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Effects of iron on the thermoelastic properties of MgSiO3 perovskite

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(Mg,Fe)SiO{sub}3{/sub} perovskite is thought to be the most abundant phases in the Earth lower mantle. Mineral physical studies on this phase is therefore of significant importance in investigating structure and dynamics of the Earth deep mantle. However, due to some technical difficulties for the iron-bearing phases, its high-P,T thermodynamics are yet to be well understood both experimentally and theoretically. In particular, all the ab initio studies on (Mg,Fe)SiO{sub}3{/sub} perovskite conducted so far are limited at the static condition in contrast to pure MgSiO{sub}3{/sub}.

Here, we present the results of a computational study on the thermodynamic properties of Fe-bearing MgSiO{sub}3{/sub} perovskite up to 150GPa. We perform density functional calculations beyond conventional methods based on the internally consistent LDA+U technique (Tsuchiya et al., 2006, Phys. Rev. Lett.) to describe local interactions between the d-states in Fe in more appropriately, that give rise to Hubbard splitting. In this study, Fe is incorporated as substitutional single-point defects, which can be present in the different oxidation states (+2 or +3) and different spin states (low or high). We calculate the phonon dispersion relations of the iron-bearing phases based on the direct method, where the force constant matrices are determined by directly applying small but finite atomic displacements, similarly to our previous study in Fe-bearing MgSiO{sub}3{/sub} post-perovskite (Metsue and Tsuchiya, 2011, under review). Then, we determine several important thermodynamic quantities such as the vibrational entropy, free energy, heat capacities, bulk moduli and thermal expansion coefficient within the quasiharmonic approximation. These results are compared to those reported by Tsuchiya et al. (2005, J. Geo. Res.) for pure MgSiO{sub}3{/sub} perovskite. In addition, we show that our results are in good agreement with previous experimental studies on Fe-bearing perovskite (Andrault et al., 2001, EPSL; Lundin et al., 2008, PEPI; Catalli et al., 2010, EPSL). This study points the fact that a low concentration of iron, irrespective of the spin state, affects mainly the low phonon frequency ranges of the perovskite and thus has limited effects on its thermodynamic properties.

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Keywords: perovskite, equation of states, thermodynamic properties, phonon spectra, first-principle calculations