

Lattice dynamics of MgSiO_3 perovskite

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Abstract. A lattice dynamical study of the geophysically important mineral MgSiO_3 in its orthorhombic perovskite phase, with space group Pnma (D_{2h}^{16}) has been carried out using a rigid ion model, with the potential consisting of Coulombic and short-ranged interactions. With the help of program DISPR, the ionic charges and radii were optimized using the equilibrium conditions. The resulting potential model is employed to predict the elastic constants and the phonon dispersion relations. The computed long wavelength optic modes are in good agreement with the corresponding experimental Raman and infrared active bands. The phonon density of states has been obtained and is used to evaluate the specific heat, the mean square displacements and thermal parameters of atoms.

Keywords. Lattice dynamics; MgSiO_3 perovskite; density of states; specific heat; thermal parameters.

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1. Introduction

The perovskite phases of MgSiO_3 and CaSiO_3 are generally accepted as the most abundant minerals in the earth's lower mantle (Reid and Ringwood 1975) and are believed to contribute to the seismic velocity discontinuities in the mantle at the depth of 650 km (Liu 1979). Despite its importance, useful experimental data of various physical properties under geophysically relevant conditions for MgSiO_3 perovskite are generally lacking. Theoretical predictions of the physical properties of this mineral and the variation in these properties with temperature and pressure have therefore aroused considerable interest. Computer simulations of the structure and elastic properties of MgSiO_3 perovskite have been reported by Wall *et al* (1986) and Matsui *et al* (1987). The study of relative stability of some of the possible perovskite polymorphs (Wall *et al* 1986) indicates that the orthorhombic phase is the most stable phase at all but the highest pressures (> 1.5 Mbar) where the cubic phase may be stable. X-ray diffraction measurements of the structure of polycrystalline MgSiO_3 perovskite at 1 Kbar (Yagi *et al* 1978) reveal that it is orthorhombic with space group Pnma . The theoretical study of lattice dynamics and equation of state of cubic perovskite type MgSiO_3 has been carried out by Hemley *et al* (1987); they find that the cubic structure of MgSiO_3 with space group $\text{Pm}3\text{m}$ is dynamically unstable at all pressures, with

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