $[J/K/mol]$

average_heat_capacity_v (*fractions*, *c_v*)

Averages the heat capacities at constant volume C_V by molar fractions as in eqn. (16) in *[IS92]*.

Parameters fractions : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_v : list of floats

List of heat capacities at constant volume C_V of each phase in the composite. $[J/K/mol]$

Returns c_v : float

heat capacity at constant volume of the composite C_V. $[J/K/mol]$

average_thermal_expansivity (*volumes*, *alphas*)
thermal expansion coefficient of the mineral α. $[1/K]$

8.4 Voigt-Reuss-Hill average

class burnman.averaging_schemes.**VoigtReussHill**
Bases: *burnman.averaging_schemes.AveragingScheme*

Class for computing the Voigt-Reuss-Hill average for elastic properties. This derives from burnman.averaging_schemes.averaging_scheme, and implements the burnman.averaging_schemes.averaging_scheme.average_bulk_moduli() and burnman.averaging_schemes.averaging_scheme.average_shear_moduli() functions.

average_bulk_moduli (*volumes*, *bulk_moduli*, *shear_moduli*)
Average the bulk moduli of a composite with the Voigt-Reuss-Hill average, given by:

$$K_{VRH} = \frac{K_V + K_R}{2}$$

This is simply a shorthand for an arithmetic average of the bounds given by burnman.averaging_schemes.voigt and burnman.averaging_schemes.reuss.

Parameters **volumes** : list of floats

List of the volume of each phase in the composite. $[m^3]$

bulk_moduli : list of floats

List of bulk moduli K of each phase in the composite. $[Pa]$

shear_moduli : list of floats

List of shear moduli G of each phase in the composite. Not used in this average. $[Pa]$

Returns **K** : float

The Voigt-Reuss-Hill average bulk modulus K_{VRH}. $[Pa]$

average_shear_moduli (*volumes*, *bulk_moduli*, *shear_moduli*)
Average the shear moduli G of a composite with the Voigt-Reuss-Hill average, given by:

$$G_{VRH} = \frac{G_V + G_R}{2}$$

This is simply a shorthand for an arithmetic average of the bounds given by burnman.averaging_schemes.voigt and burnman.averaging_schemes.reuss.

Parameters **volumes** : list of floats

List of the volume of each phase in the composite $[m^3]$

bulk_moduli : list of floats

List of bulk moduli K of each phase in the composite Not used in this average. $[Pa]$

shear_moduli : list of floats

List of shear moduli G of each phase in the composite $[Pa]$

Returns G : float

The Voigt-Reuss-Hill average shear modulus G_{VRH}. $[Pa]$

average_density (*volumes*, *densities*)

Average the densities of a composite, given a list of volume fractions and densitites. This is implemented in the base class, as how to calculate it is not dependent on the geometry of the rock. The formula for density is given by

$$\rho = \frac{\Sigma_i \rho_i V_i}{\Sigma_i V_i}$$

Parameters volumes : list of floats

List of the volume of each phase in the composite. $[m^3]$

densities : list of floats

List of densities of each phase in the composite. $[kg/m^3]$

Returns rho : float

Density ρ. $[kg/m^3]$

average_heat_capacity_p (*fractions*, *c_p*)

Averages the heat capacities at constant pressure C_P by molar fractions.

Parameters fractions : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_p : list of floats

List of heat capacities at constant pressure C_P of each phase in the composite. $[J/K/mol]$

Returns c_p : float

heat capacity at constant pressure C_P of the composite. $[J/K/mol]$

average_heat_capacity_v (*fractions*, *c_v*)

Averages the heat capacities at constant volume C_V by molar fractions as in eqn. (16) in *[IS92]*.

Parameters fractions : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_v : list of floats

List of heat capacities at constant volume C_V of each phase in the composite. $[J/K/mol]$

Returns **c_v** : float

heat capacity at constant volume of the composite C_V. $[J/K/mol]$

average_thermal_expansivity (*volumes*, *alphas*)
thermal expansion coefficient of the mineral α. $[1/K]$

8.5 Hashin-Shtrikman upper bound

class burnman.averaging_schemes.**HashinShtrikmanUpper**
Bases: *burnman.averaging_schemes.AveragingScheme*

Class for computing the upper Hashin-Shtrikman bound for elastic properties. This derives from burnman.averaging_schemes.averaging_scheme, and implements the burnman.averaging_schemes.averaging_scheme.average_bulk_moduli() and burnman.averaging_schemes.averaging_scheme.average_shear_moduli() functions. Implements formulas from *[WDOConnell76]*. The Hashin-Shtrikman bounds are tighter than the Voigt and Reuss bounds because they make the additional assumption that the orientation of the phases are statistically isotropic. In some cases this may be a good assumption, and in others it may not be.

average_bulk_moduli (*volumes*, *bulk_moduli*, *shear_moduli*)
Average the bulk moduli of a composite with the upper Hashin-Shtrikman bound. Implements Formulas from *[WDOConnell76]*, which are too lengthy to reproduce here.

Parameters **volumes** : list of floats

List of the volume of each phase in the composite. $[m^3]$

bulk_moduli : list of floats

List of bulk moduli K of each phase in the composite. $[Pa]$

shear_moduli : list of floats

List of shear moduli G of each phase in the composite. $[Pa]$

Returns **K** : float

The upper Hashin-Shtrikman average bulk modulus K. $[Pa]$

average_shear_moduli (*volumes*, *bulk_moduli*, *shear_moduli*)
Average the shear moduli of a composite with the upper Hashin-Shtrikman bound. Implements Formulas from *[WDOConnell76]*, which are too lengthy to reproduce here.

Parameters **volumes** : list of floats

List of the volume of each phase in the composite. $[m^3]$

bulk_moduli : list of floats

List of bulk moduli K of each phase in the composite. $[Pa]$

shear_moduli : list of floats

List of shear moduli G of each phase in the composite. $[Pa]$

Returns G : float

The upper Hashin-Shtrikman average shear modulus G. $[Pa]$

average_density (*volumes*, *densities*)

Average the densities of a composite, given a list of volume fractions and densitites. This is implemented in the base class, as how to calculate it is not dependent on the geometry of the rock. The formula for density is given by

$$\rho = \frac{\Sigma_i \rho_i V_i}{\Sigma_i V_i}$$

Parameters volumes : list of floats

List of the volume of each phase in the composite. $[m^3]$

densities : list of floats

List of densities of each phase in the composite. $[kg/m^3]$

Returns rho : float

Density ρ. $[kg/m^3]$

average_heat_capacity_p (*fractions*, *c_p*)

Averages the heat capacities at constant pressure C_P by molar fractions.

Parameters fractions : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_p : list of floats

List of heat capacities at constant pressure C_P of each phase in the composite. $[J/K/mol]$

Returns c_p : float

heat capacity at constant pressure C_P of the composite. $[J/K/mol]$

average_heat_capacity_v (*fractions*, *c_v*)

Averages the heat capacities at constant volume C_V by molar fractions as in eqn. (16) in *[IS92]*.

