Phase stability and thermal equations of state of Fe_3S and Fe_2S polymorphs to Earth's core pressures and high temperatures

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Abstract

The seismologically-determined density profile and dynamics of Earth's iron-rich core can only be explained by incorporating a small but significant light element component such as sulfur. Understanding the phase stability and pressure-temperature-volume relationships of iron-rich sulfides to core conditions is critical for assessing the core's composition. In this *in-situ* X-ray diffraction study, we determined the high *P-T* stability fields of Fe_3S and Fe_2S polymorphs to outer core pressures and high temperatures and fit their thermal equations of state. Between 26 and 140 GPa and at moderate temperatures, a *Pnma* Fe_2S structure coexists with Fe and FeO. Upon heating, below 85 GPa, the *Pnma* Fe_2S phase transitions to $I\bar{4}$ Fe_3S. Above 85 GPa, the *Pnma* Fe_2S phase transitions to a $P\bar{6}2m$ Fe_2S structure at high temperatures. This phase is stable on the liquidus to 142 GPa. We fit thermal equations of state for $I\bar{4}$ Fe_3S and *Pnma* Fe_2S to 75 GPa and 137 GPa respectively and determined the following isothermal bulk moduli (K_0) and pressure derivatives (K_0'): K_0 = 124±2 GPa and K_0' = 5.2±0.1 for Fe_3S and K_0 = 149±11 GPa and K_0' = 5.1±0.3 for Fe_2S. Fe_3S was found to compress isotropically while the *Pnma* Fe_2S phase displayed anisotropic compressibility. Extrapolating the adiabatic density curves of Fe_3S and *Pnma* Fe_2S to outer core conditions, we concluded that 15-18 wt% S is required to account for the density deficit at the core-mantle boundary. Based on the phase relations determined in this study, Fe_2S, not Fe_3S is stable at outer core pressures and high temperatures and could play a critical role in the thermodynamics of Earth's core.