

Magnetic transition of FeS at high pressures

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Introduction

The high-pressure behaviour of iron sulfide (FeS) has been investigated by both high-pressure experiments and *ab initio* simulations in many previous studies. Troilite (FeS I) is a stable phase, which was confirmed as the antiferromagnetic mineral, at ambient conditions. With increasing pressure, a structural transition from troilite to the MnP-type structure (FeS II), which is also antiferromagnetic, was observed. The magnetic spin direction of the low-P MnP-type phase is perpendicular to the *b* axis. The next structural transition, accompanied by a disappearance of the magnetic moment, is to a monoclinic structure (FeS III). In this study, the high-pressure phases of iron sulfide were investigated using a laser-heated diamond anvil cell combined with a synchrotron X-ray diffraction method.

Experimental

High-pressure X-ray diffraction experiments were performed using a laser-heated diamond anvil cell high-pressure apparatus. Synthetic powdered FeS were loaded into a 150 μm diameter holes that were drilled into a rhenium gasket. NaCl was used as pressure calibrant [1]. The samples were heated with a laser to overcome any potential kinetic effects on possible phase transitions. The samples were probed using an angle-dispersive X-ray diffraction technique at the synchrotron beam lines BL13A, Photon Factory in Japan [2]. A monochromatic incident X-ray beam was used. The X-ray beams were collimated to a diameter of 15-30 μm , and the angle-dispersive X-ray diffraction patterns were obtained on an imaging plate.

Results and Discussion

The sample was compressed to 60 GPa, and was then heated to 1000-2000 K to relax the differential stress and synthesize a high-pressure phase of FeS. During the heating stage, new diffraction peaks appeared, and these remained stable after the temperature quench. The new peaks could not be indexed using known high-pressure phases of FeS [3]. This indicated that the new high-pressure phase (FeS VI) could be synthesized at 60 GPa and high temperatures. The diffraction peaks of FeS VI were reasonably indexed by MnP-type structure with an orthorhombic symmetry, which is the same as FeS II. As the large volume reduction was observed between FeS II and FeS VI, the magnetic transition is likely to occur without any structural transition. The lattice parameters at 56.3 GPa and 300 K, for example, are $a = 5.153(3)$ \AA , $b = 4.938(4)$ \AA and $c = 3.088(1)$ \AA , with a unit cell volume of

$78.59(9)$ \AA^3 for the orthorhombic cell [3]. The pressure-volume data were used for a least-squares fit of the Birch-Murnaghan equation of state. Accordingly, the data were constrained by fixing K_0' equal to 4. Using all the data for FeS VI, K_0 and V_0 were 156 (6) GPa and 99.5 (7) \AA^3 , respectively. At 40 GPa and room temperature, the relative volume change from FeS III to FeS VI was 1% [3]. The detailed structure of the Martian interior remains an open question because of a lack of observational data. The estimated Martian core pressure is 36-48 GPa. If stoichiometric FeS exists in the Martian core, the stable phase could be FeS V within the outer core. As we discovered the new phase transformation in FeS at 40 GPa, our study indicates that the Martian core may have two layers, with orthorhombic FeS VI possibly occurring at the inner core of the Mars.

References

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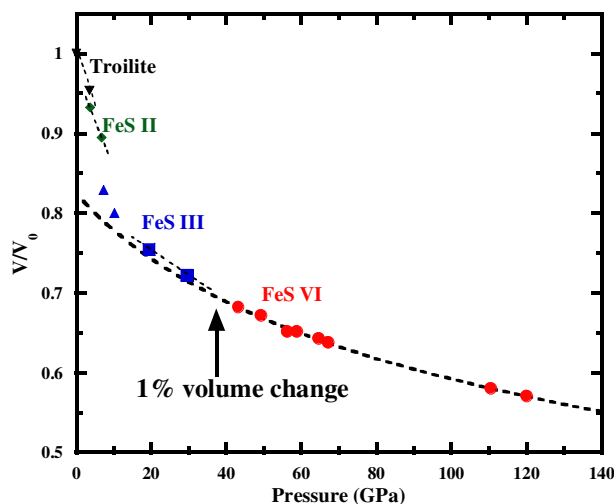


Figure 1. Relative volume of FeS phases as a function of pressure. Abbreviations of symbols are as follows: red circles, orthorhombic phase (FeS VI); blue squares, monoclinic phase (FeS III). Upper and lower triangles and diamonds are volumes of FeS phases from Nelmes et al. [4].