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Ab-initio determination of high-pressure and high-temperature thermoelastic and thermodynamic properties of low-spin $(Mg_{1-x}Fe_x)O$ ferropericlase with x in the range [0.06, 0.59]

Isacco Scanavino* and Mauro Prencipe

Dipartimento di Scienze della Terra, Università di Torino, Via Valperga Caluso 35, 10125 Torino, Italy

Abstract

In this work, we calculate the thermo-elastic properties of $(Mg_{1-x}Fe_x)O$ ferropericlase, with x in the [0.06, 0.59] range, and the thermodynamic properties of ferropericlase having the specific stoichiometric composition $(Mg_{0.54}Fe_{0.46})O$, at pressures and temperatures, which are those typical of the Earth's lower mantle. We follow an ab-initio quantum-mechanical approach, with the use of the WC1LYP hybrid Hartree-Fock/density functional theory (HF/DFT) functional, within the framework of the quasi-harmonic approximation. Iron is assumed to be in the low-spin configuration, as it proved to be the most stable spin arrangement at the thermo-baric conditions of the deepest lower mantle. The choice of the low-spin configuration, and the use of an ab-initio approach, make this work unique as it is the first time that such a technique is applied for the calculation of the vibrational and thermodynamic properties of the low-spin ferropericlase.

We observe a linear increase of the bulk modulus and a linear decrease of the cell volume as iron content increases. More precisely, for x = 0.46, at ambient condition $K_T = 205.57$ GPa, $K'_T = 4.242$, and $V_T = 72.216$ Å^3; for x = 0.03, at the same conditions, $K_T = 167.42$ GPa, $K'_T = 4.085$, and $V_T = 75.145$ Å^3.

Some thermodynamic parameters and the thermal expansion (C_V, C_P, S, α) for $(Mg_{0.54}Fe_{0.46})O$ are calculated both at ambient condition [$C_V = 36.11$ J/(mol·K), $C_P = 36.38$ J/(mol·K), $S = 26.62$ J/(mol·K), $\alpha = 1.97\times10^{-5}$ K^{-1}], and at simultaneous high-pressure and high-temperature conditions as a function of the geobar and geotherm curves. The data here proposed can be seen as possible bounds to the values of thermoelastic and thermodynamic parameters employed in the construction of geophysical models and the same data could be used to revise the velocity of the seismic waves in the lower mantle.

Keywords: Ferropericlase, lower mantle, thermoelastic properties, thermodynamic properties