Temperature dependence of elastic moduli of β-$(Mg, Fe)_2SiO_4$

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Abstract

The elastic moduli of polycrystalline wadsleyite, β-$(Mg_{0.91}Fe_{0.09})_2SiO_4$, were measured up to 470 K by means of the resonant sphere technique. The adiabatic bulk (K_S) and shear (μ) moduli were found to be 165.72(6) and 105.43(2) GPa at room temperature. The average slopes (dK_S/dT and $d\mu/dT$) in the range were determined to be –0.0175(3) and –0.0159(1) GPa/K. We estimated that the *P*-, *S*-wave velocity and density jumps for the α- to β-phase transformation at the 410-km depth condition were 9.5, 11.2 and 5.4 %, respectively. These results suggest that the olivine component at the depth should be 52 and 42 volume % for *P*- and *S*-waves.

1. Introduction

The 410-km discontinuity in the upper mantle is thought to be caused by the transformation of olivine (α-phase) to wadsleyite (β-phase) (*Ringwood*, 1975). Pyroxene may transform to garnet phase [cf. *Irifune and Isshiki*, 1998]. But this may affect slopes of velocities and may be excluded in discussion based on the discontinuous change. Comparing the velocity jumps caused by this transformation with those from the seismological observations, we may infer the volume ratio of the olivine component in the upper mantle. Therefore the elastic moduli and their pressure and temperature derivatives for the α- and β-phases have been measured in many studies [e.g., *Kumazawa and Anderson,* 1969*, Sawamoto et al.,* 1984]. The temperature derivatives of elastic moduli of the α-phase have been obtained by means of the resonance method in a wide range of temperatures [*Isaak et al.,* 1989, *Isaak*, 1992]. Recently, those of the β-phase were obtained with the ultrasonic interferometry [*Li et al.,* 1998]. In our foregoing paper [*Katsura et al.,* 2001], we reported temperature derivatives of elastic moduli for a polycrystalline β-phase specimen in a rather narrow temperature range of 278 to 318 K. But the errors of the temperature derivatives for the β-phase in these reports were larger in one order of magnitude than those for the α-phase and so, the elastic moduli at mantle temperature were simply estimated by linear extrapolation. *Katsura et al.,* [2001] did not discuss the mantle composition. For discussion of mantle constitution, we need measurements of elastic moduli of the β-phase in much wider temperature range and also a method other than linear extrapolation to estimate the elastic moduli at high temperature. In the present paper, we report the elastic moduli of the β-phase measured under more stable conditions by the resonance method [*Suzuki et al.,* 1992a] in wider temperature range of 298 to 470 K, and try to apply an equation which represents better the temperature dependence of elastic moduli.

2. Measurement

The β-phase specimen is the same as that of *Katsura et al.* [2001]. The specimen was synthesized and sintered from San Carlos olivine using a Kawai-type high-pressure apparatus. Pressure, temperature and duration time for the synthesis and sintering were 14(1) GPa, 1400 K and 1 hour. The polycrystalline specimen was confirmed to be uniform under microscope and good in crystallinity from the narrow widths of x-ray diffraction peaks. The electron microprobe analyses were made for the specimen and the Fe/(Mg+Fe) ratio was found to be 0.091(3), which was the same as that of starting material. After shaping, the diameter of the sphere specimen was 2.250(2) mm at room temperature. With the data of mass and volume, bulk density was calculated to be 3.60(1) g/cm^3. This bulk density is in good agreement with X-ray density, 3.57(3) g/cm^3 [*Sinogeikin et al.,* 1998], suggesting that our specimen is nearly pore-free.

The resonant spectra of the specimen at room temperature were measured by the common frequency scanning method, or the CW method [*Suzuki et al.,* 1992b]. The frequency range of measurement was from 1.8 to 5.0 MHz with 10 Hz intervals. The resonant frequency shifts caused by supporting force for the specimen were corrected by using the contacting sphere theory [*Yoneda,* 2002].

Data acquisition at high temperature was made for the damping waveform of the specimen stimulated by high voltage pulses, which was generally called the FT method [*Suzuki et al.,* 1994]. The oscillatory waveform data of the specimen was stacked and averaged up over five thousand times to reduce random noises from circumstances. The resonant spectrum was obtained by the FFT analysis, in which frequency resolution was 100 Hz. Buffer rods were used to protect transducers from high temperature [*Goto and Anderson,* 1988]. Example of the oscillatory waveforms is shown in Figure 1A, and the resonant spectrum in Figure 1B. The temperature range was from 298 to 470 K, in which data acquisition was made almost at every 10 K. Temperature fluctuation during measurements was within 1 K. The diameter and density of the specimen at high temperature were corrected by thermal expansion data of *Suzuki et al.* [1980]. The resonant frequencies obtained at high temperatures were reduced by the correction terms at the ambient condition. The elastic moduli (adiabatic bulk (K_S) and shear (μ) moduli) at every temperature were calculated from the resonant frequencies by the least squares method.