Parameters fractions : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_v : list of floats

List of heat capacities at constant volume C_V of each phase in the composite. $[J/K/mol]$

Returns c_v : float

heat capacity at constant volume of the composite C_V. $[J/K/mol]$

average_thermal_expansivity (*volumes*, *alphas*)
thermal expansion coefficient of the mineral α. $[1/K]$

8.6 Hashin-Shtrikman lower bound

class burnman.averaging_schemes.**HashinShtrikmanLower**
Bases: *burnman.averaging_schemes.AveragingScheme*

Class for computing the lower Hashin-Shtrikman bound for elastic properties. This derives from burnman.averaging_schemes.averaging_scheme, and implements the burnman.averaging_schemes.averaging_scheme.average_bulk_moduli() and burnman.averaging_schemes.averaging_scheme.average_shear_moduli() functions. Implements Formulas from *[WDOConnell76]*. The Hashin-Shtrikman bounds are tighter than the Voigt and Reuss bounds because they make the additional assumption that the orientation of the phases are statistically isotropic. In some cases this may be a good assumption, and in others it may not be.

average_bulk_moduli (*volumes*, *bulk_moduli*, *shear_moduli*)
Average the bulk moduli of a composite with the lower Hashin-Shtrikman bound. Implements Formulas from *[WDOConnell76]*, which are too lengthy to reproduce here.

Parameters **volumes** : list of floats

List of the volume of each phase in the composite. $[m^3]$

bulk_moduli : list of floats

List of bulk moduli K of each phase in the composite. $[Pa]$

shear_moduli : list of floats

List of shear moduli G of each phase in the composite. $[Pa]$

Returns **K** : float

The lower Hashin-Shtrikman average bulk modulus K. $[Pa]$

average_shear_moduli (*volumes*, *bulk_moduli*, *shear_moduli*)
Average the shear moduli of a composite with the lower Hashin-Shtrikman bound. Implements Formulas from *[WDOConnell76]*, which are too lengthy to reproduce here.

Parameters **volumes** : list of floats

List of volumes of each phase in the composite. $[m^3]$.

bulk_moduli : list of floats

List of bulk moduli K of each phase in the composite. $[Pa]$.

shear_moduli : list of floats

List of shear moduli G of each phase in the composite. $[Pa]$

Returns **G** : float

The lower Hashin-Shtrikman average shear modulus G. $[Pa]$

average_density (*volumes*, *densities*)

Average the densities of a composite, given a list of volume fractions and densitites. This is implemented in the base class, as how to calculate it is not dependent on the geometry of the rock. The formula for density is given by

$$\rho = \frac{\Sigma_i \rho_i V_i}{\Sigma_i V_i}$$

Parameters **volumes** : list of floats

List of the volume of each phase in the composite. $[m^3]$

densities : list of floats

List of densities of each phase in the composite. $[kg/m^3]$

Returns **rho** : float

Density ρ. $[kg/m^3]$

average_heat_capacity_p (*fractions*, *c_p*)

Averages the heat capacities at constant pressure C_P by molar fractions.

Parameters **fractions** : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_p : list of floats

List of heat capacities at constant pressure C_P of each phase in the composite. $[J/K/mol]$

Returns **c_p** : float

heat capacity at constant pressure C_P of the composite. $[J/K/mol]$

average_heat_capacity_v (*fractions*, *c_v*)

Averages the heat capacities at constant volume C_V by molar fractions as in eqn. (16) in *[IS92]*.

Parameters **fractions** : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_v : list of floats

List of heat capacities at constant volume C_V of each phase in the composite. $[J/K/mol]$

Returns **c_v** : float

heat capacity at constant volume of the composite C_V. $[J/K/mol]$

average_thermal_expansivity (*volumes*, *alphas*)

thermal expansion coefficient of the mineral α. $[1/K]$

8.7 Hashin-Shtrikman arithmetic average

class burnman.averaging_schemes.**HashinShtrikmanAverage**

Bases: *burnman.averaging_schemes.AveragingScheme*

Class for computing arithmetic mean of the Hashin-Shtrikman bounds on elastic properties. This derives from burnman.averaging_schemes.averaging_scheme, and implements the burnman.averaging_schemes.averaging_scheme.average_bulk_moduli() and burnman.averaging_schemes.averaging_scheme.average_shear_moduli() functions.

average_bulk_moduli (*volumes*, *bulk_moduli*, *shear_moduli*)

Average the bulk moduli of a composite with the arithmetic mean of the upper and lower Hashin-Shtrikman bounds.

Parameters **volumes** : list of floats

List of the volumes of each phase in the composite. $[m^3]$

bulk_moduli : list of floats

List of bulk moduli K of each phase in the composite. $[Pa]$

shear_moduli : list of floats

List of shear moduli G of each phase in the composite. Not used in this average. $[Pa]$

Returns **K** : float

The arithmetic mean of the Hashin-Shtrikman bounds on bulk modulus K. $[Pa]$

average_shear_moduli (*volumes*, *bulk_moduli*, *shear_moduli*)

Average the bulk moduli of a composite with the arithmetic mean of the upper and lower Hashin-Shtrikman bounds.

Parameters **volumes** : list of floats

List of the volumes of each phase in the composite. [m^3].

bulk_moduli : list of floats

List of bulk moduli K of each phase in the composite. Not used in this average. $[Pa]$

shear_moduli : list of floats

List of shear moduli G of each phase in the composite. $[Pa]$

Returns **G** : float

The arithmetic mean of the Hashin-Shtrikman bounds on shear modulus G. $[Pa]$

average_density (*volumes*, *densities*)

Average the densities of a composite, given a list of volume fractions and densitites. This is

implemented in the base class, as how to calculate it is not dependent on the geometry of the rock. The formula for density is given by

$$\rho = \frac{\Sigma_i \rho_i V_i}{\Sigma_i V_i}$$

Parameters **volumes** : list of floats

List of the volume of each phase in the composite. $[m^3]$

densities : list of floats

List of densities of each phase in the composite. $[kg/m^3]$

Returns **rho** : float

Density ρ. $[kg/m^3]$

average_heat_capacity_p (*fractions*, *c_p*)

Averages the heat capacities at constant pressure C_P by molar fractions.

Parameters **fractions** : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_p : list of floats

List of heat capacities at constant pressure C_P of each phase in the composite. $[J/K/mol]$

Returns **c_p** : float

heat capacity at constant pressure C_P of the composite. $[J/K/mol]$

average_heat_capacity_v (*fractions*, *c_v*)

Averages the heat capacities at constant volume C_V by molar fractions as in eqn. (16) in *[IS92]*.

Parameters **fractions** : list of floats

List of molar fractions of each phase in the composite (should sum to 1.0).

c_v : list of floats

List of heat capacities at constant volume C_V of each phase in the composite. $[J/K/mol]$

Returns **c_v** : float

heat capacity at constant volume of the composite C_V. $[J/K/mol]$

average_thermal_expansivity (*volumes*, *alphas*)

thermal expansion coefficient of the mineral α. $[1/K]$

CHAPTER

NINE

GEOTHERMS

burnman.geotherm.**brown_shankland**(*pressure*)

Geotherm from *[BS81]*. NOTE: Valid only above 270 km

Parameters **pressure** : list of floats

The list of pressures at which to evaluate the geotherm. $[Pa]$

Returns **temperature** : list of floats

The list of temperatures for each of the pressures. $[K]$

burnman.geotherm.**anderson**(*pressure*)

Geotherm from *[And82a]*.

