Constraints on the \( P-V-T \) equation of state of MgSiO\(_3\) perovskite

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ABSTRACT

Equation of state fits to experimental \( P-V-T \) data were examined by the inversion of synthetic data sets using the thermoelastic parameters of MgSiO\(_3\) perovskite. Our results show that by extending the pressure and temperature range to 130 GPa and 2500 K, the volume dependence of the Gr"uneisen parameter, \( q = \partial \ln \gamma / \partial \ln V \), could be resolved to \( \sim 10\% \) under the best circumstances. However, simulations also showed strong correlation between the bulk modulus, \( K_m \), and its pressure derivative, \( K_m' \), and \( q \) within the currently accepted uncertainty of elastic parameters for MgSiO\(_3\) perovskite. We considered the effect of random error based on the reported uncertainty for different measurement techniques. Even though the laser heated diamond-anvil cell (LHDAC) technique has significantly larger temperature uncertainty, the ability to extend the pressure and temperature ranges allows for improved resolution of higher order thermodynamic parameters. However, systematic error from temperature inhomogeneity in the LHDAC sample could result in overestimation of \( q \). We also performed Birch-Murnaghan-Debye (BMD) equation of state (EOS) fits for currently available data sets. Consistent with the simulation results, combining recent LHDAC (Fiquet et al. 1998) and resistance heated diamond-anvil cell (RHDAC) (Saxena et al. 1999) with lower \( P-T \) measurements (Ross and Hazen 1989; Wang et al. 1994; Utsumi et al. 1995; Funamori et al. 1996) we obtained \( q = 2.0(3) \) and \( \gamma_0 = 1.42(4) \). The difference between \( q = 2.0(3) \) and the normally assumed value of \( q = 1 \) strongly affects calculated values for higher order thermoelastic parameters [e.g., \( \alpha, \partial K_m / \partial T \), and \( \partial K_m' / \partial T \)] as well as first order parameters, such as density and bulk modulus at lower mantle conditions. However, possible systematic error sources need to be further investigated and measurements at higher \( P-T \) conditions promise to yield better constraints on the thermoelastic parameters of MgSiO\(_3\) perovskite.

INTRODUCTION

The lower mantle plays an important role in understanding the dynamics and evolution of the Earth. However, fundamental questions about this region remain unanswered. Recent studies have uncovered new evidence of chemical stratification or heterogeneity in the deep lower mantle (Kellogg et al. 1999; van der Hilst and Kárauson 1999). Tomographic images appear to show subducting slabs penetrating into the lower mantle (van der Hilst et al. 1997), but the ultimate fate of these slabs is uncertain (Kesson et al. 1998; Hirose et al. 1999). The D\(^*\) region at the base of the mantle has been shown to be a region of complex seismic behavior the origin of which is not well understood (Williams et al. 1998).

Due to the lack of direct samples from the lower mantle, seismic observations and laboratory measurements are the only available means to understanding this region. MgSiO\(_3\) perovskite is believed to be the major constituent of the Earth’s lower mantle (Liu 1976; Knittle and Jeanloz 1987; Tomioka and Fujino 1997). Thus, the physical and chemical properties of this material are crucial to understanding those of the lower mantle.

The \( P-V-T \) equation of state (EOS) plays a central role in study of the Earth’s deep interior. Using the EOS, we can calculate the densities and bulk wave velocities of candidate materials at lower mantle \( P-T \) conditions. By fitting the densities and wave velocities to seismic observations, one can test models for the bulk chemistry of the lower mantle (e.g., Stixrude et al. 1992; Wang et al. 1994; Hemley et al. 1992; Bina 1995; Jackson 1998). In addition, the EOS enables us to determine the depth dependence of important thermoelastic parameters such as thermal expansivity and temperature sensitivity of the bulk modulus. The latter is necessary for comparing seismic bulk velocity profiles to laboratory data. The importance of the pressure dependence of thermal expansivity for planetary interiors was recognized early on by O. L. Anderson (1967). Recent work by Anderson and colleagues has provided important insights into thermal expansivity in general, and the thermodynamic properties of MgSiO\(_3\) perovskite in particular (e.g., Anderson et al. 1990; Anderson and Masuda 1994; Anderson et al. 1995; Anderson 1998).

The \( P-V-T \) EOS is obtained by fitting experimentally measured volumes at various \( P-T \) conditions. Static \( P-V-T \) EOS data have been reported using different types of experimental apparatus which cover different \( P-T \) ranges and have different experimental precision. For the large volume press (LVP), typical uncertainties are \( \sim 2-4\% \) for pressure, \( \sim 0.1\% \) for volume, and \( \sim 1\% \) for temperature (Wang et al. 1994; Funamori et al. 1996). Recently, new methods using the diamond cell combined with laser or resistance heating have been used to obtain \( P-V-T \) EOS.