Mantle Phase Changes Detected from Stochastic Tomography

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Abstract

Stochastic tomography, made possible by dense deployments of seismic sensors, is used to identify previously undetected and poorly detected changes in the composition and mineral structure of Earth's mantle. This technique inverts the spatial coherence of amplitudes and travel times of body waves to determine the depth and lateral dependence of the spatial spectrum of seismic velocity. The inverted spectrum is interpreted using predictions from the thermodynamic stability of different compositions and mineral phases as a function of temperature and pressure, in which the metamorphic temperature derivative of seismic velocities can be used as a proxy for the effects of heterogeneity induced in a region undergoing a phase change. Peaks in the metamorphic derivative of seismic velocity are found to closely match those found from applying stochastic tomography to elements of Earthscope and FLEX arrays. Within ± 12 km, peaks in the fluctuation of P velocity at 425, 500, and 600 km depth beneath the western US agree those predicted by a mechanical mixture of harzburgite and basalt in a cooler mantle transition zone. A smaller peak at 250 km depth may be associated with chemical heterogeneity induced by dehydration of subducted oceanic sediments, and a peak at 775 km depth with a phase change in subducted basalt. Non-detection of a predicted endothermic phase change near 660 km is consistent with its width being much less than 10 km. These interpretations of the heterogeneity spectrum are consistent with the known history of plate subduction beneath North America.

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Key Points:

- Stochastic tomography can capture higher order phase and chemical changes undetectable from reflection imaging.
- The heterogeneity spectrum of the upper mantle is marked by peaks associated with depth regions undergoing phase or compositional change.
- The upper mantle beneath the western US is consistent with a history of subduction and slab stagnation in the transition zone.

Abstract

Stochastic tomography, made possible by dense deployments of seismic sensors, is used to identify previously undetected and poorly detected changes in the composition and mineral structure of Earth's mantle. This technique inverts the spatial coherence of amplitudes and travel times of body waves to determine the depth and lateral dependence of the spatial spectrum of seismic velocity. The inverted spectrum is interpreted using predictions from the thermodynamic stability of different compositions and mineral phases as a function of temperature and pressure, in which the metamorphic temperature derivative of seismic velocities can be used as a proxy for the effects of heterogeneity induced in a region undergoing a phase change. Peaks in the temperature derivative of seismic velocity are found to closely match those found from applying stochastic tomography to elements of Earthscope and FLEX arrays. Within $\pm$ 12 km, peaks in the fluctuation of P velocity at 425, 500, and 600 km depth beneath the western US agree those predicted by a mechanical mixture of harzburgite and basalt in a cooler mantle transition zone. A smaller peak at 250 km depth may be associated with chemical heterogeneity induced by dehydration of subducted oceanic sediments, and a peak at 775 km depth with a phase change in subducted basalt. Non-detection of a predicted endothermic phase change near 660 km is consistent with its width being much less than 10 km. These interpretations of the heterogeneity spectrum are consistent with the known history of plate subduction beneath North America.

Plain Language Summary

Fluctuations in amplitude and traveltimes of seismic P waves from deep earthquakes observed at the US Array of seismic stations are inverted for a depth dependent spectrum of the intensity of P wave velocity fluctuations. Peaks with depth of this spectrum correlate with the depths predicted for changes in the arrangements of atoms of the silicate minerals comprising the upper 1000 km of Earth's mantle. The structure of the peaks agrees with the known history of tectonic plate subduction beneath the western US.

1 Introduction

The best-known solid phase changes in Earth's silicate mantle are commonly detected from the reflection and conversion of body waves interacting with rapid, near discontinuous, changes in velocity and density occurring at or near 410 and 660 km depth (e.g., *Shearer*, 1991; *Niu et al.*, 2005). These phase changes also produce multi-pathed body waveforms between 15^0 -35^0 great circle range (e.g., Burdick and Helmberger, 1978; *Chu et al.*, 2012). The steepness of the inferred P and S velocity gradients between 410 and 660 km in reference Earth models, however, cannot be explained by plausible silicate mantle chemistry without the existence of at least one more phase change between 410 and 660 km. When the tools of mineral physics are applied to a constrained composition of the Earth's mantle, up to two additional phase changes are predicted to occur between the 410 to 660 km. Several other phase changes are also predicted above and below this zone, each having a unique behavior in their Clapeyron slope and the widths in depth over which each occurs (Fig. 1a). The widths of more than half of these are on the order of 15 to 60 km, making it difficult to detect them from reflected and converted body waves having similar or shorter wavelengths. A serendipitous seismological discovery from the inversion of P wave coherences across the USArray (Cormier et al., 2020) reveals that many these phase changes are marked by peaks in the depth-dependency of the mantle heterogeneity spectrum that correlate with peaks in the temperature derivatives of seismic velocities predicted by thermodynamic models of mantle composition and phase. Stixrude and Lithgow-Bertelloni

(2005 2007) have demonstrated that small lateral variations in temperature (<150^o K) allow the peaks in the predicted temperature derivatives to capture the depth zone in which two competing mineral phases my coexist that are capable of scattering seismic body waves (Fig.2). These peaks in the metamorphic component of the temperature derivatives can be used to identify and interpret peaks in narrow depth ranges of the mantle heterogeneity spectrum. This heterospectrum can be inverted from fluctuations in travel time and amplitudes of seismic waves observed across dense networks of seismic stations by a process known as stochastic tomography. In this paper, our objective is to interpret the seismological results from stochastic tomography applied to seismic arrays located in the western US (Cormier et al., 2020) using the predictions of the thermodynamic code Hefesto (Stixrude and Lithgow-Bertelloni, 2005, 2207) for the temperature derivatives of the P wave velocity. We assume mantle models of both equilibrium pyrolite and mechanical mixtures of harzburgite and basalt, and examine the effects of temperature and subduction. Before we begin interpretations in section 4, we review the principles and assumptions of stochastic tomography in section 2. In section 3 we discuss the filtering and depth averaging of the metamorphic temperature derivatives predicted by Hefesto required to match the sensitivity achievable with stochastic tomography. Readers primarily interested our interpretation of the detected phase changes may best begin by reading sections 4 and 5, which focus on the interpretation of our results, referring as needed, to the methods of inversion and analysis in sections 2 and 3.

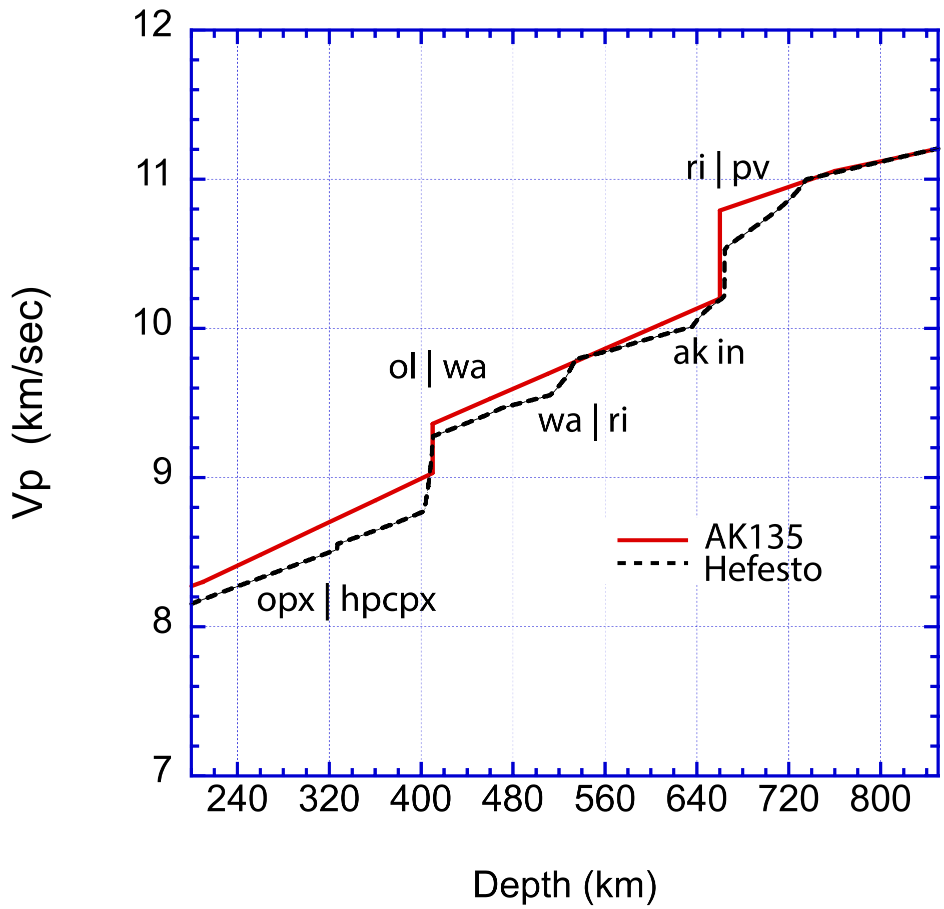

Figure 1. Dashed black line: P velocity of the upper mantle predicted by the thermodynamic modeling code Hefesto for a pyrolite composition along a 1600° K isentrope. Red solid line: P velocity of the AK135 model (Montagner and Kennett, 1995). Sharp, near vertical changes in slope occur for phase changes at 410 km and 660 km. Milder changes in slope predicted by Hefesto denote phase changes that occur over broader regions of depth. (Note: The generally slower Hefesto P velocities shown here, compared to a reference Earth model, are due to an average Earth geotherm cooler than the assumed 1600° K isentrope in the conductive zone near Earth's surface and cool perturbations due to slab stagnations in the transition zone (section 4).)