Parameters **pressure** : list of floats

The list of pressures at which to evaluate the geotherm. $[Pa]$

Returns **temperature** : list of floats

The list of temperatures for each of the pressures. $[K]$

burnman.geotherm.**adiabatic**(*pressures*, *T0*, *rock*)

This calculates a geotherm based on an anchor temperature and a rock, assuming that the rock's temperature follows an adiabatic gradient with pressure. This amounts to integrating:

$$\frac{\partial T}{\partial P} = \frac{\gamma T}{K_s}$$

where γ is the Grueneisen parameter and K_s is the adiabatic bulk modulus.

Parameters **pressures** : list of floats

The list of pressures in $[Pa]$ at which to evaluate the geotherm.

T0 : float

An anchor temperature, corresponding to the temperature of the first pressure in the list. $[K]$

rock : burnman.composite

Material for which we compute the adiabat. From this material we must compute average Grueneisen parameters and adiabatic bulk moduli for each pressure/temperature.

Returns temperature: list of floats

The list of temperatures for each pressure. $[K]$

burnman.geotherm.**dTdP**(*temperature*, *pressure*, *rock*)

ODE to integrate temperature with depth for a composite material Assumes that the minerals exist at a common pressure (Reuss bound, should be good for slow deformations at high temperature), as well as an adiabatic process. This corresponds to conservation of enthalpy. First consider compression of the composite to a new pressure P+dP. They all heat up different amounts dT[i], according to their thermoelastic parameters. Then allow them to equilibrate to a constant temperature dT, conserving heat within the composite. This works out to the formula:

$$dT/dP = T * \frac{\Sigma_i(X[i] * C_p[i] * \gamma[i]/K[i])}{\Sigma(X[i] * C_p[i])}$$

Where $X[i]$ is the molar fraction of phase i, C_p is the specific heat at constant pressure, γ is the Gruneisen parameter and K is the bulk modulus. This function is called by *burnman.geotherm.adiabatic()*, and in general it will not be too useful in other contexts.

Parameters **pressure** : float

The pressure at which to evaluate dT/dP. $[Pa]$

temperature : float

The temperature at which to evaluate dT/dP. $[K]$

rock : burnman.composite

Material for which we compute dT/dP.

Returns **dT/dP** : float

Adiabatic temperature gradient for the composite at a given temperature and pressure. $[K/Pa]$

CHAPTER

TEN

THERMODYNAMICS

Burnman has a number of functions and classes which deal with the thermodynamics of single phases and aggregates.

10.1 Lattice Vibrations

10.1.1 Debye model

burnman.debye.**debye_fn**(*x*)
Evaluate the Debye function. Takes the parameter xi = Debye_T/T

burnman.debye.**debye_fn_cheb**(*x*)
Evaluate the Debye function using a Chebyshev series expansion coupled with asymptotic solutions of the function. Shamelessly adapted from the GSL implementation of the same function (Itself adapted from Collected Algorithms from ACM). Should give the same result as debye_fn(x) to near machine-precision.

burnman.debye.**entropy**(*T*, *debye_T*, *n*)
Entropy due to lattice vibrations in the Debye model [J/K]

burnman.debye.**heat_capacity_v**(*T*, *debye_T*, *n*)
Heat capacity at constant volume. In J/K/mol

burnman.debye.**helmholtz_free_energy**(*T*, *debye_T*, *n*)
Helmholtz free energy of lattice vibrations in the Debye model. It is important to note that this does NOT include the zero point energy of vibration for the lattice. As long as you are calculating relative differences in F, this should cancel anyways. In Joules.

burnman.debye.**jit**(*fn*)

burnman.debye.**thermal_energy**(*T*, *debye_T*, *n*)
calculate the thermal energy of a substance. Takes the temperature, the Debye temperature, and n, the number of atoms per molecule. Returns thermal energy in J/mol

10.1.2 Einstein model

burnman.eos.einstein.**thermal_energy**(*T*, *einstein_T*, *n*)
calculate the thermal energy of a substance. Takes the temperature, the Einstein temperature, and n,

the number of atoms per molecule. Returns thermal energy in J/mol

burnman.eos.einstein.**heat_capacity_v**(*T*, *einstein_T*, *n*)
Heat capacity at constant volume. In J/K/mol

10.2 Solution models

burnman.solutionmodel.**kd**(*x*, *y*)

class burnman.solutionmodel.**SolutionModel**
Bases: object

This is the base class for a solution model, intended for use in defining solid solutions and performing thermodynamic calculations on them. All minerals of type burnman.SolidSolution use a solution model for defining how the endmembers in the solid solution interact.

A user wanting a new solution model should define the functions below. In the base class all of these return zero, so if the solution model does not implement them, they essentially have no effect, and then the Gibbs free energy and molar volume of a solid solution are just the weighted arithmetic averages of the different endmember values.

excess_gibbs_free_energy(*pressure*, *temperature*, *molar_fractions*)
Given a list of molar fractions of different phases, compute the excess Gibbs free energy of the solution. The base class implementation assumes that the excess gibbs free energy is zero.

Parameters **pressure** : float

Pressure at which to evaluate the solution model. [Pa]

temperature : float

Temperature at which to evaluate the solution. [K]

molar_fractions : list of floats

List of molar fractions of the different endmembers in solution

Returns **G_excess** : float

The excess Gibbs free energy

excess_partial_gibbs_free_energies(*pressure*, *temperature*, *molar_fractions*)
Given a list of molar fractions of different phases, compute the excess Gibbs free energy for each endmember of the solution. The base class implementation assumes that the excess gibbs free energy is zero.

Parameters **pressure** : float

Pressure at which to evaluate the solution model. [Pa]

temperature : float

Temperature at which to evaluate the solution. [K]

molar_fractions : list of floats

List of molar fractions of the different endmembers in solution

Returns **partial_G_excess** : numpy array

The excess Gibbs free energy of each endmember

excess_volume (*pressure*, *temperature*, *molar_fractions*)

Given a list of molar fractions of different phases, compute the excess volume of the solution. The base class implementation assumes that the excess volume is zero.

Parameters **pressure** : float

Pressure at which to evaluate the solution model. [Pa]

temperature : float

Temperature at which to evaluate the solution. [K]

molar_fractions : list of floats

List of molar fractions of the different endmembers in solution

Returns **V_excess** : float

The excess volume of the solution

excess_enthalpy (*pressure*, *temperature*, *molar_fractions*)

Given a list of molar fractions of different phases, compute the excess enthalpy of the solution. The base class implementation assumes that the excess enthalpy is zero.

Parameters **pressure** : float

Pressure at which to evaluate the solution model. [Pa]

temperature : float

Temperature at which to evaluate the solution. [K]

molar_fractions : list of floats

List of molar fractions of the different endmembers in solution

Returns **H_excess** : float

The excess enthalpy of the solution

excess_entropy (*pressure*, *temperature*, *molar_fractions*)

Given a list of molar fractions of different phases, compute the excess entropy of the solution. The base class implementation assumes that the excess entropy is zero.

Parameters **pressure** : float

Pressure at which to evaluate the solution model. [Pa]

temperature : float

Temperature at which to evaluate the solution. [K]

molar_fractions : list of floats

List of molar fractions of the different endmembers in solution

Returns **S_excess** : float

The excess entropy of the solution

class burnman.solutionmodel.**IdealSolution**(*endmembers*)

Bases: *burnman.solutionmodel.SolutionModel*

A very simple class representing an ideal solution model. Calculate the excess gibbs free energy due to configurational entropy, all the other excess terms return zero.

excess_partial_gibbs_free_energies(*pressure*, *temperature*, *molar_fractions*)

activity_coefficients(*pressure*, *temperature*, *molar_fractions*)

activities(*pressure*, *temperature*, *molar_fractions*)

excess_enthalpy(*pressure*, *temperature*, *molar_fractions*)

Given a list of molar fractions of different phases, compute the excess enthalpy of the solution. The base class implementation assumes that the excess enthalpy is zero.

