Thermoelasticity of iron- and aluminum-bearing bridgmanite

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We report *ab initio* (LDA + U_{SC}) calculations of thermoelastic properties of iron (ferrous, Fe^{2+}, and ferric, Fe^{3+}) and aluminum Al-bearing bridgmanite ($MgSiO_3$ perovskite), the main Earth forming phase, at relevant pressure and temperature conditions and compositions. Results of aggregate elastic moduli and acoustic velocities for the Mg end-member (x=0) agree very well with the latest high-pressure and high-temperature experimental measurements. In the Fe^{2+}-bearing system, pressure induced lateral displacement of Fe^{2+} reproduces the trend of changes in equation of state parameters observed in recent experimental study, which otherwise were attributed to high- to intermediate spin state crossover. In the case of Fe^{3+}-bearing bridgmanite, the high-spin (S=5/2) to low-spin (S=1/2) crossover of Fe^{3+} in Si-site leads to a significant volume collapse and elastic anomalies across the spin crossover region. The presence of aluminum in Fe^{3+}-bearing system suppresses the elastic anomalies otherwise present in the system. Calculated elastic properties along a lower mantle model geotherm suggest that the elastic behavior of bridgmanite with simultaneous substitution of Fe_2O_3 and Al_2O_3 in equal proportions or with Al_2O_3 in excess should be similar to that of $(Mg,Fe^{2+})SiO_3$ bridgmanite. However, excess of Fe_2O_3 should produce elastic anomalies in the crossover pressure region.