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Ab initio study of structural, elastic and thermodynamic properties of Fe_3S at high pressure: Implications for planetary cores

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Abstract

Using density functional theory electronic structure calculations, the equation of state, thermodynamic and elastic properties, and sound wave velocities of Fe_3S at pressures up to 250 GPa have been determined. Fe_3S is found to be ferromagnetic at ambient conditions but becomes non-magnetic at pressures above 50 GPa. This magnetic transition changes the *c*/*a* ratio leading to more isotropic compressibility, and discontinuities in elastic constants and isotropic sound velocities. Thermal expansion, heat capacity, and Grüneisen parameters are calculated at high pressures and elevated temperatures using the quasiharmonic approximation. We estimate Fe-Fe and Fe-S force constants, which vary with Fe environment, as well as the $^{56}Fe/^{54}Fe$ equilibrium reduced partition function in Fe_3S and compare these results with recently reported experimental values. Finally, our calculations under the conditions of the Earth's inner core allow us to estimate a S content of 2.7 wt% S, assuming the only components of the inner core are Fe and Fe_3S, a linear variation of elastic properties between end-members Fe and Fe_3S, and that Fe_3S is kinetically stable. Possible consequences for the core-mantle boundary of Mars are also discussed.

Keywords: Fe_3S, first-principles calculations, high pressure, thermodynamic properties