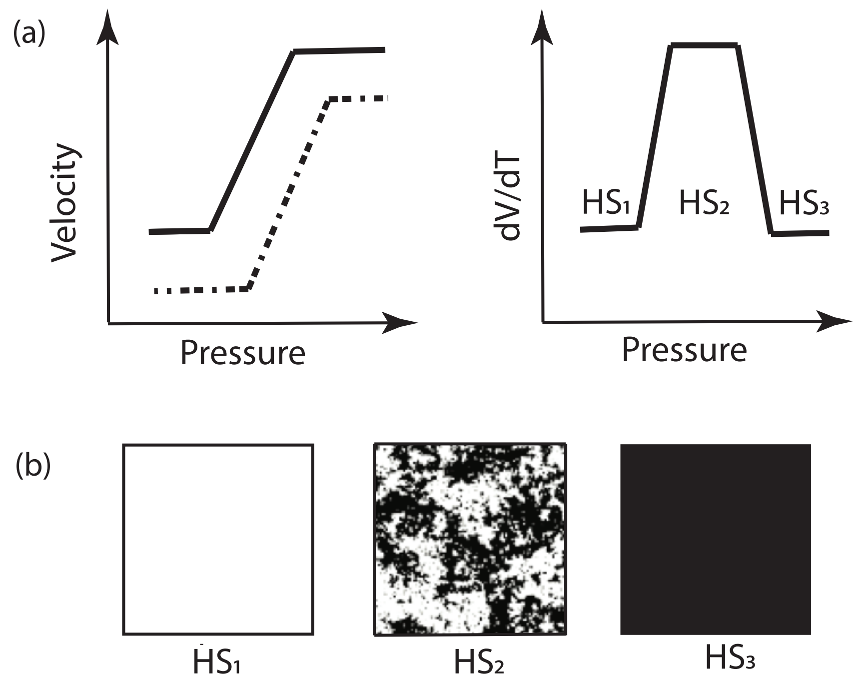

Figure 2. (a) Illustration of how a change in velocity over a zone of exothermic phase change affects its temperature derivative assuming a positive Clapeyron slope. Upper left: the solid line is the velocity change at lower temperature and the dotted line is the velocity change at higher temperature. Upper right: computed difference derivative of velocity with respect to temperature. (b) Realizations of the how the heterospectrm may change with depth across a phase change. The example shown here is inspired by Ising models of electron spin statistics for a ferromagnetic transition (Blundell and Blundell, 2014).

2 Stochastic Tomography

2.1 Theory and data

Small-scale heterogeneities, unresolvable by conventional tomography, have detectible signatures in the fluctuation of amplitudes and travel times observed across seismic arrays. Numerical simulations have shown that small-scale heterogeneity in the upper mantle can affect the wavefront of an incident teleseismic wave beneath an array. Small differences in the angle of approach of wavefronts, on the order of a several degrees or less, can produce unique signatures in amplitude and phase fluctuations due to differences in the sensitivity of the wavefronts to the small-scale structure (e.g., Zheng & Wu 2008; Tkalčić et al., 2010). Measurement of these fluctuations between array elements can be exploited to invert for the spectrum of heterogeneity beneath the array with techniques that have been named stochastic tomography (Wu & Flatté, 1990; Wu & Xie, 1991, Zheng & Wu, 2008).

Transmission fluctuation coherence measurements (eqs. 1a-d) are the starting point for stochastic tomography. We consider the recorded fields due to two plane waves, PW1 and PW2. We use $U_1(x_1)$ for the recorded field at x_1 for PW1. Likewise, we use $U_2(x_2)$ for the recorded field at x_2 for PW2. Both fields propagate through the same heterogeneous medium. We also consider their corresponding reference fields (no heterogeneities), $U_{1ref}(x_1)$ and $U_{2ref}(x_2)$, respectively. We can write the seismic fields in amplitude and phase terms, for example, $U_1 = u_1 \exp[i\omega t] = u_1 \exp[i\phi]$ and $U_{1ref} = u_{1ref} \exp\left[i\omega t_{ref}\right] = u_{1ref} \exp\, [i\phi_{ref}]$. Similar representations are applied to PW2. A Rytov approximation provides the relationship between the scattered field and the reference field: $U_1 = U_{1ref} e^{\Psi_1}$. The complex function ψ has a real part, which is the logarithmic amplitude, and an imaginary part, which is the phase (or traveltime) difference with respect to the reference value. In our work, the observables are the ratios of log amplitude and travel time differences (eqs. 1c-d) from those computed in a reference Earth model. Transverse coherence functions are constructed as a function of the lag distance x between pairs of receivers. The brace brackets in eqs. 1a-b, define the logarithmic amplitude $\left\langle u_1 u_2 \right\rangle$ and $\left\langle \phi_1 \phi_2 \right\rangle$ phase coherences by averaging measurements for a specific lag distance over all combinations of two receivers in an array separated by that lag distance. Non-dimensional coherence values range from zero (amplitude and traveltime fluctuations) at neighboring receivers to 1 for perfect correlation of amplitudes and to 2π for perfect correlation of phase.

$$
\begin{aligned}
&(1a) \quad \langle u_1 u_2 \rangle = \frac{1}{2}\mathrm{Re}\langle \psi_1 \psi_2^* \rangle + \frac{1}{2}\mathrm{Re}\langle \psi_1 \psi_2 \rangle \\
&(1b) \quad \langle \phi_1 \phi_2 \rangle = \frac{1}{2}\mathrm{Re}\langle \psi_1 \psi_2^* \rangle - \frac{1}{2}\mathrm{Re}\langle \psi_1 \psi_2 \rangle, \qquad \textit{where} \\
&(1c) \quad \psi(\omega) = \ln(u / u_{ref}) + i\omega(t - t_{ref}) \\
&(1d) \quad u = \frac{\psi + \psi^*}{2} \quad \textit{and} \quad \phi = \frac{\psi - \psi^*}{2i}
\end{aligned}
$$

To construct the complex functions $\psi(\omega)$, we measure u and u_{ref} from observed and synthetic seismograms around the direct P waves from the outputs of a multi-taper filter at 0.7 Hz, and measure the traveltime difference $t - t_{ref}$ from cross-correlation of observed and predicted reference waveforms.

Stochastic tomography assumes that the functional behaviors of the coherences with lag distance are due to the interference of plane waves scattered by random heterogeneities having an unknown power spectrum as a function of wavenumber and depth. The transverse coherences can be written as an integral over horizontal wavenumber and depth, with an integrand containing the power spectrum (eqs. 2a-c).

$$
\begin{aligned}
&(2a) \quad \langle u_1 u_2 \rangle = (2\pi)^{-1} \int_0^H d\xi a_1(\xi) a_2(\xi) \int_0^\infty J_0\left[(\kappa R(\xi)\right] \sin\left[\omega\theta_1(\xi)\right] \sin\left[\omega\theta_2(\xi)\right] P(\xi,\kappa)\kappa d\kappa \\
&(2b) \quad \langle \phi_1 \phi_2 \rangle = (2\pi)^{-1} \int_0^H d\xi a_1(\xi) a_2(\xi) \int_0^\infty J_0\left[(\kappa R(\xi)\right] \cos\left[\omega\theta_1(\xi)\right] \cos\left[\omega\theta_2(\xi)\right] P(\xi,\kappa)\kappa d\kappa \\
&(2c) \quad \langle u_1 \phi_2 \rangle = (2\pi)^{-1} \int_0^H d\xi a_1(\xi) a_2(\xi) \int_0^\infty J_0\left[(\kappa R(\xi)\right] \sin\left[\omega\theta_1(\xi)\right] \cos\left[\omega\theta_2(\xi)\right] P(\xi,\kappa)\kappa d\kappa
\end{aligned}
$$

In eqs. 2a-c, P is the power spectrum as a function of depth ξ and horizontal wavenumber κ. H is the thickness of a heterogeneous layer. Functions a_1, a_2, θ_1, and θ_2 are defined in Cormier et al. (2020). The function R appearing in the argument of the Bessel function J_0 is the horizontal distance between the pair of rays arriving at a specific lag distance at depth ξ. The average sum of a coherence measurement at each lag from many sources at different distances and azimuths can, in principle, be sensitive to the effects of scatterers whose size may be on the order of or less than the spacing of array elements.

