Physics of the Earth and Planetary Interiors 182 (2010) 107–112

Contents lists available at ScienceDirect

Physics of the Earth and Planetary Interiors

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

The temperature dependence of the elasticity of Fe-bearing wadsleyite

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ARTICLE INFO

Article history:
Received 15 February 2010
Received in revised form 9 June 2010
Accepted 28 June 2010

Edited by: G. Helffrich

Keywords:
Wadsleyite
Elastic properties
Resonant ultrasound spectroscopy
Seismic discontinuities
Mantle composition

ABSTRACT

Data are presented on the elastic properties of β-$(Mg_{0.92}Fe_{0.08})_2SiO_4$ (iron-bearing wadsleyite) from 295 K to 640 K at ambient pressure. Elasticity measurements were made on hot-pressed polycrystals using resonant ultrasound spectroscopy (RUS). Multiple temperature excursions were done with data retrieved during both heating and cooling cycles. Room temperature (RT) values for the adiabatic bulk (K_S) and shear (G) moduli are 170.8(1.2) GPa and 108.9(0.4) GPa, respectively. The average derivatives over the temperature (T) range studied are $(\partial K_S/\partial T)_P = -1.75(0.07) \times 10^{-2}$ GPa K^{-1} and $(\partial G/\partial T)_P = -1.55(0.06) \times 10^{-2}$ GPa K^{-1}. Comparison of these results with those from our recent study of Mg-endmember wadsleyite shows no measurable difference in the average $(\partial K_S/\partial T)_P$ or $(\partial G/\partial T)_P$ from RT to 640 K due to Fe content. Slight nonlinearity in the temperature dependences of both K_S and G are observed, such that second order fits for both $K_S(T)$ and $G(T)$ are statistically justified. Whereas, the current nonlinearity in $G(T)$ for β-$(Mg_{0.92}Fe_{0.08})_2SiO_4$ is similar to that observed for β-Mg_2SiO_4, second order effects in $K_S(T)$ were not observed previously for wadsleyite.

1. Introduction

Reliable data on the elasticity of all candidate minerals for Earth's mantle are necessary to understand compositional, structural, and thermal features of that region. The elastic properties of wadsleyite [β-$(Mg,Fe)_2SiO_4$], a high pressure polymorph of olivine [α-$(Mg,Fe)_2SiO_4$], are of special importance for interpreting geophysical processes in Earth's transition zone and for constraining mineral models of the entire mantle. Indeed, seismic discontinuities at 410 km depth, the upper boundary to the transition zone, have generally been associated with elastic changes resulting from the α- to β-phase transition at that depth. These discontinuities could provide powerful controls on acceptable mantle mineral models, especially on the amount of olivine, if the elastic properties of both the α- and β-phases are known at the temperature and pressure of 410-km depth.

Considerable experimental efforts have gone towards determining the adiabatic bulk (K_S) and shear (G) moduli at elevated temperature (T) and/or pressure (P) for α-$(Mg,Fe)_2SiO_4$ with $X_{Fe} \equiv [Fe]/([Fe]+[Mg])$ ranging from 0 to about 0.1 (Isaak et al., 1989; Isaak, 1992; Zaug et al., 1993; Li et al., 1996; Zha et al., 1996, 1998; Abrahamson et al., 1997; Darling et al., 2004). There are also several reports on the elasticity of β-$(Mg,Fe)_2SiO_4$ (Sawamoto et al., 1984; Gwanmesia et al., 1990b; Zha et al., 1997; Li et al., 1996, 1998, 2001; Sinogeikin et al., 1998; Katsura et al., 2001; Mayama et al., 2004; Liu et al., 2005; Isaak et al., 2007; Liu et al., 2009). Nevertheless, questions remain on the temperature dependence of elasticity for the β-phase, and possible effects, if any, that variations in X_{Fe} have on the temperature effects.

