Physics of the Earth and Planetary Interiors 250 (2016) 46–63

Contents lists available at ScienceDirect

Physics of the Earth and Planetary Interiors

journal homepage: www.elsevier.com/locate/pepi

Seismic signature of a hydrous mantle transition zone

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ARTICLE INFO

Article history:
Received 2 April 2015
Received in revised form 2 November 2015
Accepted 18 November 2015
Available online 2 December 2015

Keywords:
Water
Transition zone
Seismology
Mineral physics

ABSTRACT

Although water has a major influence on tectonic and other geodynamic processes, little is known about its quantity and distribution within the deep Earth. In the last few decades, laboratory experiments on nominally anhydrous minerals (NAMs) of the transition zone have shown that these minerals can contain significant amounts of water, up to 3.3 wt%. In this study, we investigate if it is possible to use seismic observations to distinguish between a hydrous and anhydrous transition zone. We perform an extensive literature search of mineral experimental data, to generate a compilation of the water storage capacities, elastic parameters and phase boundary data for potentially hydrous minerals in the transition zone, and use thermodynamic modelling to compute synthetic seismic profiles of density, V_P and V_S at transition zone temperatures and pressures. We find that large uncertainties on the mineral phase equilibria (ca. 2 GPa) and elastic properties produce a wide range of seismic profiles. In particular, there is a lack of data at temperatures corresponding to those along a 1300 °C adiabat or hotter, which may be expected at transition zone pressures. Comparing our hydrous transition zone models with equivalent profiles at anhydrous conditions, we see that the depths of the 410 and 660 discontinuities cannot at present be used to map the water content of the transition zone due to these uncertainties. Further, while average velocities and densities inside the transition zone clearly decrease with increasing water content, there is a near-perfect trade-off with increases in temperature. It is therefore difficult to distinguish thermal from water effects, and the conventional view of a slow and thick transition zone for water and slow and thin transition zone for high temperature should be regarded with caution. A better diagnostic for water may be given by the average velocity gradients of the transition zone, which increase with increasing water content (but decrease for increasing temperature). However the significance of this effect depends on the degree of water saturation and partitioning between the NAMs. Since seismology is better able to constrain the thickness of the transition zone than velocity gradients, our study indicates that the most useful input from future mineral physics experiments would be to better constrain the phase relations between hydrous olivine and its high-pressure polymorphs, especially at high temperatures. Additionally, the uncertainties on the mineral seismic properties could be reduced significantly if the experimentally-observable correlations between bulk and shear moduli and their corresponding pressure derivatives would be published.

1. Introduction

One of the prime characteristics that distinguishes the Earth from other terrestrial planets is the substantial amount of liquid water at its surface. Water plays a major role in the dynamics of our planet and is fundamental to the existence of organic life. Yet while the water cycle at the Earth's surface and atmosphere is widely studied and understood, little is known about the quantity, distribution or behaviour of water within the Earth. We know that water enters the mantle via subduction and is released via volcanism, but precisely how it cycles between those places is essentially unknown. Water has a large influence on the physical properties of rocks. It reduces their strength, viscosity and melting point (Chen et al., 1998; Hirschmann, 2006), which in turn yields major consequences for large-scale processes such as volcanic activity, plate tectonics (Regenauer-Lieb et al., 2001) and possibly the generation of very deep (400–600 km) earthquakes (Richard et al., 2007). Therefore, in order to gain a better understanding of these processes, it is essential to constrain how much water is stored in the mantle and its distribution. This, in turn, requires us to determine the change in water solubility with respect to pressure, temperature and mineral type, and the effect which water has on the physical properties of mantle minerals.

The present-day total water volume found in oceans is about 0.025% of the total mass of the Earth, but this fraction may have

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http://dx.doi.org/10.1016/j.pepi.2015.11.005
0031-9201/

been significantly higher during the early stages of the Earth's existence, ~4.5 billion years ago (Drake, 2005). This poses the question of what happened to the excess water; did it escape the atmosphere into space, or is a significant amount of water currently stored within the deep Earth? Field studies provide both supporting and opposing results for the latter: a recent study by Pearson et al. (2014) on a ringwoodite inclusion in a diamond found that the ringwoodite had a water content of 1.5 wt%, indicating that the mantle is (at least locally) subject to hydration. On the other hand, geochemical analysis of volcanic rocks by Dixon et al. (2002), together with numerical models of the deep mantle by Rupke et al. (2006), suggest that the deeper mantle is predominantly anhydrous.

Laboratory experiments in the last two decades on the water storage capacity of major mantle minerals previously thought to be anhydrous, the so called 'nominally anhydrous minerals' (NAMs), have shown that they actually have the capacity to absorb small weight percentages of water, in the form of structurally bound (OH–) ions. When integrated over the whole volume of the Earth, the mantle could therefore, theoretically, contain significant amounts of water, up to several times the total water volume currently found in the oceans (Smyth and Jacobsen, 2006). Two minerals in particular, wadsleyite and ringwoodite, have been found to have a significant water storage capacity of up to several weight percent (Ohtani et al., 2000; Chen et al., 2002). These high-pressure polymorphs of olivine make up about 60% of the transition zone, a region in the mantle between approximately 410 and 660 km depth which is characterised by high velocity gradients. The transition zone is bounded on both sides by sharp increases in velocity, the so-called '410' and '660' discontinuities, which are thought to arise from the phase transition of olivine to wadsleyite, and the decomposition of ringwoodite into perovskite and magnesiowüstite, respectively. Since wadsleyite and ringwoodite have much greater water storage capacity than the overlying olivine or underlying perovskite, the transition zone could be a major water reservoir, where water entering the mantle by subduction becomes trapped between the relatively dry minerals above and below the transition zone (the so-called 'transition-zone water filter' of Bercovici and Karato (2003)).

