

High-pressure thermoelasticity of minerals from first-principles

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I present the recent results on the thermoelastic properties of MgSiO_3 perovskite and MgO , two most abundant minerals in the Earth's lower mantle, at high pressure obtained within the framework of density functional perturbation theory (DFPT) [Karki *et al.*, *Science* 286, 1705, 1999; *Phys. Rev. B* 61, 8793, 2000; *Nature*, submitted, 2000]. In essence, the method exploits the calculated volume dependence of the phonon spectrum to determine the thermal contribution to the crystal's free energy (within the quasi-harmonic approximation), $F(V, T)$, from which all thermodynamical and thermoelastic quantities of interest can be derived [e.g., Wallace, *Thermodynamics of Crystals*, 1972]. These include the thermal expansivity, bulk modulus, heat capacity and entropy. In case of MgO , we also studied the temperature dependence of individual elastic constants at high pressures by calculating phonon dispersion for strained lattices. Our extensive and successful comparison with available experimental data demonstrates that the quasi-harmonic approximation combined with DFPT phonon calculations provides an important theoretical approach for exploring materials properties at the pressure-temperature conditions which are difficult to reproduce in the laboratory. I briefly discuss the geophysical implications of thus predicted mineral properties by comparing them with the seismological observations [e.g., Dziewonski and Anderson, *Phys. Earth. Planet. Int.* 25, 297, 1981; Lay *et al.* *Nature* 392, 461, 1998] towards extracting useful information about the composition, temperature and dynamics of the deep interior.