3. Result

In the spectrum data at room temperature, we found the lower 13 resonant modes for the specimen. The modes were well assigned with isotropic oscillation. The half-widths of resonant peaks were about 1 kHz. At high temperatures, the lower 9 modes (Fig. 1B) were found through buffer rods. Although higher frequency modes were not detected because of their smaller amplitudes, we had a sufficient number of modes for reduction of the isotropic elastic moduli. Figure 2 shows examples of resonant frequency changes against temperature. The differences of resonant frequencies between heating and cooling processes are very small to be 0.05 % maximum. Figure 3 shows the elastic moduli of the β-phase as a function of temperature. The present results in Figure 3 show smooth changes of elastic moduli against temperature. Their derivatives were obtained by fitting a linear function to the data between 298 and 470 K. The errors of the temperature derivatives were estimated by taking account of not only residuals from the linear fitting but also errors of elastic moduli being deduced from observed frequencies at every temperature. The K_S and μ and their temperature derivatives (dK_S/dT and $d\mu/dT$) of the β-phase are shown in Table 1, along with data from other sources [e.g., *Sawamoto et al.* 1984].

The elastic moduli of the β-phase at room temperature obtained in this study are about 2.5 % smaller than those obtained by *Sinogeikin et al.* [1998]. The reason is not well known but differences in measuring technique, chemical composition and structure of the specimens etc.

are possible. Compared with our previous results [*Katsura et al.,* 2001], the present slopes of elastic moduli against temperature are larger and their errors are smaller in one order of magnitude. This situation is probably due to the wider temperature range and smooth temperature changes of elastic moduli in the present study as compared to those in previous one, in which the elastic moduli against temperature are somewhat scattered because the S/N ratio of resonant spectra is small, due to the smaller force supporting the specimen and the vibration of the temperature chamber. The present value of dK_S/dT is somewhat different from that for the end member β-phase obtained by *Li et al.* [1998]. This discrepancy may be not due to the effect of different Fe content, when we remind that the difference is only 10 % in the α-phase [*Isaak et al.,* 1989, *Isaak*, 1992]. The larger slope of dK_S/dT than that of $d\mu/dT$ in the present study is also found in the relative materials of the α-phase [*Isaak et al.,* 1989, *Isaak*, 1992] and ringwoodite (γ-phase) [*Jackson et al.,* 2000, *Sinogeikin et al.,* 2001] as well as alminate spinel $MgAl_2O_4$ [*Suzuki et al.*, 2000a], whereas the slopes in *Li et al.* [1998] show the opposite tendency. *Li et al.* [1998] succeeded in difficult measurements of travel times through a small specimen in a solid pressure medium and simultaneously determined the pressure and temperature derivatives of elastic moduli from the set of travel time data. On the other hand, the present measurements were made simply as a function of temperature. Then, three-digit significant figures of slopes are listed in Table 1 with errors.

4. Discussion

We calculated the seismic wave velocity and density jumps at 410-km depth (e.g., 13.8 GPa and 1673 K) for a hypothetical pure olivine mantle from the present results. The elastic moduli at high temperatures were estimated by using not linear extrapolation but the modified

