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P–V–T relation of MgO derived by simultaneous elastic wave velocity and in situ X-ray measurements: A new pressure scale for the mantle transition region

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ABSTRACT

Simultaneous elastic wave velocity and in situ synchrotron X-ray measurements on polycrystalline MgO were carried out with a V/V_0 between ~0.9 and 1.0, which corresponds to the pressures up to 23.6 GPa in our *P–V–T* relation of MgO, and temperatures up to 1650 K using a multi-anvil apparatus. The experimentally observed adiabatic bulk modulus and unit-cell volume led to the first pressure-scale-independent *P–V–T* relation of MgO. We obtained a pressure derivative of the isothermal bulk modulus ($K'_{T0} = 4.35(10)$) and a volume dependent Grüneisen parameter ($q_0 = 1.5(5)$), which reproduces the existing pressure-scale-independent data set (temperature dependence of elastic properties at ambient pressure and shock compression). Thus the present experimental and analytical procedure based on simultaneous elastic wave velocity and in situ X-ray diffraction measurements can give strong constraints on *P–V–T* equations of states (EoS) of minerals without any pressure scale. The present *P–V–T* EoS of MgO determined at pressure and temperature conditions comparable to the mantle transition region should be an important pressure scale to accurately determine the phase transition boundaries in this region. Application of the present pressure scale to the post-spinel transition boundary yields a transition pressure of 23.0 GPa at 1873 K, which is only marginally lower than that of the 660 km discontinuity.

1. Introduction

Accurate determination of pressure in mineral physics observations is crucial to understand the nature of the Earth's interior. In situ synchrotron X-ray observations have been used to determine the phase transformation pressures of mantle minerals [e.g. Irifune et al., 1998; Murakami et al., 2004], where the pressures are evaluated based on unit-cell volume changes in pressure reference materials, such as Au, Pt, NaCl, and MgO, using *P–V–T* equations of state (EoS) [e.g. Decker, 1971; Jamieson et al., 1982; Anderson et al., 1989; Speziale et al., 2001; Shim et al., 2002; Tsuchiya, 2003]. Thus the establishment of accurate *P–V–T* EoS is vital in experimental studies of the Earth's interior, and great efforts have been made to determine the *P–V–T* EoS based on the Hugoniot and static compression curves [e.g. Jamieson et al., 1982; Anderson et al., 1989; Speziale et al., 2001; Shim et al., 2002], and also on theoretical studies [e.g. Tsuchiya, 2003; Wu et al., 2008]. However, serious disagreement in pressure estimates has been noted among earlier studies [e.g. Litasov et al., 2005; Hirose, 2006; Irifune and Tsuchiya, 2007], yielding a number of conflicting results on the phase transition pressures of the major mantle minerals such as the post-spinel transitions [e.g. Irifune et al., 1998; Katsura et al., 2003; Fei et al., 2004].

Although shock-wave experiments provide the scale-free P–V–(T) data along the Hugoniot curves, it is difficult to establish the *P–V–T* EoS solely from the shock-wave data, because of a strong correlation between the key parameters of the pressure derivative of the isothermal bulk modulus K'_T and the volume dependence of the Grüneisen parameter γ. Previous studies therefore fixed either K'_T or volume dependence of γ to derive the *P–V–T* EoS, inevitably leading to significant uncertainties in the EoS. Since it is difficult to experimentally determine the volume dependence of γ, determination of K'_T has been attempted to establish the EoS using static compression data [e.g. Speziale et al., 2001; Shim et al., 2002]. However, the determination of K'_T in this manner requires a pressure scale. In order to avoid this chicken-and-egg problem, we need direct determination of K'_T without any pressure scales, which can be realized by simultaneous measurements of unit-cell volume and elastic wave velocity changes of a pressure reference material at high pressures.

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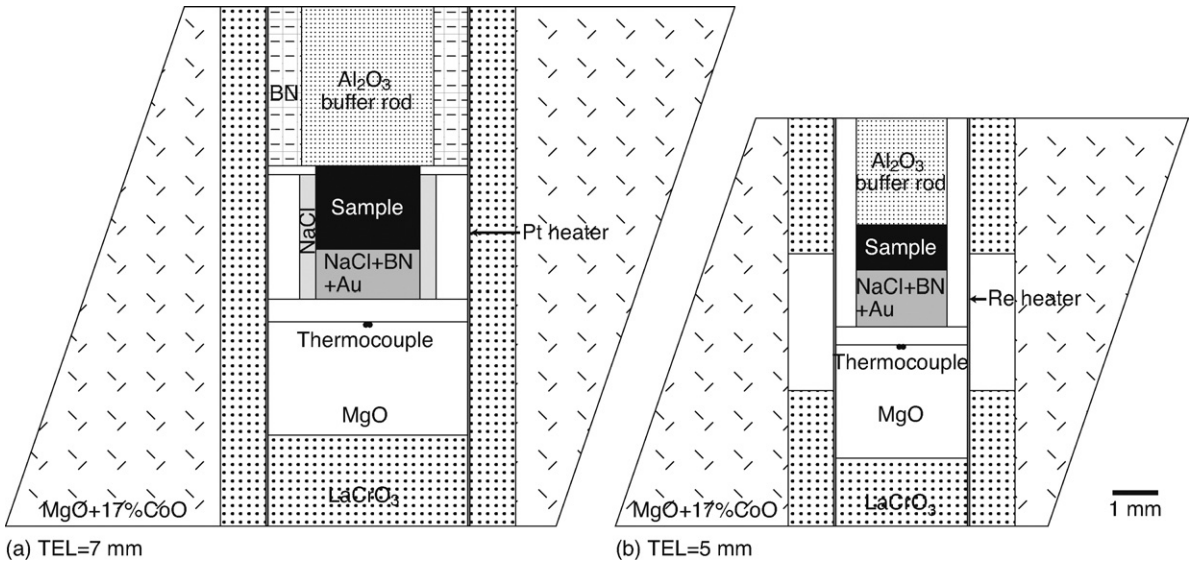

Fig. 1. Illustrations of the cell assembly used in the present experiments for the truncation edge length (TEL) of WC anvils of 7 mm (a) and 5 mm (b).

