

MD simulated equations of state of the NaCl-B1 and B2 phases

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In high-temperature and high-pressure experiments, known equations of state (EOS) of standard materials, such as NaCl, MgO, and Au are generally used to measure pressure in the systems concerned. However, severe discrepancies are reported between proposed pressure scales especially at high temperatures, and thus critical crosschecks on these pressure scales are strongly required. Here, we use the molecular dynamics (MD) method to simulate accurately the T-P-V EOS of NaCl over wide temperature and pressure ranges. The MD method is particularly useful and powerful for the simulation at high temperatures where anharmonicity of atomic vibrations is important.

The interatomic potential includes pairwise additive Coulomb, van der Waals, and repulsive interactions. In addition, the breathing shell model (BSM) is used for our MD simulation, in which the repulsive radii of Cl ions are allowed to deform isotropically under the effects of other ions. Quantum corrections to the MD results are made using the Wigner-Kirkwood expansion of free energy. Required energy parameters, including the Cl breathing parameters, were derived empirically to reproduce the observed volume, volume thermal expansivity, volume compression, and elasticity data of the B1 phase, as well as the measured volume compression of the B2 phase at room temperature.

The MD simulations with BSM are found to be very successful in reproducing accurately these measured properties of both the B1 and B2 phases over wide temperature and pressure ranges. We present the MD simulated T-P-V EOS of the B2 phase up to 150 GPa, and 3000 K.