



ELASTICITY AND WAVE VELOCITIES OF MGSiO₃-PEROVSKITE AT LOWER MANTLE CONDITIONS

R. Wentzcovitch

Department of Chemical Engineering and Materials Science, University of Minnesota,
Minneapolis, MN 55455, USA (wentxcov@cems.umn.edu/Fax: 01-612-626-7246)

The elastic-constants and wave-velocities of MgSiO₃-perovskite (Mg-pv) have been determined throughout the lower mantle's (LM) pressure/temperature (P,T) regime by means of first principles computations of its vibrational density of states at various strained configurations and free energy calculations within the quasi-harmonic approximation (QHA). The latter was tested a posteriori and shown to be valid at expected conditions. This completes the series of calculations of the thermoelastic properties of Mg-pv that are necessary to 1) narrow down constraints on LM's composition and thermal state, 2) shed light on the origin of the 3D-velocity structures, and 3) address temperature effects on the anisotropy of this phase.