Li et al. (1998, 2001) reported values of $(\partial K_S/\partial T)_P = -1.2(1) \times 10^{-2}$ GPa K^{-1} and $(\partial G/\partial T)_P = -1.7(1) \times 10^{-2}$ GPa K^{-1} for polycrystalline β-Mg_2SiO_4 using ultrasonic interferometry at simultaneous elevated pressure and temperature. Liu et al. (2005) reanalysed the Li et al. (1998, 2001) data and obtained refined values for $(\partial K_S/\partial T)_P$ and $(\partial G/\partial T)_P$ of $-1.29(17) \times 10^{-2}$ GPa K^{-1} and $-1.58(10) \times 10^{-2}$ GPa K^{-1}, respectively. Recently, Liu et al. (2009), using techniques and analyses similar to those utilized by Li et al. (1998, 2001) and Liu et al. (2005), reported results for temperature and pressure effects on the elasticity of wadsleyite with $X_{Fe} = 0.13$. Liu et al. (2009) found $(\partial K_S/\partial T)_P = -1.35(10) \times 10^{-2}$ GPa K^{-1} and $(\partial G/\partial T)_P = -1.44(18) \times 10^{-2}$ GPa K^{-1}. When uncertainties are taken into account, these derivatives appear indistiguishable from those determined by Liu et al. (2005) on endmember wadsleyite, i.e., $X_{Fe} = 0.0$.

In contrast to ultrasonic interferometry studies at simultaneously elevated pressure and temperature discussed above are two resonant ultrasound spectroscopy (RUS) studies at ambient pressure and high temperature. Mayama et al. (2004),

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doi:10.1016/j.pepi.2010.06.014

using polycrystalline wadsleyite with $X_{Fe} = 0.09$, found the average $(\partial K_S/\partial T)_P = -1.75(3) \times 10^{-2}$ GPa K^{-1} and $(\partial G/\partial T)_P = -1.59(1) \times 10^{-2}$ GPa K^{-1} from 298 K to 470 K. Measurements by Isaak et al. (2007) on endmember wadsleyite from 295 to 660 K produced average values of $(\partial K_S/\partial T)_P = -1.71(5) \times 10^{-2}$ GPa K^{-1} and $(\partial G/\partial T)_P = -1.57(3) \times 10^{-2}$ GPa K^{-1}.

So, while there appears to be near covergence on $(\partial G/\partial T)_P$ for wadsleyite, whether or not iron is present, there are significant differences in $(\partial K_S/\partial T)_P$ when comparing between the two types of studies. The Isaak et al. (2007) magnitude of $(\partial K_S/\partial T)_P$ is 33% higher than found by Lui et al. (2005), both using Fe-free material. Furthermore, we regard the similarities in the average $(\partial K_S/\partial T)_P$ and $(\partial G/\partial T)_P$ between the Mayama et al. (2004) and Isaak et al. (2007) reports as tenuous. Their room temperature values for K_S and G were both a few GPa lower than found from single-crystals (Sinogeikin et al., 1998). Furthermore, inspection of graphical data displayed by Mayama et al. (2004) clearly show systematic nonlinear behavior, even though they do not discuss this effect. If the nonlinearity in the Mayama et al. (2004) data were to persist to 660 K (the highest temperature used by Mayama et al. was 470 K), the magnitude of their averages for $(\partial K_S/\partial T)_P$ and $(\partial G/\partial T)_P$ from RT to 660 K would increase significantly, voiding the apparent agreement with the Isaak et al. (2007) data.

Finally, Isaak et al. (2007) identified and quantified second-order temperature effects in $G(T)$ of endmember wadsleyite which would significantly impact efforts to model mantle composition if nonlinearity persists to higher temperature. Additional measurements are needed to determine whether the nonlinearity is also observed in iron-bearing wadsleyite.

In light of some ambiguities in the temperature effects of wadsleyite elastic properties, we made new elasticity measurements from 295 K to 640 K for an Fe-bearing hot-pressed polycrystalline wadsleyite sample. The temperature range in this report is similar to that reported for endmember wadsleyite (Isaak et al., 2007) and twice the range used by Mayama et al. (2004) for their Fe-bearing sample at ambient pressure. In constrast, the Liu et al. (2009) study reports measurements up to 1073 K, but not along isobars. Each datum is at a different pressure. The present study has significantly denser data than obtained in the earlier Isaak et al. (2007) experiments because data from the present study were collected during both the heating and cooling cycles, and for multiple temperature excursions.

