Unified analyses for P-V-T EOS of MgO: A solution for P-scale problems in high P-T experiments

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Periclase (MgO) has no phase transition at least up to 200 GPa and also has the very high melting-temperatures above 3000 K. For the wide stability ranges, various models of P-V-T equation of state (EOS) of MgO have been proposed as internal pressure standards for high-pressure experiments. Within the previously proposed EOS models, an EOS model of Speziale et al. (2001) is popularly used as the pressure-scale in high P-T experiments. However, the EOS model of Speziale et al. not only has problems for reproducing the high-T properties of MgO at 1 atm but also depends on the other pressure-scale proposed for ruby. Therefore, the Speziale et al.'s MgO-scale are less adequate for a primary pressure standard. Here we report unified analyses for various pressure-scale-free data sets to determine a primary P-V-T EOS of MgO applicable to a pressure standard in high P-T experiments.

The unified analyses were carried out for various pressure-scale-free experimental data sets measured at 1 atm-196 GPa and 300-3700 K, which are zero-pressure thermal expansion data, zero-pressure and high-temperature adiabatic bulk modulus (KS) dada, room-temperature and high-pressure KS data, and shock compression data. Several EOS models were tested based on the Mie-Gruneisen-Debye description for the thermal pressures with the Vinet and the third-order Birch-Murnaghan equations for the 300-K isothermal compression. Through least-squares analyses with prerequisite zero-pressure and room-temperature properties of V0, KS0, alpha0, and CP0, we simultaneously optimized K'T0 and gamma(V) required to represent the P-V-T EOS.

Two EOS models were determined in this study with seven parameters. The two EOS models can reproduce all the analyzed data with the total RMS residuals of 0.8 GPa in pressure. Among the several proposals for the EOS model of MgO, only our two models and the model of Wu et al. (2008) are able to reproduce the shock compression data correctly. The two EOS models determined in this study are consistent each other within typical uncertainties in the high P-T experiments to the condition of the Earth's core-mantle boundary. These EOS models are completely independent from other pressure-scales and applicable to primary pressure-calibration standards in high P-T experiments.