Earth and Planetary Science Letters 481 (2018) 41–47

Contents lists available at ScienceDirect

Earth and Planetary Science Letters

www.elsevier.com/locate/epsl

Single-crystal elasticity of $MgAl_2O_4$-spinel up to 10.9 GPa and 1000 K: Implication for the velocity structure of the top upper mantle

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ARTICLE INFO

Article history:
Received 11 August 2017
Received in revised form 4 October 2017
Accepted 5 October 2017
Available online xxxx
Editor: P. Shearer

Keywords:
$MgAl_2O_4$-spinel
single-crystal elasticity
high pressure-temperature
Brillouin scattering
top upper mantle
velocity

ABSTRACT

The combined effect of pressure and temperature on the single-crystal elasticity of $MgAl_2O_4$-spinel has been studied using Brillouin scattering and X-ray diffraction up to 10.9 GPa and 1000 K in externally-heated diamond anvil cells. The obtained single-crystal elastic moduli of $MgAl_2O_4$-spinel at ambient conditions are consistent with literature values and follow a linear increase with pressure at high temperatures. More importantly, the pressure dependence of the elastic moduli at high temperatures is much smaller than that at 300 K, indicating a stronger temperature effect on the elastic moduli of $MgAl_2O_4$-spinel at high pressures. Our new results were applied to model the sound velocity of $MgAl_2O_4$-spinel at relevant pressure and temperature conditions of the top upper mantle, showing that $MgAl_2O_4$-spinel has the greatest velocity and the V_P/V_S ratio among major mantle minerals. We further modeled the velocity of spinel-peridotite at the top upper mantle. Varying the composition of spinel-peridotite can lead to up to 2.1% variation in V_P and 1.3% in V_S. The top upper mantle with greater V_P and V_S should contain more olivine and spinel but less orthopyroxene. The velocity of the top upper mantle is thus strongly correlated with the composition of the region. Our results are thus important in understanding the composition and velocity of the top upper mantle.

1. Introduction

$MgAl_2O_4$-rich spinel with a space group of $Fd\bar{3}m$ is a common mineral in the Earth's top upper mantle and an important host for Al and other trivalent cations in the region (Sickafus et al., 1999; Yoneda, 1990). In the peridotite xenolith from alkaline volcanics and kimberlites in the lithosphere beneath cratonic areas, the content of $MgAl_2O_4$-rich spinel is 1–4 wt.% (e.g. Downes et al., 1992; Foley et al., 2006; Furnes et al., 1986; Raye et al., 2011; Rudnick et al., 2004; Titus et al., 2007). The plagioclase-spinel and spinel-garnet transition are two important phase transitions at the top upper mantle, which are applied to study the pressure history of mantle peridotites during the uplift process (Fumagalli and Klemme, 2015; Su et al., 2010). In the CaO–MgO–Al_2O_3–SiO_2 (CMAS) system, $MgAl_2O_4$-spinel can be formed from the transition from plagioclase at 0.6–0.8 GPa and 900–1200 °C, while it further transforms into garnet at 1.5 to 2.5 GPa between 1000 and 1400 °C (e.g. Gasparik, 1984; Green and Hibberson, 1970; Klemme and O'Neill, 2000; Kushiro and Yoder, 1966; Milholland and Presnall, 1998; O'Neill, 1981; Walter et al., 2002; Ziberna et al., 2013). The presence of Cr can greatly increase the stability of $MgAl_2O_4$-spinel relative to both plagioclase and garnet (Borghini et al., 2009; Evans and Frost, 1975; Fumagalli and Klemme, 2015; Klemme, 2004; Su et al., 2010). When the mole percentage of Cr [Cr/(Cr + Al)] in $Mg(Cr, Al)_2O_4$ is less than 70 mol.%, every addition of 10 mol.% Cr can increase the stability pressure of spinel by 0.28 GPa at 1000–1400 K (O'Neill, 1981; Webb and Wood, 1986). Previous high pressure studies have found that $MgAl_2O_4$-spinel decomposes into a mixture of MgO and Al_2O_3 above 15 GPa at 1500 °C (Irifune et al., 1991; Liu, 1980). Yet at 26–28 GPa and 1300–1900 °C, $MgAl_2O_4$-spinel transforms into a new denser phase with a structure similar to that of $CaFe_2O_4$ (Akaogi et al., 1999; Davies and Gaffney, 1973; Enomoto et al., 2009; Irifune et al., 1991; Ono et al., 2009; Schäfer et al., 1983; Wang, 1968). $MgAl_2O_4$-rich spinel and its high pressure phase were proposed to be potential carriers of Al to the Earth's deep interior (Davies and Gaffney, 1973; Funamori et al., 1998; Irifune et al., 1991; Wang, 1968). Experimental studies on the physical properties of $MgAl_2O_4$-spinel, in particular the elasticity, at high pressure and

