

Unified phase transition boundaries of Mg₂SiO₄ polymorphs at the mantle transition region

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Phase transitions of olivine to wadsleyite, ringwoodite, and perovskite (+periclase) have been considered to correspond to major seismic discontinuities in the mantle transition region (410 km, 520 km, 660 km discontinuity, respectively), and these phase transitions play important role in the structure and dynamics of the Earth's mantle transition region. Although a lot of efforts have been made to precisely determine the phase transition boundaries from in situ high-pressure X-ray experiments, it has been noted that the choice of pressure scale strongly influences on the resultant phase transition boundaries. Here we unified the pressure scales of MgO, Au, and NaCl, which were often used in in situ X-ray experiments, based on pressure-scale-independent P-V-T relation of MgO determined by simultaneous ultrasonic and in situ X-ray measurement at both high pressures (up to 23.6 GPa) and high temperatures (up to 1650 K), which are comparable to those of the mantle transition region.

We used unit-cell volume data of Au and NaCl measured simultaneously in the ultrasonic and in situ X-ray measurement of MgO, and compared the pressures determined by pressure-scale-independent method with those estimated from pressure scale proposed by previous studies. We observed almost no difference in the estimated pressures at the pressures below 10 GPa, while the data shows marked variations in the pressures above 10 GPa. Anderson's and Shim's pressure scale of Au yields markedly lower pressure (up to ~1.5 GPa) than that determined by pressure-scale-independent method. In contrast, pressure scale of Au proposed by Tsuchiya (2003) showed good agreement with our pressure scale determined by pressure-scale-independent method. We therefore adopted Tsuchiya's pressure scale to unify high-pressure experimental data obtained using Au as a pressure standard. Pressure scale of NaCl by Decker (1971) and Birch (1986) also showed lower pressure (up to ~1.0 GPa) than those of our pressure scale particularly at higher pressure than ~10 GPa. In order to make unified pressure scale for determining unified phase transition boundary, we fitted our P-V-T data of NaCl into the Mie-Gruneisen equation with the Debye model using a unified formulation proposed by Stixrude and Lithgow-Bertelloni (2005). The data was well fitted with a root-mean-square misfit value of 0.19 GPa, and then we applied this equation-of-state to pressure estimation of high-pressure experimental data observed using NaCl as a pressure standard.

We recalculated olivine-wadsleyite (Morishima et al., 1994; Katsura et al., 2004), wadsleyite-ringwoodite (Suzuki et al., 2000; Inoue et al., 2006), ringwoodite-perovskite (+MgO) (Irifune et al., 1998; Katsura et al., 2003; Fei et al., 2004) transition boundaries of Mg₂SiO₄ obtained by high-pressure in situ X-ray experiments using Au, NaCl, or MgO as a pressure standard. As a result of unification of pressure scale, we observed good agreement among these previous studies. In particular, serious disagreements have been reported among the studies of the ringwoodite-perovskite transition boundaries in Mg₂SiO₄ determined by using Au (Irifune et al., 1998; Katsura et al., 2003) and MgO (Fei et al., 2004) pressure scales. The unified pressure scale yields good agreement in the phase transition boundary between Katsura et al. (2003) and Fei et al. (2004), although recalculated phase transition boundary based on the result of Irifune et al. (1998) shows slightly lower phase transition pressures. The unified ringwoodite-perovskite transition boundaries

in Mg₂SiO₄ locates at ~23 GPa at 1600 °C, which is only marginally lower than that of the 660 km discontinuity.

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