Parameters **pressure** : float

Pressure at which to evaluate the solution model. [Pa]

temperature : float

Temperature at which to evaluate the solution. [K]

molar_fractions : list of floats

List of molar fractions of the different endmembers in solution

Returns **H_excess** : float

The excess enthalpy of the solution

excess_entropy(*pressure*, *temperature*, *molar_fractions*)

Given a list of molar fractions of different phases, compute the excess entropy of the solution. The base class implementation assumes that the excess entropy is zero.

Parameters **pressure** : float

Pressure at which to evaluate the solution model. [Pa]

temperature : float

Temperature at which to evaluate the solution. [K]

molar_fractions : list of floats

List of molar fractions of the different endmembers in solution

Returns **S_excess** : float

The excess entropy of the solution

excess_gibbs_free_energy(*pressure*, *temperature*, *molar_fractions*)

Given a list of molar fractions of different phases, compute the excess Gibbs free energy of the solution. The base class implementation assumes that the excess gibbs free energy is zero.

Parameters **pressure** : float

Pressure at which to evaluate the solution model. [Pa]

temperature : float

Temperature at which to evaluate the solution. [K]

molar_fractions : list of floats

List of molar fractions of the different endmembers in solution

Returns **G_excess** : float

The excess Gibbs free energy

excess_volume(*pressure*, *temperature*, *molar_fractions*)

Given a list of molar fractions of different phases, compute the excess volume of the solution. The base class implementation assumes that the excess volume is zero.

Parameters **pressure** : float

Pressure at which to evaluate the solution model. [Pa]

temperature : float

Temperature at which to evaluate the solution. [K]

molar_fractions : list of floats

List of molar fractions of the different endmembers in solution

Returns **V_excess** : float

The excess volume of the solution

class burnman.solutionmodel.**AsymmetricRegularSolution**(*endmembers*, *alphas*, *enthalpy_interaction*, *volume_interaction=None*, *entropy_interaction=None*)

Bases: *burnman.solutionmodel.IdealSolution*

Solution model implementing the asymmetric regular solution model formulation (Holland and Powell, 2003)

excess_partial_gibbs_free_energies(*pressure*, *temperature*, *molar_fractions*)

excess_volume(*pressure*, *temperature*, *molar_fractions*)

excess_entropy(*pressure*, *temperature*, *molar_fractions*)

excess_enthalpy(*pressure*, *temperature*, *molar_fractions*)

activity_coefficients(*pressure*, *temperature*, *molar_fractions*)

activities(*pressure*, *temperature*, *molar_fractions*)

excess_gibbs_free_energy(*pressure*, *temperature*, *molar_fractions*)

Given a list of molar fractions of different phases, compute the excess Gibbs free energy of the solution. The base class implementation assumes that the excess gibbs free energy is zero.

Parameters **pressure** : float

Pressure at which to evaluate the solution model. [Pa]

temperature : float

Temperature at which to evaluate the solution. [K]

molar_fractions : list of floats

List of molar fractions of the different endmembers in solution

Returns **G_excess** : float

The excess Gibbs free energy

class burnman.solutionmodel.**SymmetricRegularSolution**(*endmembers*, *enthalpy_interaction*, *volume_interaction=None*, *entropy_interaction=None*)

Bases: *burnman.solutionmodel.AsymmetricRegularSolution*

Solution model implementing the symmetric regular solution model

activities(*pressure*, *temperature*, *molar_fractions*)

activity_coefficients(*pressure*, *temperature*, *molar_fractions*)

excess_enthalpy(*pressure*, *temperature*, *molar_fractions*)

excess_entropy(*pressure*, *temperature*, *molar_fractions*)

excess_gibbs_free_energy(*pressure*, *temperature*, *molar_fractions*)

Given a list of molar fractions of different phases, compute the excess Gibbs free energy of the solution. The base class implementation assumes that the excess gibbs free energy is zero.

Parameters **pressure** : float

Pressure at which to evaluate the solution model. [Pa]

temperature : float

Temperature at which to evaluate the solution. [K]

molar_fractions : list of floats

List of molar fractions of the different endmembers in solution

Returns **G_excess** : float

The excess Gibbs free energy

excess_partial_gibbs_free_energies(*pressure*, *temperature*, *molar_fractions*)

excess_volume(*pressure*, *temperature*, *molar_fractions*)

class burnman.solutionmodel.**SubregularSolution**(*endmembers*, *enthalpy_interaction*, *volume_interaction=None*, *entropy_interaction=None*)

Bases: *burnman.solutionmodel.IdealSolution*

Solution model implementing the subregular solution model formulation (Helffrich and Wood, 1989)

excess_partial_gibbs_free_energies(*pressure*, *temperature*, *molar_fractions*)

excess_volume(*pressure*, *temperature*, *molar_fractions*)

excess_entropy(*pressure*, *temperature*, *molar_fractions*)

excess_enthalpy(*pressure*, *temperature*, *molar_fractions*)

activity_coefficients(*pressure*, *temperature*, *molar_fractions*)

activities(*pressure*, *temperature*, *molar_fractions*)

excess_gibbs_free_energy(*pressure*, *temperature*, *molar_fractions*)

Given a list of molar fractions of different phases, compute the excess Gibbs free energy of the solution. The base class implementation assumes that the excess gibbs free energy is zero.

Parameters **pressure** : float

Pressure at which to evaluate the solution model. [Pa]

temperature : float

Temperature at which to evaluate the solution. [K]

molar_fractions : list of floats

List of molar fractions of the different endmembers in solution

Returns **G_excess** : float

The excess Gibbs free energy

10.3 Chemistry parsing

burnman.processchemistry.**read_masses**()

A simple function to read a file with a two column list of elements and their masses into a dictionary

burnman.processchemistry.**dictionarize_formula**(*formula*)

A function to read a chemical formula string and convert it into a dictionary

burnman.processchemistry.**formula_mass**(*formula*, *atomic_masses*)

A function to take chemical formula and atomic mass dictionaries and

burnman.processchemistry.**dictionarize_site_formula**(*formula*)

A function to take a chemical formula with sites specified by square brackets and return a standard dictionary with element keys and atoms of each element per formula unit as items.

burnman.processchemistry.**process_solution_chemistry**(*formulae*)

This function parses a set of endmember formulae containing site information, e.g.

['[Mg]3[Al]2Si3O12', '[Mg]3[Mg1/2Si1/2]2Si3O12']

It outputs the bulk composition of each endmember (removing the site information), and also a set of variables and arrays which contain the site information. These are output in a format that can easily be used to calculate activities and gibbs free energies, given molar fractions of the phases and pressure and temperature where necessary.