These integrals can be discretized and set-up as a linearized inverse problem in which the squared difference of the observed coherences and predicted coherences of an unknown power spectrum are minimized. The discretized forms of eqs.2a-c and the object function to be minimized are given in Appendix B of Cormier et al. (2020).

The coherence data we chose to invert were 3 groups of deep focus earthquakes (Marianas, Tonga-Kermedec, and South America) observed by elements of the US array, transportable array, and FLEX arrays deployed in the western US (Fig. 3). Deep focus events were chosen to avoid the effects of heterogeneity concentrated in the upper mantle near the source and to eliminate the effects of near source reflections. P waveforms of 21,205 deep focus earthquakes having moment magnitudes Mw 5.8-6.2 were downloaded from the Data Management Center of IRIS. About 40% of these had sufficiently high signal to noise ratios and simple apparent source-time functions to include in the coherence measurements. Within each earthquake group, measured coherences are averaged at all receiver pairs corresponding to a specific lag. Wavefront healing due to propagation from the source to the teleseismic receivers and averaging coherences at each lag over all earthquakes aid in eliminating any source-side heterogeneity effects. A joint inversion of data comprising 3 wavefronts arriving from widely different azimuths, whose rays cross at variable depths beneath the array, makes it possible to achieve a sensitivity to heterogeneity scales on the order of the smallest spacing (10 km) of array elements.

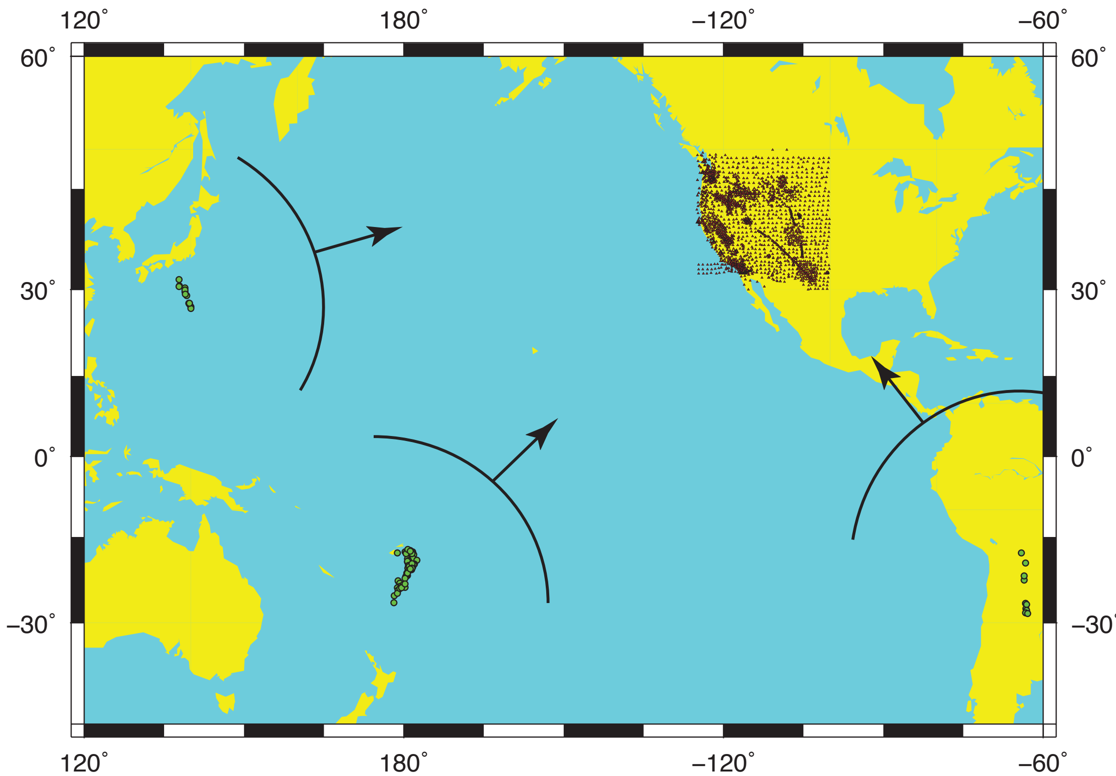

Figure 3. Hypocenters (green dots) of three deep-focus earthquake groups and US and FLEX Array seismic stations (black triangles) used in the inversion of P wave coherence for the upper mantle heterogeneity spectrum.

The inclusion of the effects of the specific earthquake source-time functions and radiation patterns in u_{ref} are essential to isolating the effects of forward scattering from those of the source. To achieve this for each event the reference synthetic seismogram u_{ref} at each array element was computed from the IRIS Syngine service (Nissen-Meyer, et al., 2014; https://service.iris.edu/irisws/syngine) in the AK135-F Earth model (Montagner & Kennett, 1995) using the known moment tensor solution for each event from the GCMT service (Ekstrom et al., 2012; https://www.globalcmt.org) and an empirical source time function determined by stacking P waves from each event in the 40^{o} to 90^{o} distance range. In conjunction with this paper we also provide a link to Python and Matlab scripts to assist researchers in designing experiments with stochastic tomography (Tian and Cormier, 2020). These example scripts treat the effects of earthquake moment tensors and source-time functions on the reference wavefields defining coherence measurements.

2.2 Single layer inversion

As a first step it is useful to factor out the wavenumber dependence from a depth dependent spectrum and compare its spectrum against published, non-depth dependent, stochastic models of upper mantle heterogeneity. For understanding how lateral temperature differences drive mantle heterogeneity such a comparison can also provide some constraints on the compositional and temperature variations in the upper mantle. The coherence of broadband (0.02 to 2 Hz) body waves can provide information at scale lengths intermediate between those estimated from global travel-time tomography and the coda of higher-frequency body waves.

We thus first inverted for a uniform heterogeneity spectrum with depth in which the shape of the power spectrum was defined by 4 parameters described in Cormier et al. (2020). To recognize that the sensitivity of our coherence data peaked around a narrow band in wavenumber, we employed a parameterization of the heterogeneity spectrum that consisted of a product of a low pass and high pass filter in wavenumber (Klimes, 2002). Fig. 4a compares our inverted spectrum for the upper 1000 km of the mantle to an overlapping band estimated by Mancinelli et al. (2016) from scattered, low-frequency (<0.2 Hz), coda of teleseismic body waves. The two spectra nearly coincide in a narrow wavenumber band centered near 0.065 km^{-1}. The dominant frequency (0.7 Hz) of our P wave data in this wavenumber corresponds to a 100 km wavelength in the upper mantle. At this center frequency, scattering will primarily be the Mie type in the forward direction, with sensitivity strongest to heterogeneities having a scale between 10 to 100 km. A minimum detection threshold of 10 km scale agrees with the highest resolution achievable by stochastic tomography with our smallest sensor spacings. It also agrees with our detections and non-detections of phase changes predicted from thermodynamic modeling (section 3).

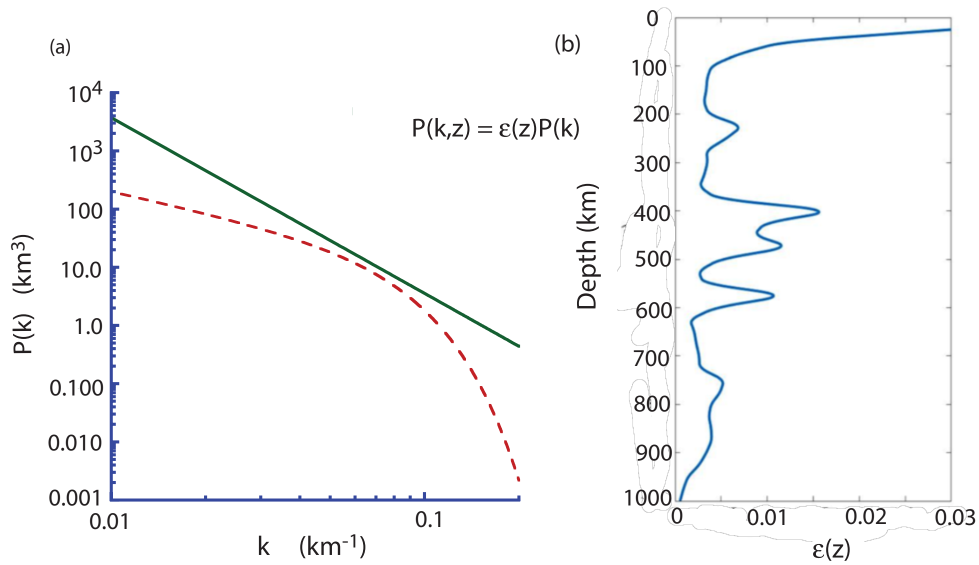

Figure 4. (a) Left: uniform power spectrum density of P velocity fluctuation for the upper 1000 km of Earth's mantle determined from stochastic tomography (dashed red line) compared to an overlapping portion of Mancinelli et al's (2016) estimates for this depth range in the frequency band of teleseismic body waves, (solid green line), in which Mancinelli et al.'s 1-D spectrum has been converted to a 3-D isotropic spectrum for a von Kármán medium using formulas in Sato et al. (2012). (b) Left: smoothed depth-dependent model of this spectrum determined from stochastic tomography applied to the mantle beneath the western US (Cormier et al., 2020).