2. Experimental procedures

A polycrystalline wadsleyite [β-$(Mg,Fe)_2SiO_4$] specimen with $X_{Fe} = 0.08$ was fabricated by hot-pressing (Gwanmesia et al., 1990a, 1993) from powder ground from single-crystal San Carlos olivine. The hot-pressing experiments were carried out in the 1500-ton multi-anvil Presnall press apparatus (Haemyeong et al., 2006) at the Geophysical Laboratory of the Carnegie Institution of Washington D.C. Synchrotron *x*-ray diffraction analysis confirmed that the recovered material had fully transformed to the wadsleyite structure. The bulk density (ρ) of the recovered material was determined to be 3.581(3) g/cm^3 by Archimedes' immersion measurement which is very close to 3.57 g/cm^3 obtained from X-ray diffraction observations on a single-crystal of similar composition (Sinogeikin et al., 1998).

The recovered wadsleyite polycrystalline sample was nearly cylindrical with both diameter and height of a few millimeters. The specimen was ground into a small right-rectangular parallelepiped using diamond compounds of increasingly fine grit. The edge lengths (in mm) of the prepared specimen were 1.965(1), 1.667(1), and 1.416(2), where numbers in parenthesis represent uncertainty in the last digit.

The adiabatic bulk and shear moduli of the right-rectangular wadsleyite specimen were determined using the right-rectangular parallelepiped resonance (RPR) version of resonant ultrasound spectroscopy (RUS), similar to procedures outlined in Isaak et al. (2007) and references therein. Frequencies in the range of 1.25–4.05 MHz were scanned in the current experiments on Fe-wadsleyite.

Isaak et al. (2007) describe data acquisition procedures at elevated temperature. For Fe-wadsleyite, frequency scans were performed at discrete intervals while heating and cooling during four temperature excursions. Run A was from room temperature (294.5 K) to 500 K. Runs B and C were from room temperature to 640 K, and run D was from 340 K to 640 K. Run B was done 5 days after A. Run C was then done 14 days after B, while D immediately followed C. Indeed, run D was initiated at 340 K just as C had cooled down to that temperature. Values of K_S and G were determined from 34 modal frequencies. The same set of 34 frequencies was used to deduce K_S and G, and consequently $(\partial K_S/\partial T)_P$ and $(\partial G/\partial T)_P$, for each temperature run.

The estimated uncertainty in temperature is ±3 K at the highest temperature (640 K) which introduces an error of slightly less than 1% in the temperature derivatives of elastic moduli. Thermal expansion (α_V) data for Mg-endmember wadsleyite (Inoue et al., 2004) were used to account for changes in specimen edge lengths and density at elevated temperature in reducing the spectral data. There may be small difference in the thermal expansion between Mg-endmember and the Fe-bearing wadsleyite used in the current experiments. The computed K_S and G, however, are not very sensitive to variations in α_V. For example, systematically overestimating α_V by 10% over the temperature range studied would cause the magnitudes of $(\partial K_S/\partial T)_P$ and $(\partial G/\partial T)_P$ to be overestimated by less than 1%.

The RUS data reduction scheme assumes a completely unconstrained vibrating specimen. We performed several spectral measurements at room temperature with the holding force exerted by the transducers on the specimen ranging from the weight of 0.5–5.0 g and then extrapolated results to zero holding force. When making spectral measurements during each temperature excursion, care was taken to insure that a force corresponding to a weight of 5 g was used to hold the specimen between the transducers. From the room temperature measurements, we determined the effect of 5-g weight support force is to increase the apparent measured values for K_S and G by only 0.5 GPa and 0.2 GPa, respectively, above what would be measured with zero grams holding force. Accordingly, values for K_S and G cited at each temperature have all been corrected by 0.5 GPa and 0.2 GPa, respectively.

3. Results

All results for $K_S(T)$ and $G(T)$ obtained during the four temperature excursions described in the preceding section are shown in Figs. 1 and 2. Representative uncertainties for K_S and G are illustrated at 400 K in these figures. The uncertainties in K_S and G are nearly constant over the temperature range, indicating that random experimental error at each datum has little adverse effect on our determination of the temperature derivatives of K_S and G. Errors associated with K_S and G at each temperature are calculated from the slight mismatch of the 34 modal frequencies used to determine two elastic properties. The mismatch, in turn, is due mostly to imperfections of the sample which is assumed to be a perfectly isotropic and homogenous right-rectangular parallelepiped when performing data reduction.

An important feature of both Figs. 1 and 2 is that measurements of the temperature dependences of K_S and G are fairly reproducible. Uncertainties in $(\partial K_S/\partial T)_P$ and $(\partial G/\partial T)_P$ are about 5%. These