Wachtman's equation [*Anderson*, 1966, *Suzuki et al.,* 2000b], and the seismic wave velocity and density were obtained by the third-ordered finite strain-equation [*Davies and Dziewonski*, 1975], referring to pressure derivatives of K_S and μ [*Zha et al.,* 2000]. On the other hand, it was suggested that the Fe/(Mg+Fe) ratio in olivine might vary during the transformation from the α- to β-phases around 410-km depth [*Irifune and Isshiki*, 1998]. Then we also calculated the seismic wave velocity and density jumps for this model, and compared results from the two Fe content models. The first model is that the Fe/(Mg+Fe) ratio in the phases is constant, to be 9 mol%, the same as composition of the specimen used in the present study, and designated as the Fe constant model hereafter. The second one is that the Fe/(Mg+Fe) ratio varies from 7.5 to 11.5 mol% at the transition by Fe partitioning between the phases and garnet [*Irifune and Isshiki*, 1998], the Fe partitioned model. In order to obtain the seismic velocities at the 410-km depth conditions, the elastic moduli reported for single crystals were adopted as reference values and the present data were used only as their temperature dependence. The data used in calculations and the results for the two Fe models are shown Table 2. The jumps of compressional (*P*), shear (*S*) wave velocities and density for the α- to β-phase transformation at 410-km depth were obtained to be 9.5, 11.2 and 5.4 % for the Fe constant model and 8.1, 8.8 and 7.3 % for the Fe partitioned model, respectively. The Fe partitioned model consists of two parts of velocity increase, a steeply increasing part in a rather narrow pressure interval (say 0.2 GPa) and a gradually increasing part. If we apply the former part to the observed seismic velocity jump, this may infer the maximum content of olivine component in that depth of the mantle. When we adopt velocity jumps of 4.9 and 4.6 % for *P*- and *S*-waves at the 410-km discontinuity [*Walck*, 1984, *Grand and Helmberger*, 1984], and assume the jumps are only due to the phase transformation, then the olivine component from *P*- and *S*-waves are about 52(15) and 42(10) volume % for the Fe constant model and 61(15) and 54(10) volume % for the Fe partitioned model, respectively. The error bounds were estimated by the higher or lower limits of the elastic moduli and their slopes. It is found that olivine component around the 410-km depth increases about 10 volume % in numerals by introducing Fe partitioning between the phases and garnet, though *Irifune and Isshiki* [1998] suggested that olivine component should increase 4-5 volume % as estimated at ambient condition.

Shearer and Flanagan [1999] discussed the relationship between the jumps of density and *P*- or *S*-wave velocity at the 410-km discontinuity from observation of reflected phases and showed a possible range of jumps within the confidence ellipsoids. Using the present data, the olivine component within the ellipsoids is estimated to be 45-55 volume % for *P*-wave and 45-60 volume % for *S*-wave, respectively, irrespective of the Fe models. Therefore combining the density jump with velocity ones, the possible range of olivine component becomes 45-60 volume %.

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Figure caption

Figure 1. An example of the oscillatory waveform (A) at high temperature and its spectrum (B) for the β-phase specimen. The symbols represent resonant isotropic oscillation modes.

Figure 2. Examples of temperature dependence of resonant frequencies for ${}_0T_2$ and ${}_0S_2$ modes of the β-phase specimen. The open circles and squares represent heating and cooling processes, respectively.

Figure 3. Temperature dependence of elastic moduli of the β-phase. The open circles and squares represent adiabatic bulk and shear moduli, respectively. Error bars are shown.

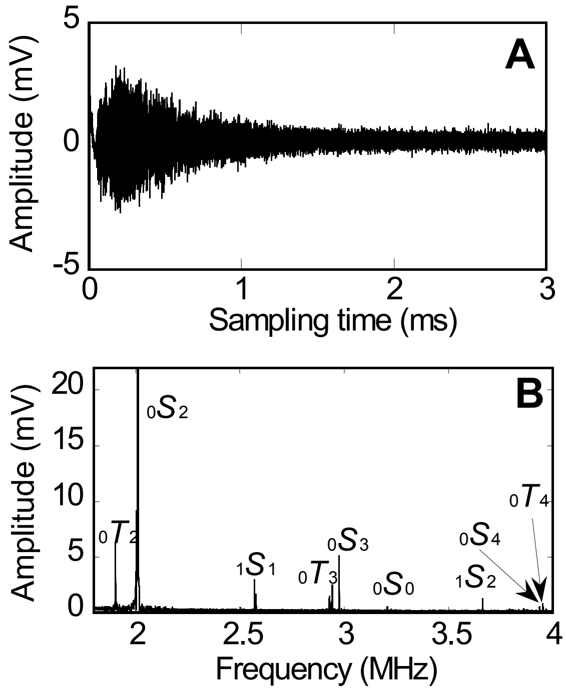
Table 1. Elastic moduli and their temperature derivatives of the β-phase. The x, K_S^*, μ^*, P and T represent Fe/(Mg+Fe) ratio, dK_S/dT, $d\mu/dT$, pressure and temperature ranges in measurement, respectively.

x(mol%)	K_S(GPa)	K_S^*(GPa/K)	μ (GPa)	μ^*(GPa/K)	P(GPa)	T(K)	reference
0	174		114		0	298	*Sawamoto et al.* [1984]
0	172(2)	–0.012(1)	113(1)	–0.017(1)	0-7	298-873	*Li et al.* [1998]
8	170(3)		108(2)		0	298	*Sinogeikin et al.* [1998]
9	165.7(1)	–0.016(3)	105.66(3)	–0.012(1)	0	278-318	*Katsura et al.* [2001]
9	165.72(6)	–0.0175(3)	105.43(2)	–0.0159(1)	0	298-470	this study