Parameters **formulae** : list of strings

List of chemical formulae with site information

Returns **solution_formulae** : list of dictionaries

List of endmember formulae is output from site formula strings

n_sites : integer

Number of sites in the solid solution. Should be the same for all endmembers.

sites : list of lists of strings

A list of elements for each site in the solid solution

n_occupancies : integer

Sum of the number of possible elements on each of the sites in the solid solution. Example: A binary solution [[A][B],[B][C1/2D1/2]] would have n_occupancies = 5, with two possible elements on Site 1 and three on Site 2

endmember_occupancies : 2d array of floats

A 1D array for each endmember in the solid solution, containing the number of atoms of each element on each site.

site_multiplicities : array of floats

The number of each site per formula unit To simplify computations later, the multiplicities are repeated for each element on each site

burnman.processchemistry.**compositional_array**(*formulae*)

Parameters **formulae** : list of dictionaries

List of chemical formulae

Returns **formula_array** : 2D array of floats

Array of endmember formulae

elements : List of strings

List of elements

burnman.processchemistry.**ordered_compositional_array**(*formulae*, *elements*)

Parameters **formulae** : list of dictionaries

List of chemical formulae

elements : List of strings

List of elements

Returns **formula_array** : 2D array of floats

Array of endmember formulae

10.4 Chemical potentials

burnman.chemicalpotentials.**chemical_potentials**(*assemblage*, *component_formulae*)

The compositional space of the components does not have to be a superset of the compositional space of the assemblage. Nor do they have to compose an orthogonal basis.

The components must each be described by a linear mineral combination

The mineral compositions must be linearly independent

Parameters **assemblage** : list of classes

List of material classes set_method and set_state should already have been used the composition of the solid solutions should also have been set

component_formulae [list of dictionaries] List of chemical component formula dictionaries No restriction on length

Returns **component_potentials** : array of floats

Array of chemical potentials of components

burnman.chemicalpotentials.**fugacity**(*standard_material*, *assemblage*)

Parameters **standard_material: class**

Material class set_method and set_state should already have been used material must have a formula as a dictionary parameter

assemblage: list of classes

List of material classes set_method and set_state should already have been used

Returns **fugacity** : float

Value of the fugacity of the component with respect to the standard material

burnman.chemicalpotentials.**relative_fugacity**(*standard_material*, *assemblage*, *reference_assemblage*)

Parameters **standard_material: class**

Material class set_method and set_state should already have been used material must have a formula as a dictionary parameter

assemblage: list of classes

List of material classes set_method and set_state should already have been used

reference_assemblage: list of classes

List of material classes set_method and set_state should already have been used

Returns **relative_fugacity** : float

Value of the fugacity of the component in the assemblage with respect to the reference_assemblage

CHAPTER

ELEVEN

SEISMIC

11.1 Base class for all seismic models

class burnman.seismic.**Seismic1DModel**

Bases: object

Base class for all the seismological models.

evaluate(*vars_list*, *depth_list*)

Returns the lists of data for a Seismic1DModel for the depths provided

Parameters **vars_list** : array of str

Available variables depend on the seismic model, and can be chosen from 'pressure','density','gravity','v_s','v_p','v_phi','G','K','QG','QK'

depth_list : array of floats

Array of depths [m] to evaluate seismic model at.

Returns Array of values shapes as (len(vars_list),len(depth_list)).

internal_depth_list(*mindepth=0.0*, *maxdepth=1e+99*)

Returns a sorted list of depths where this seismic data is specified at. This allows you to compare the seismic data without interpolation. The depths can be bounded by the mindepth and maxdepth parameters.

Parameters **mindepth** : float

Minimum depth value to be returned [m]

maxdepth

Maximum depth value to be returned [m]

Returns **depths** : array of floats

Depths [m].

pressure(*depth*)

Parameters **depth** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **pressure** : float or array of floats

Pressure(s) at given depth(s) in [Pa].

v_p (*depth*)

Parameters **depth** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **v_p** : float or array of floats

P wave velocity at given depth(s) in [m/s].

v_s (*depth*)

Parameters **depth** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **v_s** : float or array of floats

S wave velocity at given depth(s) in [m/s].

v_phi (*depth*)

Parameters **depth_list** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **v_phi** : float or array of floats

bulk sound wave velocity at given depth(s) in [m/s].

density (*depth*)

Parameters **depth** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **density** : float or array of floats

Density at given depth(s) in [kg/m^3].

G (*depth*)

Parameters **depth** : float or array of floats

Shear modulus at given for depth(s) in [Pa].

K (*depth*)

Parameters **depth** : float or array of floats

Bulk modulus at given for depth(s) in [Pa]

QK (*depth*)

Parameters **depth** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **Qk** : float or array of floats

Quality factor (dimensionless) for bulk modulus at given depth(s).

QG(*depth*)

Parameters **depth** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **QG** : float or array of floats

Quality factor (dimensionless) for shear modulus at given depth(s).

depth(*pressure*)

Parameters **pressure** : float or array of floats

Pressure(s) [Pa] to evaluate depth at.

Returns **depth** : float or array of floats

Depth(s) [m] for given pressure(s)

gravity(*depth*)

Parameters **depth** : float or array of floats

Depth(s) [m] to evaluate gravity at.

Returns **gravity** : float or array of floats

Gravity for given depths in [m/s^2]

11.2 Class for 1D Models

class burnman.seismic.**SeismicTable**

Bases: *burnman.seismic.Seismic1DModel*

This is a base class that gets a 1D seismic model from a table indexed and sorted by radius. Fill the tables in the constructor after deriving from this class. This class uses *burnman.seismic.Seismic1DModel*

Note: all tables need to be sorted by increasing depth. self.table_depth needs to be defined Alternatively, you can also overwrite the _lookup function if you want to access with something else.

internal_depth_list(*mindepth=0.0*, *maxdepth=10000000000.0*)

pressure(*depth*)

gravity(*depth*)

v_p(*depth*)

v_s(*depth*)

QK(*depth*)

QG(*depth*)

density(*depth*)

depth(*pressure*)

radius(*pressure*)

G(*depth*)

Parameters **depth** : float or array of floats

Shear modulus at given for depth(s) in [Pa].

K(*depth*)

Parameters **depth** : float or array of floats

Bulk modulus at given for depth(s) in [Pa]

evaluate(*vars_list*, *depth_list*)

Returns the lists of data for a Seismic1DModel for the depths provided

Parameters **vars_list** : array of str

Available variables depend on the seismic model, and can be chosen from 'pressure','density','gravity','v_s','v_p','v_phi','G','K','QG','QK'

depth_list : array of floats

Array of depths [m] to evaluate seismic model at.

Returns Array of values shapes as (len(vars_list),len(depth_list)).

v_phi(*depth*)

Parameters **depth_list** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **v_phi** : float or array of floats

bulk sound wave velocity at given depth(s) in [m/s].

11.3 Models currently implemented

class burnman.seismic.**PREM**

Bases: *burnman.seismic.SeismicTable*

Reads PREM (1s) (input_seismic/prem.txt, *[DA81]*). See also *burnman.seismic.SeismicTable*.

G(*depth*)

Parameters **depth** : float or array of floats

Shear modulus at given for depth(s) in [Pa].

K(*depth*)

Parameters **depth** : float or array of floats

Bulk modulus at given for depth(s) in [Pa]

QG(*depth*)

QK(*depth*)

density(*depth*)

depth(*pressure*)

evaluate(*vars_list*, *depth_list*)

Returns the lists of data for a Seismic1DModel for the depths provided

Parameters **vars_list** : array of str

Available variables depend on the seismic model, and can be chosen from 'pressure','density','gravity','v_s','v_p','v_phi','G','K','QG','QK'

depth_list : array of floats

Array of depths [m] to evaluate seismic model at.

