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A cotunnite-type new high-pressure phase of Fe_2S

Kenta Oka[1], Shigehiko Tateno[2], Yasuhiro Kuwayama[1], Kei Hirose[1,2,*,§], Yoichi Nakajima[3,†], Koihiro Umemoto[2], Noriyoshi Tsujino[4], and Saori I. Kawaguchi[5,‡]

[1]Department of Earth and Planetary Science, The University of Tokyo, 7-3-1 Hongo, Bunkyo, Tokyo 113-0033, Japan
[2]Earth-Life Science Institute, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro, Tokyo 152-8550, Japan
[3]Department of Physics, Kumamoto University, 2-39-1 Kurokami, Chuo, Kumamoto-shi, Kumamoto 860-8555, Japan
[4]Institute for Planetary Materials, Okayama University, 827 Yamada, Misasa, Tottori 682-0193, Japan
[5]Japan Synchrotron Radiation Research Institute, SPring-8, 1-1-1 Kouto, Sayo, Hyogo 679-5198, Japan

Abstract

We examined pressure-induced phase transitions in Fe_2S based on high-pressure and high-temperature X-ray diffraction measurements in a laser-heated diamond-anvil cell. Fe_2S is not stable at ambient pressure but is known to form above 21 GPa with the Fe_2P-type (C22) structure. Our experiments demonstrate a novel phase transition in Fe_2S from the C22 to C23 phase with the Co_2P-type cotunnite structure above ~30 GPa. The experiments also reveal a transformation from the C23 to C37 (Co_2Si-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 Fe_2S, C22 → C23 → C37, are similar to those of Fe_2P, while they are not known in oxides and halogens that often adopt the C23 cotunnite-type structure. The newly found cotunnite-type Fe_2S 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