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Phase stability and compression study of $(Fe_{0.89},Ni_{0.11})_3S$ up to pressure of the Earth's core

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Abstract

An in situ synchrotron powder X-ray diffraction study on $(Fe_{0.89},Ni_{0.11})_3S$ was conducted up to 141 GPa and 1590 K. $(Fe_{0.89},Ni_{0.11})_3S$ has a tetragonal structure, which is the same structure as Ni-free Fe_3S. Fitting a third-order Birch-Murnaghan equation of state to data at ambient temperature yielded a bulk modulus of K_0 = 138.1(7.2) GPa and its pressure derivative K_0' = 4.5(3) with a zero pressure volume V_0 = 375.67(4) Å^3. The density of $(Fe_{0.89},Ni_{0.11})_3S$ under the core-mantle boundary condition is 1.7% greater than that of Fe_3S. The axial ratio (*c/a*) of $(Fe_{0.89},Ni_{0.11})_3S$ decreases with increasing pressure. The addition of nickel to Fe_3S leads to a softening of the *c*-axis. Assuming that the nickel content of the outer core is about 5 at%, we estimated 12.3–20.8 at% sulfur in the outer core for the given 6–10% density deficit between the outer core and pure iron at 136 GPa.

Keywords: Earth's core, core-mantle boundary, Fe-FeS system, phase relation, equation of state, laser-heated diamond-anvil cell