Temperature-pressure-volume equation of state of Mg2SiO4 spinel

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(Mg,Fe)2SiO4 spinel is widely considered to be the most abundant phase in the mantle transition zone. Previosly (Matsui, 1999), we have shown that by combining the molecular dynamics (MD) method with quantum corrections to the MD results, it is possible to simulate very accurately the structural and elastic properties of the olivine, modified-spinel, and spinel forms of Mg2SiO4 over wide temperature and pressure ranges. Here we propose to use the MD simulated T-P-V EOS of Mg2SiO4 spinel as an internal pressure calibration standard at T up to 2000 K, and P up to 25-30 GPa.

The interionic potential is taken to be the sum of pairwise additive Coulomb, van der Waals, and repulsive interactions. In addition, in order to take account of many-body forces in crystals, the breathing shell model (BSM) is used for MD simulation, in which the repulsive radii of O ions are allowed to deform isotropically under the effects of other ions in the crystal. Quantum corrections to the MD pressures are made using the Wigner-Kirlwood expansion of the free energy.

Katsura et al.(2004) have made in situ synchrotron X-ray diffraction experiments of Mg2SiO4 spinel at high temperatures and high pressures with a multi-anvil apparatus(SPEED-Mk.II) at Spring-8. They used the MgO scale by Matsui et al.(2000) for the pressure estimation. In this work we compared in detail the MgO and Mg2SiO4 spinel scales, based on the data by Katsura et al.(2004), and found that the MgO and Mg2SiO4 spinel scales are generally quite consistent at temperatures between 1500 and 2000 K, and pressures between 18 and 23 GPa, with the average differences between the two scales being 0.1 to 0.2 GPa at these temperature and pressure ranges.