

A cotunnite-type new high-pressure phase of Fe₂S

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ABSTRACT

We examined pressure-induced phase transitions in Fe₂S based on high-pressure and high-temperature X-ray diffraction measurements in a laser-heated diamond-anvil cell. Fe₂S is not stable at ambient pressure but is known to form above 21 GPa with the Fe₂P-type (C22) structure. Our experiments demonstrate a novel phase transition in Fe₂S from the C22 to C23 phase with the Co₂P-type cotunnite structure above ~30 GPa. The experiments also reveal a transformation from the C23 to C37 (Co₂Si-type) phase above ~130 GPa. While the C23 and C37 structures exhibit the same crystallographic symmetry (orthorhombic *Pnma*), the coordination number of sulfur increases from nine in C23 to ten in C37. Such a sequence of pressure-induced phase transitions in Fe₂S, C22 → C23 → C37, are similar to those of Fe₂P, while they are not known in oxides and halogens that often adopt the C23 cotunnite-type structure. The newly found cotunnite-type Fe₂S phase could be present in solid iron cores of planets, including Mars.

Keywords: Iron sulfide, high pressure, high temperature, core, phase transition, cotunnite-type structure, Mars; Physics and Chemistry of Earth's Deep Mantle and Core