The MD simulation of the equation of state of MgO: Application as a pressure calibration standard at high temperature and high pressure

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ABSTRACT

Molecular dynamics (MD) simulation is used to calculate the elastic constants and their temperature and pressure derivatives, and the *T-P-V* equation of state of MgO. The interionic potential is taken to be the sum of pairwise additive Coulomb, van der Waals attraction, and repulsive interactions. In addition, to account for the observed large Cauchy violation of the elastic constants of MgO, the breathing shell model (BSM) is introduced in 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 correction to the MD pressure is made using the Wigner-Kirkwood expansion of the free energy. Required energy parameters, including oxygen breathing parameters, were derived empirically to reproduce the observed molar volume and elastic constants of MgO, and their measured temperature and pressure derivatives as accurately as possible. The MD simulation with BSM is found to be very successful in reproducing accurately the measured molar volumes and individual elastic constants of MgO over a wide temperature and pressure range. The errors in the simulated molar volumes are within 0.3% over the temperature range between 300 and 3000 K at 0 GPa, and within 0.1% over the pressure range from 0 up to 50 GPa at 300 K. The simulated bulk modulus is found to be correct to within 0.7% between 300 and 1800 K at 0 GPa. Here we present the MD simulated *T-P-V* equation of state of MgO as an accurate internal pressure calibration standard at high temperatures and high pressures.