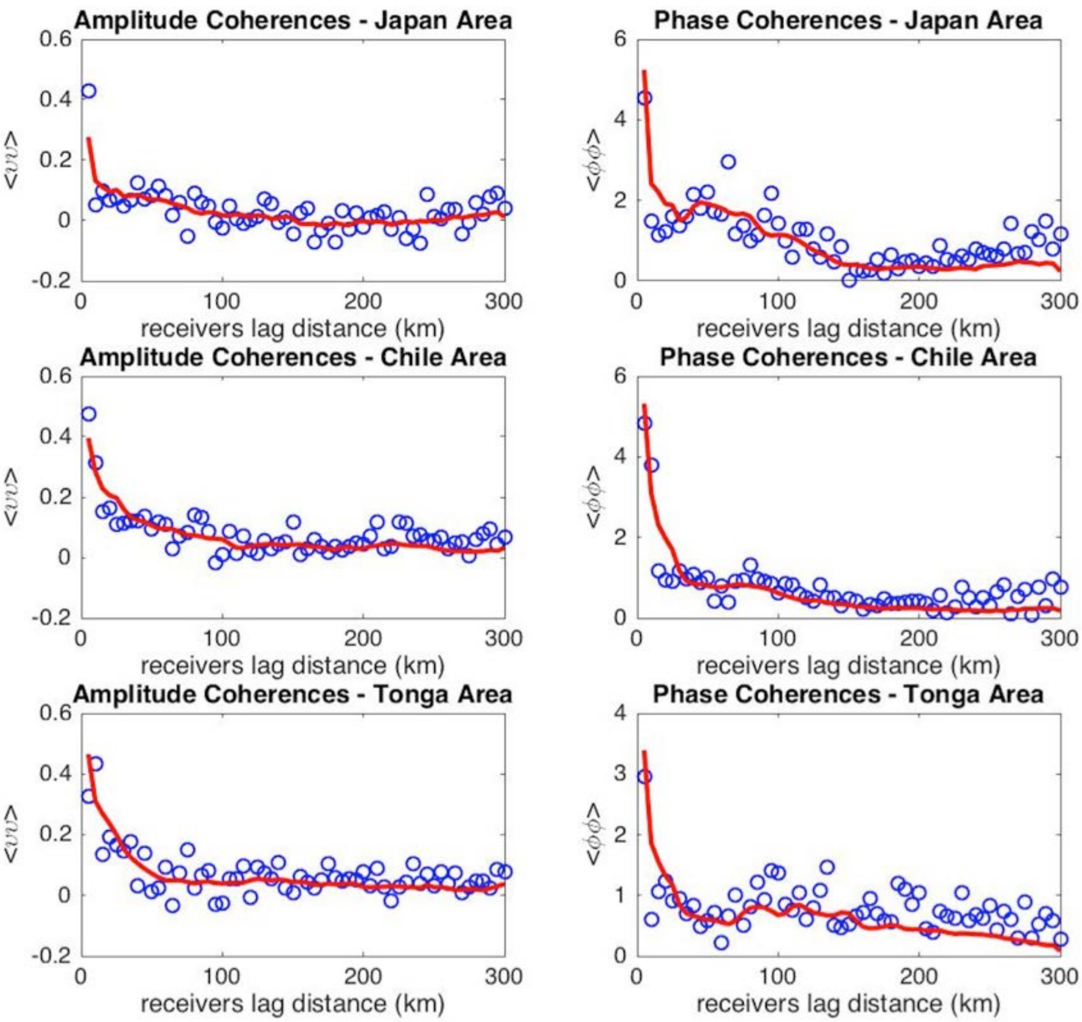

Figure 5. Observed coherences at all possible pairs of stations at specific lag distances (open circles) and predicted P wave coherence (solid lines) for a depth dependent model of mantle heterogeneity power (Fig. 4b) for the 3 epicentral regions shown in Fig. 3.

2.3 Depth dependent inversion

We next assumed that the spectral shape determined from the single layer inversion (Fig. 4a) was constant in depth but allowed its peak power to vary with depth in 40, 25 km thick, layers. Fig. 4b plots the inverted depth dependence of P velocity fluctuation. Fig. 5 compares the predicted coherences for the depth dependent model with the observed coherences for the 3 epicentral regions. Compared to the uniform model, the squared coefficient of determination of coherences for the depth dependent model increased from 0.74 to 0.80. The reduced χ^2

computed from observed and predicted coherences decreased from 1.65 to 1.05. The significantly smaller, but not less than 1, χ^2 for the depth dependent spectrum is consistent with an improved fit, but not an over-fit due to the assumption of a larger number of unknown parameters. Interpretations of the depth dependent of model heterogeneity power are given in section 4.

The 25 km thick depth intervals, which are close to the smallest sensor spacings (10 to 20 km) of the denser FLEX arrays shown in Fig. 3, agree with the resolvable spatial scale determined in sensitivity tests conducted by Wu and Xie (1991). In that study, Wu and Xie applied a stochastic tomographic inversion to numerically synthesized seismograms in media having known depth-dependent heterogeneity spectra in the presence of noise. For coherence inversions that combined wavefronts arriving from different angles (e.g., Fig. 6), they found it possible to achieve a depth resolution equal to the spacing of sensor elements.

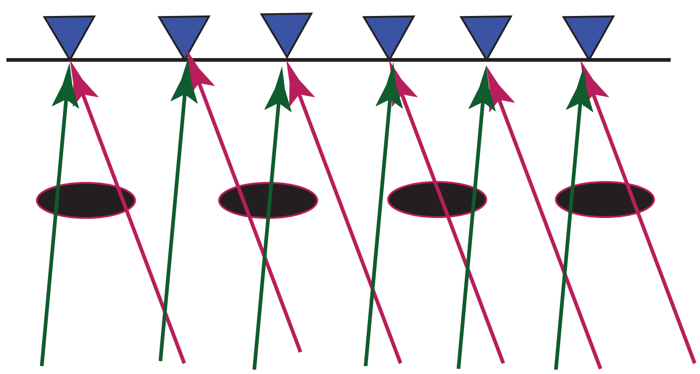

Figure 6. Illustration of how incorporation of wavefronts arriving from different directions (red and green arrows) can enhance the resolution of small-scale heterogeneity (black ellipses).

3. Hefesto: a thermodynamic model of mantle composition and phase

3.1 Temperature derivatives of seismic velocity

Hefesto is a Fortran code for computing seismic velocities, densities, and other physical properties for silicate minerals that minimize the Gibbs free energy at specific temperatures and pressures (Stixrude and Lithgow-Bertelloni, 2005, 2007, 2022). Its input consists of pressure, temperature, and a bulk composition in the SiO_2-MgO-FeO-Al_2O_3-CaO-Na_2O system, and models of the properties of 51 end-members of 22 phases and their interactions. Among its output options are elastic velocities and density, as a function of depth. Isomorphic (constant phase) temperature derivatives of elastic velocity are calculated analytically but the additional contribution of a metamorphic component in the midst of a solid phase change can be calculated from difference derivatives determined by running the code at two closely spaced temperatures (e.g., Fig. 1a and Stixrude and Lithgow-Bertelloni, 2007). In the results shown in this paper, we calculated difference derivatives of, dlnVp/dT to double precision on a 64 bit processor, assuming either adiabatic or isothermal conditions, assuming two temperatures separated by 10^o K.