Returns Array of values shapes as (len(vars_list),len(depth_list)).

gravity(*depth*)

internal_depth_list(*mindepth=0.0*, *maxdepth=10000000000.0*)

pressure(*depth*)

radius(*pressure*)

v_p(*depth*)

v_phi(*depth*)

Parameters **depth_list** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **v_phi** : float or array of floats

bulk sound wave velocity at given depth(s) in [m/s].

v_s(*depth*)

class burnman.seismic.**Slow**

Bases: *burnman.seismic.SeismicTable*

Inserts the mean profiles for slower regions in the lower mantle (Lekic et al. 2012). We stitch together tables 'input_seismic/prem_lowermantle.txt', 'input_seismic/swave_slow.txt', 'input_seismic/pwave_slow.txt'). See also *burnman.seismic.SeismicTable*.

G(*depth*)

Parameters **depth** : float or array of floats

Shear modulus at given for depth(s) in [Pa].

K(*depth*)

Parameters **depth** : float or array of floats

Bulk modulus at given for depth(s) in [Pa]

QG(*depth*)

QK(*depth*)

density(*depth*)

depth(*pressure*)

evaluate(*vars_list*, *depth_list*)

Returns the lists of data for a Seismic1DModel for the depths provided

Parameters **vars_list** : array of str

Available variables depend on the seismic model, and can be chosen from 'pressure','density','gravity','v_s','v_p','v_phi','G','K','QG','QK'

depth_list : array of floats

Array of depths [m] to evaluate seismic model at.

Returns Array of values shapes as (len(vars_list),len(depth_list)).

gravity(*depth*)

internal_depth_list(*mindepth=0.0*, *maxdepth=10000000000.0*)

pressure(*depth*)

radius(*pressure*)

v_p(*depth*)

v_phi(*depth*)

Parameters **depth_list** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **v_phi** : float or array of floats

bulk sound wave velocity at given depth(s) in [m/s].

v_s(*depth*)

class burnman.seismic.**Fast**

Bases: *burnman.seismic.SeismicTable*

Inserts the mean profiles for faster regions in the lower mantle (Lekic et al. 2012). We stitch together tables 'input_seismic/prem_lowermantle.txt', 'input_seismic/swave_fast.txt', 'input_seismic/pwave_fast.txt'). See also *burnman.seismic.Seismic1DModel*.

G(*depth*)

Parameters **depth** : float or array of floats

Shear modulus at given for depth(s) in [Pa].

K(*depth*)

Parameters **depth** : float or array of floats

Bulk modulus at given for depth(s) in [Pa]

QG(*depth*)

QK(*depth*)

density(*depth*)

depth(*pressure*)

evaluate(*vars_list*, *depth_list*)

Returns the lists of data for a Seismic1DModel for the depths provided

Parameters **vars_list** : array of str

Available variables depend on the seismic model, and can be chosen from 'pressure','density','gravity','v_s','v_p','v_phi','G','K','QG','QK'

depth_list : array of floats

Array of depths [m] to evaluate seismic model at.

Returns Array of values shapes as (len(vars_list),len(depth_list)).

gravity(*depth*)

internal_depth_list(*mindepth=0.0*, *maxdepth=10000000000.0*)

pressure(*depth*)

radius(*pressure*)

v_p(*depth*)

v_phi(*depth*)

Parameters **depth_list** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **v_phi** : float or array of floats

bulk sound wave velocity at given depth(s) in [m/s].

v_s(*depth*)

class burnman.seismic.**STW105**

Bases: *burnman.seismic.SeismicTable*

Reads STW05 (a.k.a. REF) (1s) (input_seismic/STW105.txt, *[KED08]*). See also *burnman.seismic.SeismicTable*.

G(*depth*)

Parameters **depth** : float or array of floats

Shear modulus at given for depth(s) in [Pa].

K(*depth*)

Parameters **depth** : float or array of floats

Bulk modulus at given for depth(s) in [Pa]

QG(*depth*)

QK(*depth*)

density(*depth*)

depth(*pressure*)

evaluate(*vars_list*, *depth_list*)

Returns the lists of data for a Seismic1DModel for the depths provided

Parameters **vars_list** : array of str

Available variables depend on the seismic model, and can be chosen from 'pressure','density','gravity','v_s','v_p','v_phi','G','K','QG','QK'

depth_list : array of floats

Array of depths [m] to evaluate seismic model at.

Returns Array of values shapes as (len(vars_list),len(depth_list)).

gravity(*depth*)

internal_depth_list(*mindepth=0.0*, *maxdepth=10000000000.0*)

pressure(*depth*)

radius(*pressure*)

v_p(*depth*)

v_phi(*depth*)

Parameters **depth_list** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **v_phi** : float or array of floats

bulk sound wave velocity at given depth(s) in [m/s].

v_s(*depth*)

class burnman.seismic.**IASP91**

Bases: *burnman.seismic.SeismicTable*

Reads REF/STW05 (input_seismic/STW105.txt, *[KED08]*). See also *burnman.seismic.SeismicTable*.

G(*depth*)

Parameters **depth** : float or array of floats

Shear modulus at given for depth(s) in [Pa].

K(*depth*)

Parameters **depth** : float or array of floats

Bulk modulus at given for depth(s) in [Pa]

QG(*depth*)

QK(*depth*)

density(*depth*)

depth(*pressure*)

evaluate(*vars_list*, *depth_list*)

Returns the lists of data for a Seismic1DModel for the depths provided

Parameters **vars_list** : array of str

Available variables depend on the seismic model, and can be chosen from 'pressure','density','gravity','v_s','v_p','v_phi','G','K','QG','QK'

depth_list : array of floats

Array of depths [m] to evaluate seismic model at.

Returns Array of values shapes as (len(vars_list),len(depth_list)).

gravity(*depth*)

internal_depth_list(*mindepth=0.0*, *maxdepth=10000000000.0*)

pressure(*depth*)

radius(*pressure*)

v_p(*depth*)

v_phi(*depth*)

Parameters **depth_list** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **v_phi** : float or array of floats

bulk sound wave velocity at given depth(s) in [m/s].

v_s(*depth*)

class burnman.seismic.**AK135**

Bases: *burnman.seismic.SeismicTable*

Reads AK135 (input_seismic/ak135.txt, *[KEB95]*). See also *burnman.seismic.SeismicTable*.

G(*depth*)

Parameters **depth** : float or array of floats

Shear modulus at given for depth(s) in [Pa].

K(*depth*)

Parameters **depth** : float or array of floats

Bulk modulus at given for depth(s) in [Pa]

QG(*depth*)

QK(*depth*)

density(*depth*)

depth(*pressure*)

evaluate(*vars_list*, *depth_list*)

Returns the lists of data for a Seismic1DModel for the depths provided

Parameters **vars_list** : array of str

Available variables depend on the seismic model, and can be chosen from 'pressure','density','gravity','v_s','v_p','v_phi','G','K','QG','QK'

depth_list : array of floats

Array of depths [m] to evaluate seismic model at.