Recent high-pressure elasticity measurements by ultrasonic [Li et al., 2005, 2006; Mueller et al., 2003] and Brillouin scattering [Zha et al., 2000] methods combined with synchrotron in situ X-ray observations reported some P–V relations determined without pressure scales. However, these studies were made only at 300 K, although those at high temperatures are needed for mineral physics applications relevant to the Earth's deep interior. We recently succeeded in extending the precise elastic wave velocity measurements by combining in situ X-ray and ultrasonic measurements to both pressure and temperature conditions comparable to those of the mantle transition region [Higo et al., 2008; Irifune et al., 2008]. In addition, a recent theoretical study of Stixrude and Lithgow-Bertelloni (2005) demonstrated a thermodynamically consistent formulation for the EoS of minerals, which is formulated by eight thermoelastic parameters (K_{T0}, zero pressure isothermal bulk modulus; K'_{T0}, pressure derivative of isothermal bulk modulus; G_0, zero pressure shear modulus; G'_0, pressure derivative of shear modulus; θ_0, Debye temperature at reference conditions; γ_0, Grüneisen parameter at reference conditions; q_0, volume dependence of Grüneisen parameter at reference conditions; η_{s0}, shear strain derivative of Grüneisen parameter at reference conditions). The formulation enables us to determine these thermoelastic parameters by fitting the experimentally observed elastic properties and unit-cell volumes at both high pressures and high temperatures. Here we applied these experimental and analytical techniques to derive a pressure-scale-independent P–V–T EoS of MgO up to the pressure and temperature conditions of the mantle transition region.

2. Experiments

Simultaneous ultrasonic P- (V_p) and S-wave (V_s) velocity measurements, and X-ray radiography and diffraction experiments on well-sintered polycrystalline MgO (initial grain size 9 μm, initial porosity 0.55% [cf. Barnhoorn et al., 2007]) were carried out at the BL04B1 beamline at SPring-8, Japan. The unit-cell volume of MgO was determined by energy-dispersive X-ray diffraction measurements with a Ge solid-state detector. The Ge solid-state detector was calibrated using the characteristic X-rays from metal standards (Cu, Ag, Mo, Ta, Pt, Au, and Pb). The X-ray beam was collimated to 50 μm in the horizontal dimension and 200 μm in the vertical dimension. The diffraction angle was fixed at 5° using a calibration with diffraction lines of Au before the experiments.

High-pressure and high-temperature experiments were performed using a 1500-ton multi-anvil apparatus with a Kawai-type high-pressure vessel. We used tungsten carbide anvils with a truncated edge length (TEL) of 5 mm and 7 mm and MgO + 17% CoO octahedron pressure medium with an edge length of 11 mm and 14 mm, respectively (Fig. 1). Former studies have reported ultrasonic measurements using the TEL of 7 mm, which enable us to measure P- and S-wave velocities up to ~19 GPa and 1673 K [Higo et al., 2008; Irifune et al., 2008]. Here we adopted TEL of 7 mm for the experiments with a V/V_0 range of MgO between 0.92 and 1.00, and that of 5 mm for the experiments with a V/V_0 range of MgO between 0.90 and 0.94. A platinum and rhenium foil tube heaters were used for the experiments with the TEL of 7 mm and 5 mm, respectively (Fig. 1). Temperature was monitored with a W3%Re–W25%Re thermocouple placed at the opposite side of the sample for measuring the temperature comparable to the center position of the sample. $LaCrO_3$ sleeve was used as a thermal insulator, and MgO window was placed in $LaCrO_3$ sleeve for obtaining X-ray image and diffraction of the sample. We used MgO and NaCl sleeves as the sample container to realize a quasi-hydrostatic environment. In order to further reduce the deviatoric stress, we carried out the measurements after heating. It has been reported that the use of NaCl as pressure medium markedly reduces stress on sample [e.g. Wang et al., 1998; Li et al., 1994]. Wang et al. (1998) showed the macroscopic deviatoric stress in NaCl becomes <0.05 GPa at higher temperatures than 773 K. In addition, Li et al. (1994) showed that hot-pressed polycrystalline stishovite surrounded by NaCl became free of residual stress at about 1273 K. Because almost all of our measurements were carried out after heating to 1500 K, we consider that the ultrasonic and in situ X-ray measurements were carried out in a quasi-hydrostatic environment.

Ultrasonic V_p and V_s measurements were conducted using the pulse reflection method. Both P- and S-wave signals were generated and received by a 10°Y-cut $LiNbO_3$ transducer [e.g. Li et al., 2004; Sinelnikov et al., 2004]. A disk shaped $LiNbO_3$ transducer (0.05 mm thickness and 3.2 mm diameter) with a resonant frequency of 60 MHz for P-wave and 40 MHz for S-wave was mounted on the backside of a WC anvil [cf. Higo et al., 2009]. 40 and 60 MHz electrical sine wave with an amplitude of 5 V_{pp} was generated by a waveform generator (Tektronix AWG2021). P- and S-waves generated by the $LiNbO_3$ transducer passed through the WC anvil and propagated into an Al_2O_3 buffer rod and the MgO sample. A series of reflected P- and S-wave signals from the interfaces of anvil/buffer