3.2 The metamorphic temperature derivative as a proxy for heterogeneity

Because the slope of the boundary between two stable silicate phases in P-T space is neither zero or infinite, any lateral change in temperature will also be associated with a change in the pressure (depth) of the phase boundary. This makes it possible for the temperature derivative of a to be used as a proxy for locating and measuring the width of a zone in which the two phases are competing for equilibrium (e.g, Fig. 2). Stixrude and Lithgow-Bertelloni (2007) have termed the temperature derivative of velocity in this situation the metamorphic derivative in recognition that its shape is affected by more than one form or phase of a mineral. The existence of two phases in the zone of the phase transition, with differing seismic velocities and density can scatter body waves. Hence, peaks in the predicted metamorphic component of the temperature derivative of a seismic velocity will be associated with peaks in the heterogeneity spectrum as a function of depth.

Implemented as a proxy for seismic velocity fluctuations, the values of dlnVp/dT require a conversion factor related to the mean lateral temperature variation to convert dlnVp/dT predictions to estimates of the mean fluctuations of P velocity, dVp/Vp. Stixrude and Lithgow-Bertelloini (2012) find that an upper bound of 150^o K for lateral temperature variations yield lateral velocity variations in agreement with seismic tomography in the upper mantle. Solomon (1976) also argues for 150^o K lateral temperature variations from geodynamic considerations. We apply a slightly more conservative estimate of 100^o K from comparing the scale of P velocity variations (order of 1 %) inferred from P travel time tomography to thermodynamic estimates of the isomorphic temperature derivative (the temperature derivative not in a region of a phase change). An alternative estimate of this conversion factor, not related to any assumption of lateral temperature differences, is to estimate the maximum velocity fluctuation in a phase transition zone between two competing phases. This is simply the difference in velocities between two depth sides of a phase change divided by the average of the two velocities. For the 410 km phase change, this value is 3% from the Hefesto estimated velocity changes for both pyrolite and harzburgite/basalt mixtures. This leads to the identical conversion factor of 150^{o} K at 410 km. Given the existence of uncertainties in the lateral temperature differences and the precise shape of the heterogeneity spectrum and its variation across the zone of a phase change, we estimate that the true magnitude of P velocity fluctuations within most of the phase changes occurring over zones wider than a wavelength is likely to lie between 1 to 3%.

3.3 Filtering for sensitivity compatible with stochastic tomography

A phase change that occurs over a depth range less than 6 km wide is unlikely to be detected as narrow zone of increased heterogeneity that can be resolved by stochastic tomography applied to sensor spacings between 10-20 km and coherence averaged over lag intervals 25 km and greater. The 660 km phase change from ringwoodite to ferropericlase and magnesiowustie is estimated to be 1-2 km wide in agreement with both other computational and experimental estimates in mineral physics. Another phase change near 300 km depth from ortho-pyroxine to high pressure clinopyroxene (opx to hcpx) is also quite narrow, Hefesto predicting it to occur over 8 km. Such phase changes occurring over depth zones less than 10 km width are easily detected from reflected and converted body waves. This is especially the case for 660 km phase change, which has been observed in reflections at 1-2 Hz. The non-detection of the 660 km and 300 km phase changes in our stochastic tomography inversions, sensitive to phase changes wider than 6 km, is consistent with their narrowness. To compare Hefesto predictions with our stochastic tomography inversions, we have hence applied a median filter to remove phase transitions less than a body wavelength wide, and an averaging window nearly equal to observed coherence lag intervals, to each point shown in comparison plots. This median filter, often used to remove electronic spikes in seismic recordings (Evans, 1982), was designed to remove all signals in the metatmorphic derivatives that are less than 6 km wide. Fig. 7 shows an example in which the median filter and averaging window has been applied to the Hefesto predicted temperature derivatives of P velocity.

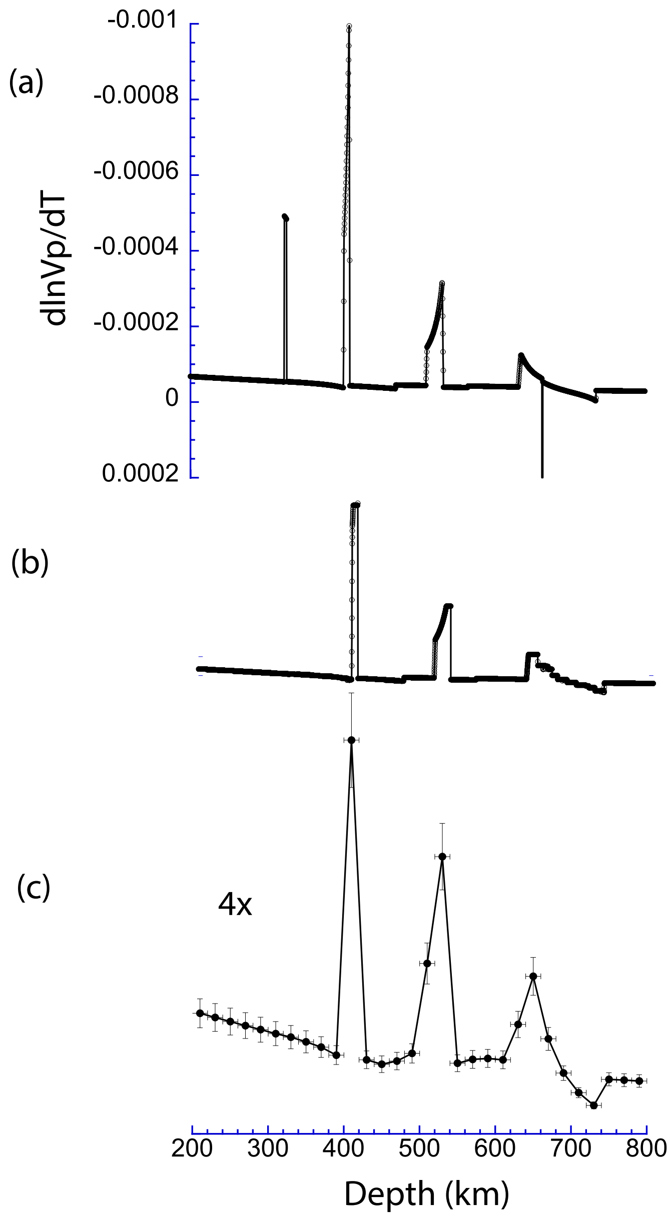

Figure 7. (a) Hefesto dlnVp/dT computed for a pyrolite model of the upper mantle; (b) followed by median filtering applied to (a) to remove signals less than 6 km wide; and (c) followed by 20 km wide depth averaging applied to (b).

4 Results

4.1 Interpretation of the depth dependent heterogeneity spectrum

Results of our inversion for a depth dependent heterogeneity spectrum for the upper 1000 km of the mantle beneath the western US for the root-mean-square (rms) P velocity fluctuations are shown in Fig. 8. These are compared with the Hefesto predictions for P velocity fluctuations derived from the temperature derivatives of P velocity. The Hefesto predictions, for both an equilibrium pyrolite composition (EA) and a mechanical mixture of harzburgite and basalt (MM), are filtered and averaged to agree with the estimated sensitivities of stochastic tomography (section 3). For the P velocity fluctuation predicted from stochastic tomography, the horizontal uncertainty bars in depth in Fig. 8 are fixed at 25 km in length to represent the spacing between averaged coherence lags, while maintaining a reduced chi-square greater than 1 calculated from predicted and observed coherences. For the P velocity fluctuations estimated from Hefesto, the horizontal uncertainty bars are the width of a 20 km moving depth average of the filtered temperature derivative of velocity. From numerical experiments recording the change in the peak value of the predicted velocity fluctuation as the starting depth of the moving average changes, the ordinate uncertainty bars are taken to be ±10% of the median peak value.