Returns Array of values shapes as (len(vars_list),len(depth_list)).

gravity(*depth*)

internal_depth_list(*mindepth=0.0*, *maxdepth=10000000000.0*)

pressure(*depth*)

radius(*pressure*)

v_p(*depth*)

v_phi(*depth*)

Parameters **depth_list** : float or array of floats

Depth(s) [m] to evaluate seismic model at.

Returns **v_phi** : float or array of floats

bulk sound wave velocity at given depth(s) in [m/s].

v_s(*depth*)

11.4 Attenuation Correction

burnman.seismic.**attenuation_correction**(*v_p*, *v_s*, *v_phi*, *Qs*, *Qphi*)

Applies the attenuation correction following Matas et al. (2007), page 4. This is simplified, and there is also currently no 1D Q model implemented. The correction, however, only slightly reduces the velocities, and can be ignored for our current applications. Arguably, it might not be as relevant when comparing computations to PREM for periods of 1s as is implemented here. Called from `burnman.main.apply_attenuation_correction()`

Parameters **v_p** : float

P wave velocity in [m/s].

v_s : float

S wave velocitiy in [m/s].

v_phi : float

Bulk sound velocity in [m/s].

Qs : float

shear quality factor [dimensionless]

Qphi: float

bulk quality factor [dimensionless]

Returns **v_p** : float

corrected P wave velocity in [m/s].

v_s : float

corrected S wave velocitiy in [m/s].

v_phi : float

corrected Bulk sound velocity in [m/s].

CHAPTER

TWELVE

MINERAL DATABASE

Mineral database

- *SLB_2005*
- *SLB_2011_ZSB_2013*
- *SLB_2011*
- *Murakami_etal_2012*
- *Murakami_2013*
- *Matas_etal_2007*
- HP_2011_ds62
- HP_2011_fluids
- HHPH_2013
- *other*

12.1 Murakami_2013

Minerals from Murakami 2013 and references therein.

class burnman.minerals.Murakami_2013.**periclase**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Murakami_2013.**wuestite**
Bases: *burnman.mineral.Mineral*

Murakami 2013 and references therein

class burnman.minerals.Murakami_2013.**mg_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Murakami_2013.**fe_perovskite**
Bases: *burnman.mineral.Mineral*

burnman.minerals.Murakami_2013.**mg_bridgmanite**
alias of *mg_perovskite*

burnman.minerals.Murakami_2013.**fe_bridgmanite**
alias of *fe_perovskite*

SLB_2011 Minerals from Stixrude & Lithgow-Bertelloni 2011 and references therein File autogenerated using SLBdata_to_burnman.py

burnman.minerals.SLB_2011.**atomic_masses = {u'Pr': 0.140908, u'Ni': 0.0586934, u'Yb': 0.173054, u'Pd'**
SOLID SOLUTIONS from inv251010 of HeFESTo

class burnman.minerals.SLB_2011.**c2c_pyroxene**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**ca_ferrite_structured_phase**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**clinopyroxene**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**garnet**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**akimotoite**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**ferropericlase**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**mg_fe_olivine**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**orthopyroxene**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**plagioclase**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**post_perovskite**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**mg_fe_perovskite**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**mg_fe_ringwoodite**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**mg_fe_aluminous_spinel**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**mg_fe_wadsleyite**(*molar_fractions=None*)
Bases: *burnman.solidsolution.SolidSolution*

class burnman.minerals.SLB_2011.**anorthite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**albite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**spinel**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**hercynite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**forsterite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**fayalite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**mg_wadsleyite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**fe_wadsleyite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**mg_ringwoodite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**fe_ringwoodite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**enstatite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**ferrosilite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**mg_tschermaks**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**ortho_diopside**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**diopside**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**hedenbergite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**clinoenstatite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**ca_tschermaks**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**jadeite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**hp_clinoenstatite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**hp_clinoferrosilite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**ca_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**mg_akimotoite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**fe_akimotoite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**corundum**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**pyrope**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**almandine**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**grossular**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**mg_majorite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**jd_majorite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**quartz**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**coesite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**stishovite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**seifertite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**mg_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**fe_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**al_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**mg_post_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**fe_post_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**al_post_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**periclase**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**wuestite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**mg_ca_ferrite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**fe_ca_ferrite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**na_ca_ferrite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**kyanite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011.**nepheline**
Bases: *burnman.mineral.Mineral*