Constraints on the physical properties of the mantle are predominantly obtained from seismic observations. Three main structural aspects of the transition zone are expected to be influenced by water and might be seen in seismic data: These are (1) the velocity profile of the transition zone, (2) the position (i.e. depth) of the '410' and '660' discontinuities and (3) the impedance contrast at the '410' and '660' discontinuities. Recent experiments on the elastic properties of NAMs indicate that both P and S wave speed decrease with increasing water content (e.g. Jacobsen and Smyth, 2006). It is thus possible that the average velocity in the hydrous transition zone will be lower than at anhydrous conditions, and that the impedance contrast at the '410' and '660' discontinuities will decrease and increase, respectively, assuming that the minerals above and below the transition zone contain significantly less water. Studies on the phase transitions between olivine and its high-pressure polymorphs indicate that the olivine–wadsleyite transition occurs at slightly lower pressures (Smyth and Frost, 2002) under hydrous conditions, and the post-spinel composition at slightly higher pressures (e.g. Litasov et al., 2005; Ghosh et al., 2013). However, this is a relatively young and active area of research, and experimental data are only available at limited (P, T) conditions. In particular, experimental data are often obtained at lower pressures than the transition zone, and whether hydrous NAMs remain slower than anhydrous NAMs at transition zone pressures depends heavily on the pressure derivatives of their elastic moduli. It is thus unclear how uncertainties in the experimental data translate into uncertainties in seismic properties, and whether the existing data are sufficiently comprehensive to allow quantitative and robust interpretation of seismic observations in terms of water content.

At the same time, mapping the water content inside the transition zone using seismology is non-trivial for two main reasons. Firstly, the seismic structure is also modified by changes in temperature and major element chemistry (e.g. Fe content), meaning that there may be a non-unique physical interpretation for a given seismic structure. Karato (2011) has argued that the influence of water on seismic velocities is so small that variations in water content may be masked by changes in temperature or chemistry, to which seismic velocities are more sensitive. Secondly, the seismic data themselves each have uncertainties and limited resolving power, and in light of this it is unclear if the differences in seismic structure between anhydrous and hydrous transition zone regions are significant enough to be resolved by seismology.

In this study we explore how the ranges and limitations of the currently-available mineral experimental data for NAMs are mapped into seismic structure. We first make a compilation of experimental observations of hydrous NAMs, and then use thermodynamic modelling to predict corresponding wave speed and density profiles through the mantle transition zone. We do this in order to quantify the effect of water on the density and wave speeds at the '410', '660' and within the transition zone, relative to uncertainties in the mineral experimental data and changes in temperature and composition. We compare our findings to real seismic observations to investigate whether, at present, seismic observations have the capacity to identify water inside the mantle transition zone. Our results can be used as a guide for future seismic and mineralogical investigations, so that they may be optimised towards mapping water inside the transition zone.

2. Methodology

In order to calculate the seismic properties of a hydrous transition zone, we need to know the elastic properties of the constituent minerals at every temperature and pressure within the transition zone. To this end, we use the equation of state (EoS) of Stixrude and Lithgow-Bertelloni (2005) to extrapolate mineral elastic properties from ambient conditions to high P and T. This EoS is essentially a third order Birch–Murnaghan finite strain extrapolation for pressure with a Mie–Grüneisen correction for temperature. The computer program *Perple_X* (Connolly, 1990, 2005) is used to solve the EoS. For a given bulk composition, set of mineral elastic properties and pressure–temperature range, *Perple_X* applies the EoS to derive the elastic properties per mineral at each point within a 2D-grid of pressure and temperature points. Simultaneously, *Perple_X* computes the stable mineral assemblage at each P–T point via a free energy minimisation. The overall physical properties of the bulk mineral assemblage are computed from a weighted average of the constituent minerals: in our case the desired properties are the Voigt–Reuss–Hill (VRH) average for P and S wave speed, and the Voigt average for density. *Perple_X* then outputs the desired properties along a given P–T path by interpolation of the local elastic properties at the nearest grid points.

The thermoelastic dataset of Stixrude and Lithgow-Bertelloni (2011) was used as the primary input for all calculations. This dataset is composed of 47 minerals and mineral end-members, each described in terms of 10 thermodynamic parameters: the Helmholtz free energy (F_0), volume (V_0), isothermal bulk modulus (K_{T0}), shear modulus (G_0), their pressure derivatives (K'_0, G'_0), Debye temperature (θ_0), Grüneisen parameter (γ_0), and two parameters related to the temperature derivatives of the bulk and shear moduli (q, η_{S0}), where the subscript '0' represents ambient conditions. These parameters have been obtained by a global inversion of experimental data allowing mineral elastic properties and phase