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嘱託研究員：松井正典(九州大学・理学部・地球惑星科学科)
受入教官：神崎正美

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Breathing shell model in molecular dynamics simulation: Application to MgO and CaO

M. Matsui
Faculty of Science, Kyushu University

Molecular dynamics (MD) simulation is used to calculate the elastic constants of both MgO and CaO at zero pressure, and their temperature dependencies, as well as the temperature-pressure-volume equation of states of the two oxides. The interionic potential is taken to be the sum of pairwise additive Coulomb, van der Waals, and repulsive interactions. In order to account for the observed large departures from the Cauthy relation of the elastic constants of the two oxides, 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, with each core and breathing shell being linked by a harmonic spring with force constant k. Required energy parameters, including k, were derived empirically to reproduce the observed molar volumes and elastic constants of the two oxides at ambient conditions, and their temperature dependencies as accurately as possible. The MD simulation with BSM is very satisfactory in reproducing accurately not only the observed large Cauthy violations, but also the measured molar volumes and individual elastic constants of the two oxides over wide temperature ranges, at zero pressure. In addition the MD simulation reproduces accurately the measured volume compression data of CaO up to 60 GPa at 300K. Here we present the MD simulated temperature -pressure-volume equation of state of CaO as a useful internal pressure calibration standard at high temperatures and high pressures.