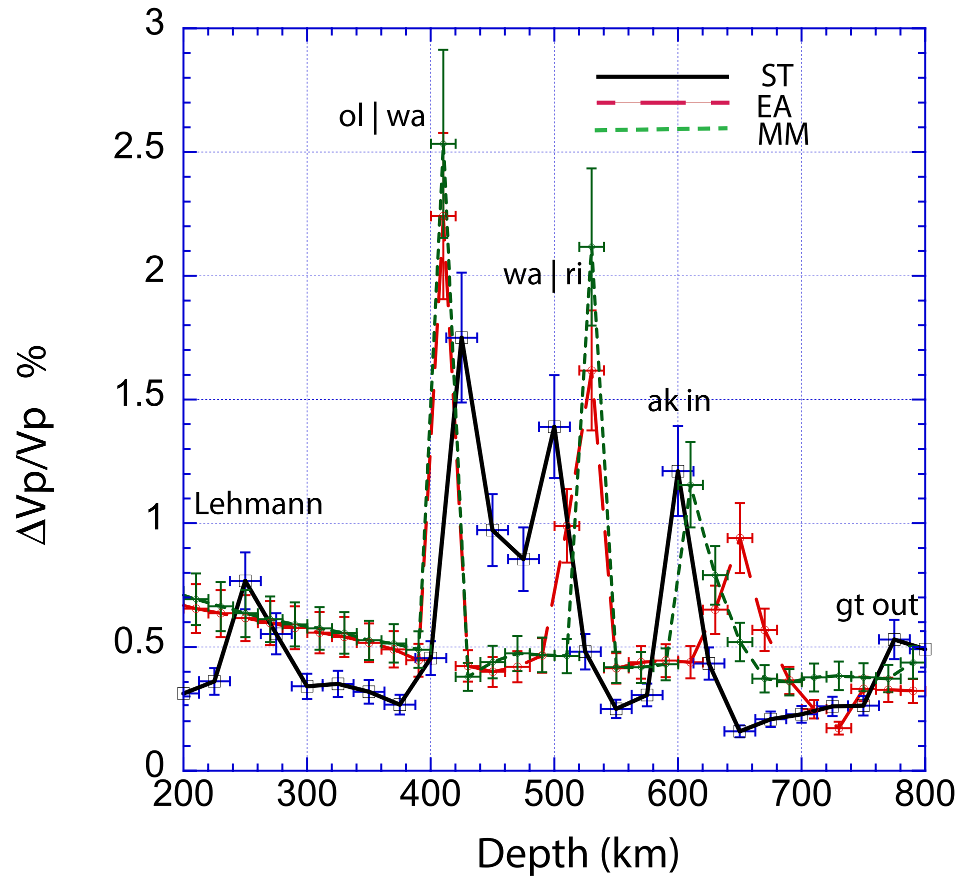

Figure 8. Solid black line (ST): the depth dependent heterogeneity spectrum for the rms fluctuation of P wave velocity in the upper 1000 km of the mantle estimated from stochastic tomography. Long dashed red line (EA): filtered temperature derivative of P velocity predicted for an equilibrium pyrolite model. Short dashed green line (MM): filtered temperature derivative of P velocity predicted for a mechanical mixture of 80% harzburgite and 20% basalt. Each thermodynamic prediction assumes an adiabatic temperature profile having a 1600° K. potential temperature. Interpreted detections of the Lehmann discontinuity and upper mantle mineral phase changes are labeled above or near peaks.

The Hefesto predicted peaks in the temperature derivative of seismic velocities are from metamorphic contributions due to changes in constituent mineral phases required to minimize Gibbs free energy. Runs are shown for an equilibrium pyrolite model and a mechanical mixture of harzburgite and basalt to simulate the effects of slab cycling. The expression of phase changes can either be sharp or spread out over a depth range bounded by two changes in the gradient of seismic velocity. If sharp (less than 10 km in width), the phase change can be easily detectable from reflected, converted, or multi-pathed body waves. In these cases the effect of lateral temperature variations will be expressed as topography on an apparent seismic reflector rather than a zone of increased heterogeneity. The predicted phase change at 660 km of ringwoodite to Mg-perovskite and magnesiowusite is one such example. Phase changes wider than 10 km in depth may not be detectable in seismic reflections or receiver functions, but will be detectable from stochastic tomography as a zone of discrete scatterers in a narrow range of depth close to the width of a peak in the filtered Hefesto prediction for the temperature derivative of P velocity. For these phase changes, the horizontal length scale of the scatterers will be related to the lateral scale of temperature variations and the vertical scale to the width of the depth (pressure) range over which the phase change occurs.

4.2 Largest peaks in the depth dependent heterogeneity spectrum

The depths and relative amplitudes of at least three of the peaks in the heterogeneity spectrum measured by stochastic tomography agree well enough with those predicted by Hefesto to have confidence in an identification of the detected phase change. These are:

(1) a peak at 425 ±12 km depth nearly matches a Hefesto predicted phase change of olivine to wadsleyite (ol | wa) at 412 km occurring over a 10 km width;
(2) a peak at 500 ±12 km depth matches a Hefesto predicted phase change of wadsleyite to ringwoodite (wa | ri) at 500 km occurring over 20 km width;
(3) in mechanical mixtures of harzburgite and basalt (MM), a peak at 600 ±12 km matches the interference of two predicted phase changes, each exothermic with positive temperature derivatives of velocity. Together they occur over a 30 km width. In equilibrium pyrolite, these phase changes are predicted to be deeper at 640 km depth.

At 600 km depth the predicted signal in the temperature derivative of velocity consists of a relatively wide peak in which the shallower wadsleyite to ringwoodite phase change interferes with an initiation of a deeper calcium perovskite phase (capv in). The 600 km initiation of akimotoite is not the deeper endothermic phase change associated with the sharp discontinuity commonly detected near 660 km. For some compositions and temperatures, Hefesto predicts the 660 km phase change to occur over two sharp, and closely spaced depths. These two deeper phase changes are too sharp to be detected by stochastic tomographic with the array and frequency band of this study. Both seismic observations and mineral physics studies (e.g., Ishii et al., 2001), predict a 660 km deep phase change to occur over a zone equal to or less than 2 km. In the median filtered Hefesto predictions shown in Figs. 7c and 8 the phase changes near 660 km vanish, but appear in the unfiltered Hefesto prediction shown in Fig 7a.

If our estimated error bars in depth are close to truth, the 600 km phase change detected from stochastic tomography favors a harzburgite rather than a pyrolite composition in the mantle transition zone. Within error bars, our stochastic tomography detection at 500 km depth for the wadsleyite to ringwoodite phase change is shallower than either the Hefesto predictions for either pyrolite or a mechanical mixture. The disagreement is similar for both compositional models, suggesting that a better agreement may be achieved either by revising the Hefesto inputs for the physical properties of individual minerals or by revising the temperature profile. Of these two inputs, the depth of phase changes is most strongly sensitive to the temperature profile. In section 5, we discuss how a negative temperature perturbation in the 410 to 660 km transition zone, consistent with a history of subduction, can bring the observed and predicted heterogeneity spectra into closer agreement.

4. 3 Smaller peaks in the depth dependent heterogeneity spectrum

4.3.1 775 km

Another peak requiring a small negative perturbation to an assumed adiabatic temperature profile having a 1600 deg K potential temperature is a peak at 775 ±12 km. This peak nearly correlates with a Hefesto predicted phase change at 795 km in mechanical mixtures of basalt and harzburgite having a basalt fraction of 18%, indicative of a phase change in subducted oceanic crust. The Hefesto predicted phase change in the temperature derivative consists of relatively weak peak having a 7 km width.

4.3.2 250 km

The heterogeneity peak at 250 km ±12 km is neither the orthopyroxene to high pressure clinopyroxene phase change predicted closer to 300 km or the X discontinuity found in many receiver function studies (Pugh, 2021), both of which are too narrow (<10 km) to be detected by stochastic tomography and the filtered Hefesto predictions shown in Figs. 7bc and 8. We instead interpret this to be a signal associated with the Lehmann discontinuity, which is frequently detected in S body wave studies at depths 220 km to 240 km beneath continents (e.g., Vinnik et al., 2015). Karato (1992) has suggested that the Lehmann discontinuity is associated with a change in rheology from dislocation creep above to diffusion creep below a 20 km wide or greater zone centered near 240 km depth for wet and/or hot conditions. This transition is also associated with a change from an anisotropic lithospheric lid to an isotropic asthenosphere. A change in anisotropy and rheology, however, is unlikely to be strongly expressed by a zone of heterogeneity capable of scattering seismic waves. Vinnik et al. (2005) have also shown that a change in rheology and anisotropy alone cannot account for the sign of the S to P conversion of S waves incident on the Lehmann discontinuity. A possible mechanism for heterogeneity in this depth region may be the hypothesis of Ono (2007), who proposes that the Lehmann is due to the effects of dehydration of subducted oceanic sediments beneath a continent. A possible supporting piece of evidence for this hypothesis is that Hefesto does not yet include the effects of H_2O content on melting and dehydration.

4.4 Modeling considerations: resolution and temperature profile

The differences between detected and predicted phase changes will depend on the accuracy of the assumptions in the thermodynamic model and the sampling and errors in the power spectrum of heterogeneity determined from stochastic tomography. The depth accuracy of the thermodynamic model depends on the validity of the assumed petrologic model, the physical properties of minerals determined from combinations of experimental observations and ab initio calculations, and the assumed temperature profile. The accuracy of the power spectrum estimated from stochastic tomography largely depends on the depth-sampling rate that can be resolved in the inversion of coherences, which depends on sensor spacing and its geometry and the azimuthal and depth distribution of seismic events.