Table 2. The data used for calculations at 410-km depth conditions (13.8 GPa and 1673 K) and results for the two Fe models. The x, K_S', μ', $K_S(T)$, $\mu(T)$, ρ, v_P and v_S represent Fe/(Mg+Fe) ratio, the pressure derivatives of K_S and μ, K_S and μ at T=1673 K, density, the compressional and shear wave velocities, respectively.

Fe model		x	K_S	$K_S(T)$	K_S'	μ	$\mu(T)$	μ'	ρ	*at 410-km depth* v_P	v_S	ρ
		mol%	GPa	GPa		GPa	GPa		g/cm^3	km/s	km/s	g/cm^3
constant model	α	9.0	129.4[a]	104.5[g]	4.2[c]	78.1[a]	59.1[g]	1.4[c]	3.353[a]	8.59	4.65	3.543
	β	9.0	170.0[b]	141.4[h]	4.3[c]	108.0[b]	82.0[h]	1.4[c]	3.602[e]	9.41	5.17	3.736
partitioned model	α	7.5	129.4[a]	104.5[g]	4.2[c]	79.0[a]	59.4[g]	1.4[c]	3.330[a]	8.62	4.68	3.519
	β	11.5	170.0[b]	141.4[h]	4.3[c]	106.0[d]	80.0[h]	1.4[c]	3.640[f]	9.32	5.09	3.775

a: *Isaak* [1992], b: *Sinogeikin et al.* [1998], c: *Zha et al.* [2000], d: *Li and Liebermann* [2000], e: the present data, f: modified for x being 11.5 % from *Hazen et al.* [1990] data, g: estimated value by the modified-Wachtman's equation fitted to the data of *Isaak* [1992], h: The present data extrapolated by the modified-Wachtman's equation.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Frequency (MHz)
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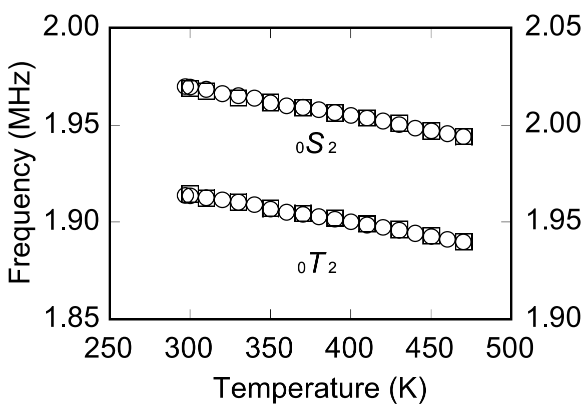
1S2
0S4
0T4

Fig. 1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Temperature (K)
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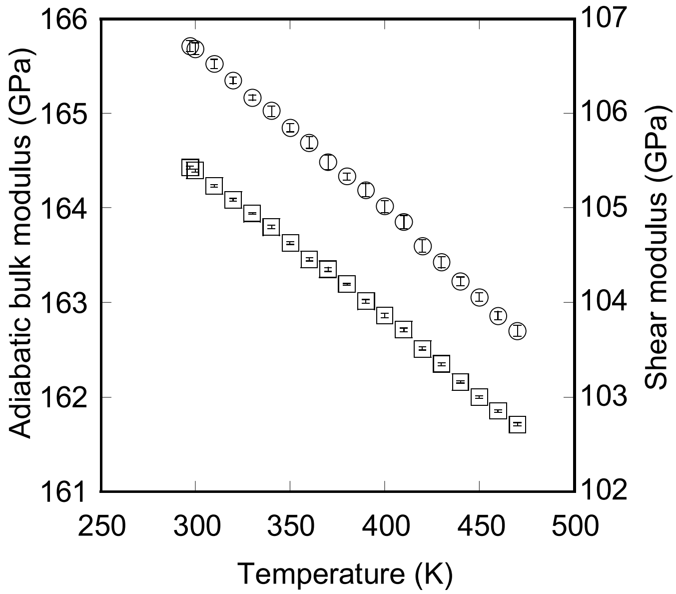
Fig. 2



166
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Temperature (K)
Adiabatic bulk modulus (GPa)
Shear modulus (GPa)

Fig. 3