

LETTERS

Structure type and bulk modulus of Fe₃S, a new iron-sulfur compound

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ABSTRACT

We performed a series of experiments in the system Fe-FeS at a pressure of 21 GPa and temperatures between 950 and 1400 °C, and we found two new iron-excess iron-sulfur compounds, Fe₃S and Fe₂S, formed at subsolidus temperatures. Powder X-ray diffraction data revealed that Fe₃S has a tetragonal cell, isostructural with Fe₃P (space group $\bar{I}4$). The tetragonal unit-cell dimensions for Fe₃S are $a = 9.144(2)$ Å and $c = 4.509(2)$ Å, with a zero-pressure density of 7.033 g/cm³. Static compression experiments on Fe₃S were carried out in a diamond-anvil cell, using synchrotron X-ray diffraction technique. A least-squares fit to the experimental data at room temperature yielded bulk modulus $K_0 = 170 \pm 8$ GPa with a corresponding pressure derivative $K_0' = 2.6 \pm 0.5$ or $K_0 = 150 \pm 2$ GPa with fixed $K_0' = 4$.