The disagreement between the detected (600 km) and predicted (660 km), last and deepest, endothermic phase change is too large to be explained by a plausible hotter mantle temperature in this broad region. A global 660 km discontinuity has been largely confirmed in many seismic studies and is generally the most robustly detected discontinuity even by reflected body waves having dominant frequencies approaching 1 Hz (e.g., Deuss et al., 2006). Its signature in receiver functions (Andrews & Deuss, 2008), however, can be complex, in agreement with the complex phase changes predicted from thermodynamic models at and near this depth (Xu et al., 2008). A partial explanation for a positive detection at 600 km but not 660 km is that the 25 km sampling rate in the inversion is simply too coarse to resolve the complex signal of two closely spaced phase changes. We thus conclude that our detection at 600 km is the transformation of high-pressure clinopyroxene to akimotoite initiating closer to 600 km than 650 km. Hao et al. (2019) predict this transition to have a width on the order of 25 km or greater. The detection of an akimototite transition at 600 km, indicative of the existence of regions of colder mantle temperatures (Hogrefe et al., 1994), coupled with a phase transition in basalt at 775 km, is consistent with the history of the subduction of the Farallon plate beneath the western US. Tomographic images of the shear velocity structure of the mantle beneath this region reveal evidence of both slab stagnation and fragmentation in the lower mantle transition zone as well as penetration beneath 660 km (Schmid et al., 2002).

4.5 Geotherm perturbation

Two isothermal runs of Hefesto (Fig. 9) demonstrate the relative sensitivity of different predicted phase transition to changes in temperature. The 410 and 660 km phase transitions are considerably less sensitive to lateral temperature variations than the calcium perovskite and akimotoite transitions near 500 and 600 km depth, respectively. Hence, if the physical properties and chemistry of these two transitions are well understood, they can potentially serve as accurate thermometers in the transition zone. Assuming that errors in of the chemistry and physical properties taken as inputs to Hefesto are small, we can estimate the temperature required to make the transition zone phase changes come into better agreement with our measurements of heterogeneity in the transition zone from stochastic tomography. The perturbation needed to achieve this (Fig. 10) requires a cooler transition zone temperature compared to that calculated for a mantle adiabat having a 1600^{o} K potential temperature. It is also worth noting that the negative temperature perturbation required to bring the akimotoite phase transition at 600 km into better agreement with a pyrolite model may not require as high a percentage of harzburgite in models having a mechanical mixture (Zhao, et al., 2022). An example applying this temperature perturbation is shown in Fig. 11. The size and form of this perturbation is similar to those proposed in mantle convection studies by Tackley (1993) and Matyska and Yuen (2002), who predict non-adiabatic perturbations to the mantle geotherm due to slab stagnation in the transition zone. In addition to the results shown here from stochastic tomography, travel time tomography also supports this condition for the subduction of the Farallon slab beneath the western US. East-west cross sections of the P wave tomographic model LLN3D are consistent with a fast, cool, region in the mantle transition zone (Fig. 12).

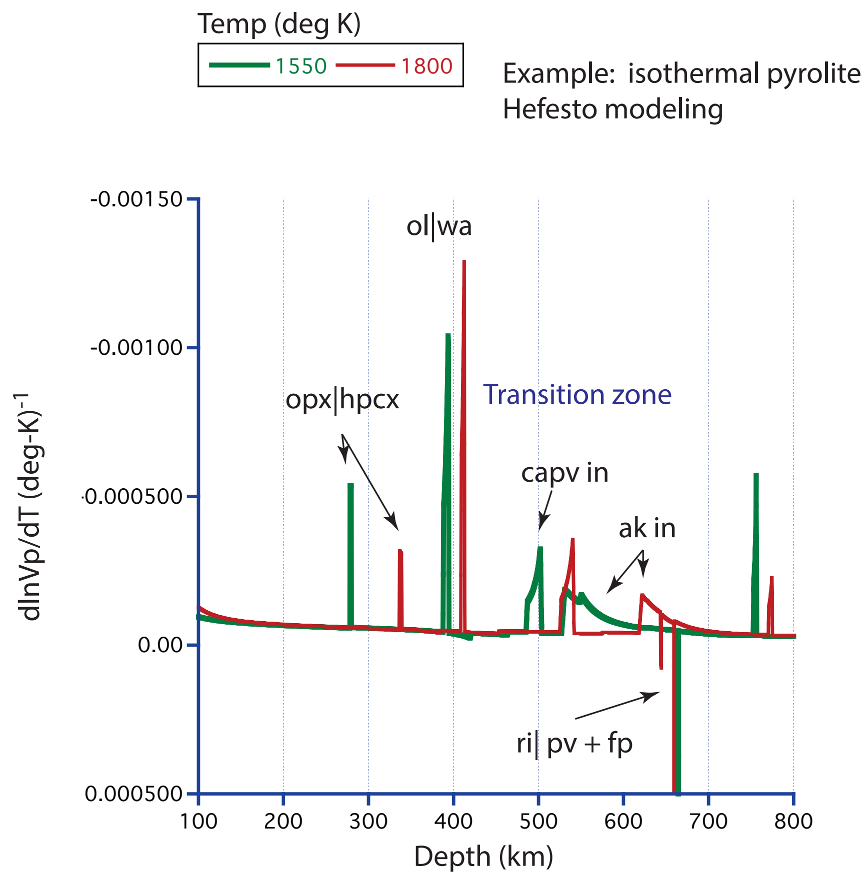

Figure 9. Isothermal calculations of dlnVp/dT for pyrolite for 1600° K. and 1800° K.

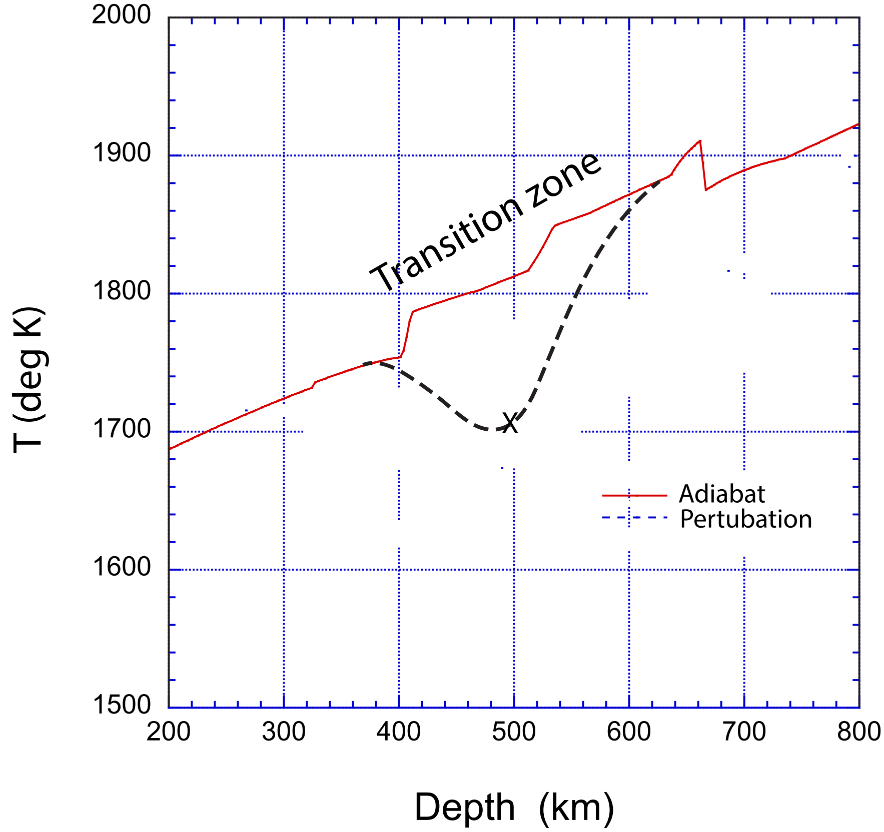

Figure 10. A perturbation (dashed) is applied in an adiabatic temperature profile in the transition zone to achieve better agreement between the peaks in heterogeneity determined from stochastic tomography and those predicted by the Hefesto thermodynamic code. The X marks the temperature perturbation needed to make depth of the wadsleyite to ringwoodite phase transition predicted from an isothermal run of Hefesto agree with the 500 km deep peak found from stochastic tomography.

