High-temperature elasticity of polycrystalline orthoenstatite (MgSiO₃)

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**ABSTRACT**

Compressional and shear wave velocities of a polycrystalline specimen of MgSiO₃ orthoenstatite have been measured by ultrasonic interferometry to 1373 K at 300 MPa in an internally heated gas-medium apparatus. The elastic wave velocities and bulk and shear moduli vary linearly with temperature to 1073 K. Below 1073 K, the temperature derivatives of the elastic moduli \([\partial K/\partial T]_P = -28.3(7)\) MPa/K and \([\partial G/\partial T]_T = -14.5(1)\) MPa/K, respectively, determined in this study are consistent with averages of single-crystal elastic constants measured using Brillouin spectroscopy by Jackson et al. (2007). The measured temperature dependence of elastic moduli, along with pressure dependence of elastic moduli, thermal expansion and calorimetric data have been assimilated into a finite-strain equation of state of the type proposed by Stixrude and Lithgow-Bertelloni (2005). This analysis suggests significant revisions to the optimal values of the zero-pressure Grüneisen parameter \(\gamma\) and its zero-pressure logarithmic volume derivative \(q_0\). The unusually high absolute values of \(\partial K/\partial P\) and \(\partial K/\partial T\) are related through the extrinsic part of the temperature derivative. Above 1073 K, a pronounced softening of the elastic wave velocities is observed, which is plausibly associated with a phase transformation for which there is microstructural evidence: The recovered specimen was found to have transformed to the low-pressure clinoenstatite polymorph.

**Keywords:** MgSiO₃ orthoenstatite, elasticity, high temperature, elastic velocity softening, phase transition

**INTRODUCTION**

To interpret seismological models of the Earth’s mantle, we need to know the elastic properties of the candidate mineral phases. From field evidence (e.g., McDonough and Rudnick 1998), the pyroxenes (Ca-poor and -rich), olivine, and garnet are suggested to be the major phases of the upper mantle. In the upper mantle, orthoenstatite, i.e., Ca-poor pyroxene, is thought to be an important phase in the harzburgite or the “depleted” mantle composition (Jordan 1978), which may present an average chemical composition for continental lithosphere. The enstatite component often exhibits an orthorhombic symmetry (space group Pnma, orthoenstatite, OEN) in the mantle specimens, for which the dominant end-members are represented in the formula (Mg,Fe)SiO₃.

Both the Mg-end-member (MgSiO₃) and (Mg,Fe)SiO₃ compositions have been widely investigated for their elastic properties (Frisillo and Barsch 1972; Ito et al. 1977; Webb and Jackson 1993; Flesch et al. 1998; Angel and Jackson 2002; Jackson et al. 2003, 2004, 2007). A key finding from such ultrasonic and X-ray diffraction studies has been the unusually high initial pressure derivative (8–11) of the bulk modulus. Kung et al. (2004) extended the experimental conditions to higher pressures and found that there is a velocity anomaly in MgSiO₃ near 12 GPa. The velocity softening behavior was attributed to a phase transition to a high-pressure polymorph (space group P2₁ca) with a displacive relationship to Pnma (Jahn 2008). A similar observation was made by Jackson et al. (2004) at high temperature (to 1400 K); P and S wave velocities along different crystallographic directions presented strong non-linear behavior at high-temperature regime (above 1000 K). From the MgSiO₃ phase diagram (e.g., Gasparik 1990), the maximum temperature in the study of Jackson et al. (2004) should approach that of the high-temperature phase transformation. It has long been known that MgSiO₃ orthoenstatite transforms into an unquenchable high-temperature phase for which the crystal structure is still in dispute—protoenstatite with orthorhombic symmetry and space group Pnma or high-temperature clinoenstatite with monoclinic symmetry and space group C2/c being observed in most studies (e.g., Smyth 1974; Murakami et al. 1982; Shimobayashi and Kitamura 1993; Yang and Ghose 1995; Ohi et al. 2010). The transition temperature revealed by various studies spans a wide range (reviewed by Jackson et al. 2004, references therein). The single-crystal Brillouin scattering measurements (Jackson et al. 2004, 2007) have provided the temperature derivatives of aggregate properties of orthoenstatite up to 1073 K and selected elastic moduli to 1400 K at ambient pressure.

Recent improvements to the experimental technique for high-temperature MHz ultrasonic interferometry allow measurement up to 1600 K at a confining pressure of 300 MPa (Jackson et al. 2005). The advantage of this technique is access to the aggregate properties by measuring an elastically isotropic polycrystalline specimen—providing ready experimental access to any