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https://doi.org/10.1016/j.epsl.2017.10.014
0012-821X/

temperature (P–T) conditions are thus important in understanding the composition and structure of the top upper mantle.

The elasticity of $MgAl_2O_4$-spinel has been extensively studied at high pressures and 300 K or high temperatures and 1 bar (Askarpour et al., 1993; Caracas and Banigan, 2009; Chang and Barsch, 1973; Chopelas, 1996; Cynn et al., 1993; Li et al., 2007; Liu et al., 1975; Speziale et al., 2016; Yoneda, 1990; Zou et al., 2013). At ambient conditions, the adiabatic bulk modulus, K_{S0}, is determined to be 196–200 GPa, and the shear modulus, G_0, is 107.8–109.0 GPa (Askarpour et al., 1993; Bruschini et al., 2015; Chang and Barsch, 1973; Liu et al., 1975; Speziale et al., 2016; Suzuki et al., 2000; Yoneda, 1990). The pressure dependences of the individual elastic moduli at 300 K have been determined up to 11 GPa using various high-pressure experimental methods, including Brillouin Spectroscopy, Ultrasonic methods and Fluorescence Sideband (Chang and Barsch, 1973; Chopelas, 1996; Speziale et al., 2016; Yoneda, 1990). Although a distinct softening in both K_S and G of $MgAl_2O_4$-spinel at pressure above 10 GPa was proposed by two studies using Ultrasonic methods (Chang and Barsch, 1973; Yoneda, 1990), such anomalous behavior in K_S and G of $MgAl_2O_4$-spinel was not observed in high-pressure studies using other methods (Chopelas, 1996; Zou et al., 2013). In addition, high-temperature studies for the elasticity of $MgAl_2O_4$-spinel at 1 bar up to 1273 K observed an order-disorder transition at ~923 K (Askarpour et al., 1993; Speziale et al., 2016; Suzuki et al., 2000). To date, only Zou et al. (2013) studied the aggregated bulk and shear moduli of $MgAl_2O_4$-spinel at simultaneously high P–T conditions up to 14 GPa and 900 K using polycrystalline sample. We still lack the experimental constraints on the single-crystal elasticity of $MgAl_2O_4$-spinel at simultaneously high P–T conditions.

In this study, we have investigated the single-crystal elasticity of $MgAl_2O_4$-spinel using Brillouin scattering combined with single-crystal X-ray diffraction at simultaneously high P–T conditions in externally heated diamond anvil cells (EHDAC). Using our new results, we compared the velocity of $MgAl_2O_4$-spinel with major mantle minerals. We also computed model velocity for spinel-peridotites to explore how the variations in composition affect the velocity structure of the earth's top upper mantle.

2. Experiments

High-quality single-crystal spinel plate with (100) orientation was purchased from the Kejing Company, China. The chemical composition of the spinel sample ($MgAl_2O_4$) was examined by electron microprobe analysis (EMPA) at the Material Center, University of Science and Technology of China. The lattice parameter of the sample determined by single-crystal X-ray diffraction (XRD) at ambient conditions is 8.0850(2) Å, yielding a density of 3.571(1) g/cm^3. The crystal was double-side polished to a platelet of ~25 μm in thickness using the 3M diamond lapping films. The sample platelet was further broken into small pieces with a size of ~100 × 100 μm for the high P–T studies. The sample crystal was loaded into the EHDACs equipped with a pair of diamonds with 500 μm culet. Two Pt foils were placed next to the sample platelet as the pressure calibrant during the high P–T measurements, while a ruby sphere was also loaded into the EHDAC as the pressure indicator when loading Ne as the pressure medium. An R-type thermocouple was attached to the diamond surface ~500 μm away from the diamond culet for temperature measurements. An alumina ceramic heater coiled by two Pt wires was used to heat the spinel crystal inside the EHDAC at high pressures.