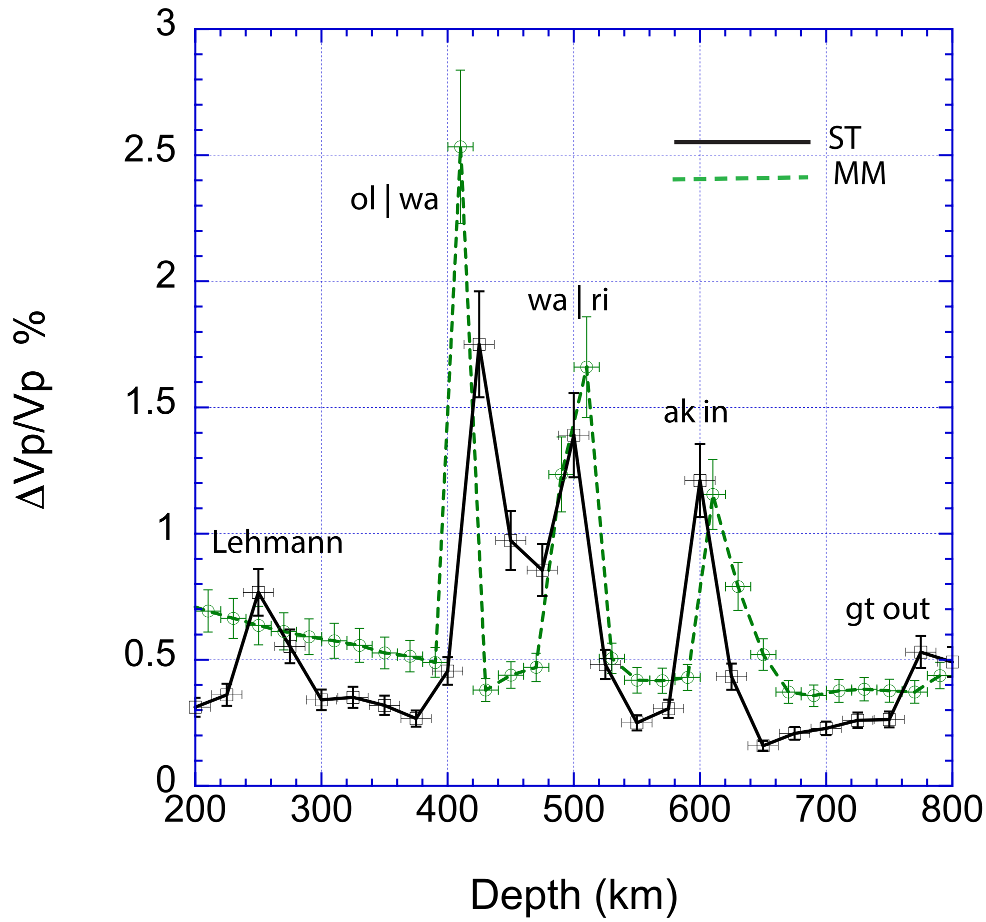

Figure 11. Solid black line (ST): mantle heterogeneity spectrum of P waves measured from stochastic tomography applied to the western US. Short green dashed line (MM): temperature derivative calculated from the Hefesto thermodynamic code for a mechanical mixture of harzburgite and basalt assuming the temperature perturbation in the transition zone shown in Figure 10.

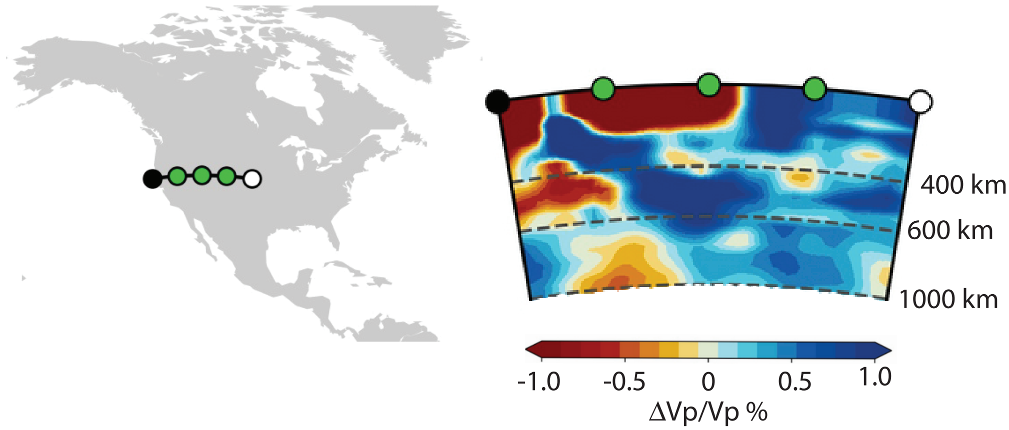

Figure 12. Cross-section of P velocity structure beneath the western US along an E-W profile centered at 50 deg latitude from the LLN3D model of Simmons et al. (2012, constructed from SubMachine web tools (Hosseini et al., 2018).

The combination of mechanisms creating slab stagnation are still actively debated, depending on slab rollback at the initial subduction zone, the fine structure of the endothermic phase change near 660 km, its Clapeyron slope, and whether there is a viscosity increase or decrease below the 660 km phase change (e.g., Mao and Zhong, 2008). The non-detection of 660 km phase change from stochastic tomography, its otherwise ubiquitous detection from reflected and converted high frequency (> 1 Hz) body waves (e.g., Whitcomb and Anderson, 1970), the narrow width of metamorphic temperature derivatives of its P and S wave velocity changes, and its topography are all consistent with it being an endothermic phase change, very narrow in width (no more than 2-10 km), with a near vertical Clapeyron slope.

5 Conclusions

From stochastic seismic tomography applied to the upper 1000 km of the western US, we have shown that its heterogeneity spectrum is characterized by a series of peaks related to narrow regions of depth in which phase or chemistry changes. We have demonstrated the stochastic seismic tomography can capture higher order phase and chemical changes in the upper mantle that are undetectable from reflection imaging. These peaks, having amplitudes on the order of 1-2% in P velocity fluctuation, strongly correlate with the majority of predicted phase changes from thermodynamic models of the upper mantle's chemistry and phase. Stochastic tomography has the potential to detect mantle phase changes that do not exhibit changes in seismic velocity and density over short depth intervals. These types of phase changes are characterized by paired changes in velocity gradient over a transition depth that may be equal to or larger than the wavelength of a body wave. Results from a depth-sampling interval of 25 km for the inverted spectrum suggest that many of these phase changes may occur over a range in depth equal to or greater than 25 km. An exception is our non-detection of the phase transition at 660 km, consistent with a transition interval in depth that may be as small as 2 km (0.1 GPa).

Our interpretation of individual peaks in the heterogeneity spectrum as a function of depth are consistent with a history of subduction and slab stagnation in the upper mantle transition zone between 400 to 660 km depth. This interpretation is based largely on the depth position and temperature dependence of the detected wadsleyite to ringwoodite transition at 500 km depth and the calcium perovskite to ringwoodite transition at 600 km depth. A stochastic tomography detection of a smaller phase transition near 250 km is interpreted to be the Lehmann discontinuity, which is unpredicted by thermodynamic modeling not containing effects of water, and which may be the signature of dehydration of subducted oceanic sediments. The depths of the 500 km, 600 km, and a 775 km phase change require a negative perturbation of a mantle adiabat in the transition zone, extending at least 100 km below the 660 km phase transition. This cool perturbation is consistent with the predictions of mantle convection suggesting slab stagnation in the transition zone, with the predictions of thermodynamic modeling incorporating perturbations to the geotherm, and with fast P velocities in the mantle transition zone found in 3-D travel time tomography of the western US.

To detect the thermodynamically predicted changes in mantle silicates with stochastic tomography, we demonstrate that a depth sampling interval of 25 km or less must be achieved. Such a resolution may generally also require an estimation of the amplitude and phase effects of source radiation patterns and source-time functions. Averaging of coherence lags over all pairs of sensors having a common lag distance over a large number of earthquakes arriving from different azimuths will enable heterogeneities having scale lengths on the order of the sensor spacing to be detected and will also tend minimize site effects at the near surface of sensors. The 10-20 km spacing of a growing number of FLEX array experiments of the US Array and the availability of waveforms from 3 widely separated groups of deep focus earthquakes, having simple source-time functions, makes this high resolution possible for at least the western US. Our location of phase changes represents an average for the western US for depths between 200 km and 1000 km, between latitudes 30º N and 50º N and longitudes 100º W and 125º W. Quantification of lateral variations in these phase changes over smaller regions of the upper mantle will depend on the densities and duration of FLEX array experiments and the availability of body wavefronts arriving from different azimuths.

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Waveform data and services for centroid moment tensors and synthetic seismograms are available from the Incorporated Research Institutions for Seismology through the web site https://www.iris.edu. Matlab and Python scripts for processing and inverting amplitude and phase coherences for single layer and depth dependent heterogeneity spectra are available from the web site listed in the Tian & Cormier (2020) entry References. The Hefesto thermodynamic mineral code is available at the web link: https://github.com/stixrude/HeFESToRepository.

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