burnman.minerals.SLB_2011.**ab**
alias of *albite*

burnman.minerals.SLB_2011.**an**
alias of *anorthite*

burnman.minerals.SLB_2011.**sp**
alias of *spinel*

burnman.minerals.SLB_2011.**hc**
alias of *hercynite*

burnman.minerals.SLB_2011.**fo**
alias of *forsterite*

burnman.minerals.SLB_2011.**fa**
alias of *fayalite*

burnman.minerals.SLB_2011.**mgwa**
alias of *mg_wadsleyite*

burnman.minerals.SLB_2011.**fewa**
alias of *fe_wadsleyite*

burnman.minerals.SLB_2011.**mgri**
alias of *mg_ringwoodite*

burnman.minerals.SLB_2011.**feri**
alias of *fe_ringwoodite*

burnman.minerals.SLB_2011.**en**
alias of *enstatite*

burnman.minerals.SLB_2011.**fs**
alias of *ferrosilite*

burnman.minerals.SLB_2011.**mgts**
alias of *mg_tschermaks*

burnman.minerals.SLB_2011.**odi**
alias of *ortho_diopside*

burnman.minerals.SLB_2011.**di**
alias of *diopside*

burnman.minerals.SLB_2011.**he**
alias of *hedenbergite*

burnman.minerals.SLB_2011.**cen**
alias of *clinoenstatite*

burnman.minerals.SLB_2011.**cats**
alias of *ca_tschermaks*

burnman.minerals.SLB_2011.**jd**
alias of *jadeite*

burnman.minerals.SLB_2011.**mgc2**
alias of *hp_clinoenstatite*

burnman.minerals.SLB_2011.**fec2**
alias of *hp_clinoferrosilite*

burnman.minerals.SLB_2011.**hpcen**
alias of *hp_clinoenstatite*

burnman.minerals.SLB_2011.**hpcfs**
alias of *hp_clinoferrosilite*

burnman.minerals.SLB_2011.**mgpv**
alias of *mg_perovskite*

burnman.minerals.SLB_2011.**mg_bridgmanite**
alias of *mg_perovskite*

burnman.minerals.SLB_2011.**fepv**
alias of *fe_perovskite*

burnman.minerals.SLB_2011.**fe_bridgmanite**
alias of *fe_perovskite*

burnman.minerals.SLB_2011.**alpv**
alias of *al_perovskite*

burnman.minerals.SLB_2011.**capv**
alias of *ca_perovskite*

burnman.minerals.SLB_2011.**mgil**
alias of *mg_akimotoite*

burnman.minerals.SLB_2011.**feil**
alias of *fe_akimotoite*

burnman.minerals.SLB_2011.**co**
alias of *corundum*

burnman.minerals.SLB_2011.**py**
alias of *pyrope*

burnman.minerals.SLB_2011.**al**
alias of *almandine*

burnman.minerals.SLB_2011.**gr**
alias of *grossular*

burnman.minerals.SLB_2011.**mgmj**
alias of *mg_majorite*

burnman.minerals.SLB_2011.**jdmj**
alias of *jd_majorite*

burnman.minerals.SLB_2011.**qtz**
alias of *quartz*

burnman.minerals.SLB_2011.**coes**
alias of *coesite*

burnman.minerals.SLB_2011.**st**
alias of *stishovite*

burnman.minerals.SLB_2011.**seif**
alias of *seifertite*

burnman.minerals.SLB_2011.**mppv**
alias of *mg_post_perovskite*

burnman.minerals.SLB_2011.**fppv**
alias of *fe_post_perovskite*

burnman.minerals.SLB_2011.**appv**
alias of *al_post_perovskite*

burnman.minerals.SLB_2011.**pe**
alias of *periclase*

burnman.minerals.SLB_2011.**wu**
alias of *wuestite*

burnman.minerals.SLB_2011.**mgcf**
alias of *mg_ca_ferrite*

burnman.minerals.SLB_2011.**fecf**
alias of *fe_ca_ferrite*

burnman.minerals.SLB_2011.**nacf**
alias of *na_ca_ferrite*

burnman.minerals.SLB_2011.**ky**
alias of *kyanite*

burnman.minerals.SLB_2011.**neph**
alias of *nepheline*

burnman.minerals.SLB_2011.**c2c**
alias of *c2c_pyroxene*

burnman.minerals.SLB_2011.**cf**
alias of *ca_ferrite_structured_phase*

burnman.minerals.SLB_2011.**cpx**
alias of *clinopyroxene*

burnman.minerals.SLB_2011.**gt**
alias of *garnet*

burnman.minerals.SLB_2011.**il**
alias of *akimotoite*

burnman.minerals.SLB_2011.**ilmenite_group**
alias of *akimotoite*

burnman.minerals.SLB_2011.**mw**
alias of *ferropericlase*

burnman.minerals.SLB_2011.**magnesiowuestite**
alias of *ferropericlase*

burnman.minerals.SLB_2011.**ol**
alias of *mg_fe_olivine*

burnman.minerals.SLB_2011.**opx**
alias of *orthopyroxene*

burnman.minerals.SLB_2011.**plag**
alias of *plagioclase*

burnman.minerals.SLB_2011.**ppv**
alias of *post_perovskite*

burnman.minerals.SLB_2011.**pv**
alias of *mg_fe_perovskite*

burnman.minerals.SLB_2011.**mg_fe_bridgmanite**
alias of *mg_fe_perovskite*

burnman.minerals.SLB_2011.**mg_fe_silicate_perovskite**
alias of *mg_fe_perovskite*

burnman.minerals.SLB_2011.**ri**
alias of *mg_fe_ringwoodite*

burnman.minerals.SLB_2011.**spinel_group**
alias of *mg_fe_aluminous_spinel*

burnman.minerals.SLB_2011.**wa**
alias of *mg_fe_wadsleyite*

burnman.minerals.SLB_2011.**spinelloid_III**
alias of *mg_fe_wadsleyite*

12.2 Matas_etal_2007

Minerals from Matas et al. 2007 and references therein. See Table 1 and 2.

class burnman.minerals.Matas_etal_2007.**mg_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Matas_etal_2007.**fe_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Matas_etal_2007.**al_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Matas_etal_2007.**ca_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Matas_etal_2007.**periclase**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Matas_etal_2007.**wuestite**
Bases: *burnman.mineral.Mineral*

burnman.minerals.Matas_etal_2007.**ca_bridgmanite**
alias of *ca_perovskite*

burnman.minerals.Matas_etal_2007.**mg_bridgmanite**
alias of *mg_perovskite*

burnman.minerals.Matas_etal_2007.**fe_bridgmanite**
alias of *fe_perovskite*

burnman.minerals.Matas_etal_2007.**al_bridgmanite**
alias of *al_perovskite*

12.3 Murakami_etal_2012

Minerals from Murakami et al. (2012) supplementary table 5 and references therein, V_0 from Stixrude & Lithgow-Bertolloni 2005. Some information from personal communication with Murakami.

class burnman.minerals.Murakami_etal_2012.**mg_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Murakami_etal_2012.**mg_perovskite_3rdorder**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Murakami_etal_2012.**fe_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Murakami_etal_2012.**mg_periclase**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Murakami_etal_2012.**fe_periclase**
Bases: *burnman.mineral_helpers.HelperSpinTransition*

class burnman.minerals.Murakami_etal_2012.**fe_periclase_3rd**
Bases: *burnman.mineral_helpers.HelperSpinTransition*

class burnman.minerals.Murakami_etal_2012.**fe_periclase_HS**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Murakami_etal_2012.**fe_periclase_LS**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Murakami_etal_2012.**fe_periclase_HS_3rd**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.Murakami_etal_2012.**fe_periclase_LS_3rd**
Bases: *burnman.mineral.Mineral*

burnman.minerals.Murakami_etal_2012.**mg_bridgmanite**
alias of *mg_perovskite*

burnman.minerals.Murakami_etal_2012.**fe_bridgmanite**
alias of *fe_perovskite*

burnman.minerals.Murakami_etal_2012.**mg_bridgmanite_3rdorder**
alias of *mg_perovskite_3rdorder*

12.4 SLB_2005

Minerals from Stixrude & Lithgow-Bertelloni 2005 and references therein

class burnman.minerals.SLB_2005.**stishovite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2005.**periclase**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2005.**wuestite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2005.**mg_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2005.**fe_perovskite**
Bases: *burnman.mineral.Mineral*

burnman.minerals.SLB_2005.**mg_bridgmanite**
alias of *mg_perovskite*

burnman.minerals.SLB_2005.**fe_bridgmanite**
alias of *fe_perovskite*

12.5 SLB_2011_ZSB_2013

Minerals from Stixrude & Lithgow-Bertelloni 2011, Zhang, Stixrude & Brodholt 2013, and references therein.

class burnman.minerals.SLB_2011_ZSB_2013.**stishovite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011_ZSB_2013.**periclase**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011_ZSB_2013.**wuestite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011_ZSB_2013.**mg_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.SLB_2011_ZSB_2013.**fe_perovskite**
Bases: *burnman.mineral.Mineral*

burnman.minerals.SLB_2011_ZSB_2013.**mg_bridgmanite**
alias of *mg_perovskite*

burnman.minerals.SLB_2011_ZSB_2013.**fe_bridgmanite**
alias of *fe_perovskite*

12.6 Other minerals

class burnman.minerals.other.**ZSB_2013_mg_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.other.**ZSB_2013_fe_perovskite**
Bases: *burnman.mineral.Mineral*

class burnman.minerals.other.**Speziale_fe_periclase**
Bases: *burnman.mineral_helpers.HelperSpinTransition*

class burnman.minerals.other.**Speziale_fe_periclase_HS**
Bases: *burnman.mineral.Mineral*

Speziale et al. 2007, Mg#=83

class burnman.minerals.other.**Speziale_fe_periclase_LS**
Bases: *burnman.mineral.Mineral*

Speziale et al. 2007, Mg#=83

class burnman.minerals.other.**Liquid_Fe_Anderson**
Bases: *burnman.mineral.Mineral*

Anderson & Ahrens, 1994 JGR

class burnman.minerals.other.**Fe_Dewaele**
Bases: *burnman.mineral.Mineral*

Dewaele et al., 2006, Physical Review Letters

CHAPTER

THIRTEEN

REFERENCES

References

The functions in the Main module operate on Materials which can be combination of different minerals from Mineral database.

CHAPTER

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INDICES AND TABLES

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