We conducted the Brillouin scattering measurements combined with single-crystal XRD at simultaneously high P–T conditions up to 10.9 GPa and 1000 K at the GSECARS of the Advanced Photon Source (APS), Argonne National Laboratory (ANL). Single-crystal XRD confirmed that the crystal platelet loaded into the EHDAC had (100) orientation. The Brillouin measurements were performed in forward scattering geometry with a scattering angle of 50° using a six-pass Sandercock tandem Fabry–Perot interferometer (Fig. 1). Acoustic velocities of spinel can be calculated from our measured Brillouin frequencies as (Fig. 1):

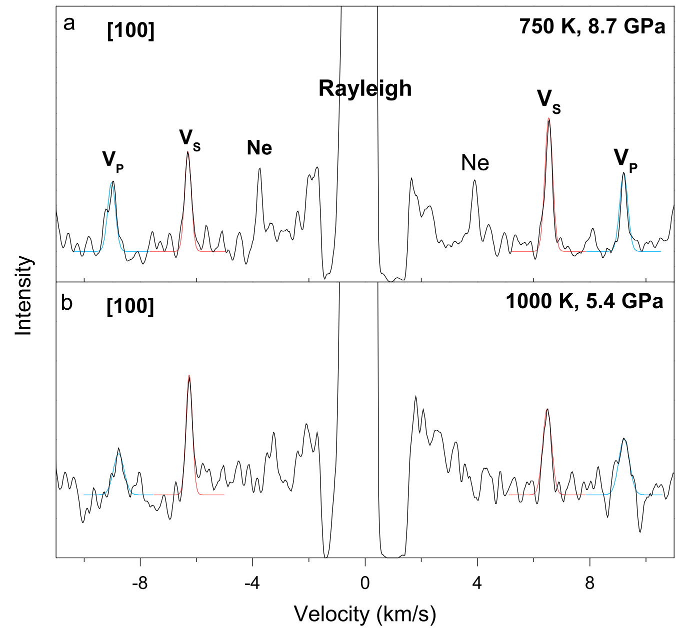

Fig. 1. Representative Brillouin spectrum at high pressure and temperature along (100) direction. a. At 750 K and 8.7 GPa; b. At 1000 K, 5.4 GPa. Black lines: collected data; red lines: fitted shear-wave, V_S; blue lines: fitted compressional-wave, V_P. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

$$v = \frac{\Delta\upsilon_B \lambda_0}{2\sin(\theta/2)} \tag{1}$$

where v is the acoustic velocity, $\Delta\upsilon_B$ is the measured Brillouin frequency shift, λ_0 is the laser wavelength of 532 nm, and θ is the external scattering angle of 50°. We also performed the XRD measurements to determine the density of spinel at each P–T condition after the Brillouin measurements. At ambient conditions, we collected the Brillouin spectra over a range of 90° at an interval of 10°. At high P–T, the Brillouin spectra were collected along (100) and (110) directions, respectively. Above 750 K at high pressures, Ar with 2% hydrogen was continuously flown into the EHDAC to avoid the potential oxidation of diamonds at high temperatures.

3. Results

$MgAl_2O_4$-spinel has cubic symmetry and its elastic tensor is fully described by three independent elastic constants. At ambient conditions, three elastic constants were obtained by fitting a set of Christoffel's equations to the measured velocities (Every, 1980):

$$\left|C_{ijkl}n_in_j - \rho v^2\delta_{ik}\right| = 0 \tag{2}$$

where C_{ijkl} is the elastic tensor with full suffix notation. In the following we will use the reduced notation, C_{ij} (Fig. 2 and Table 1). n_i, n_j are the direction cosines in the photon propagation direction, δ_{ik} is the Kronecker index, ρ is density, and v is the measured acoustic velocity. The fit to the measurements performed at ambient conditions yields $K_{S0} = 198(1)$ GPa and $G_0 = 107(1)$ GPa (Fig. 2, Table 1). At high P–T, elastic moduli of spinel were calculated using the obtained velocity data at [100] and [110] direction,