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Phase transitions of FeSi and FeS at high pressures and high temperatures

Shigeaki ONO*[1]
[1] Institute for Research on Earth Evolution (IFREE), Japan Agency for Marine-Earth Science and Technology (JAMSTEC), Yokosuka, Kanagawa 237-0061, Japan

Introduction

Iron silicide and iron sulfide are the probable candidates of the origin of the ultra-low velocity zone at the base of the Earth's mantle, which was reported by seismic studies. Iron-bearing materials may appear at the core-mantle boundary, because the liquid iron coexisting with the solid silicates. In order to understand the reaction between liquid core and the solid mantle, there have been a number of studies for the phase relations of iron-bearing materials. It is known that iron silicide and iron sulfide have some high-pressure forms as pressure increases. However, it has not investigated reasonably by high pressure experiments that what structures are stable at extreme high pressures and high temperatures corresponding to the Earth's core-mantle boundary. In this study, therefore, the high-pressure phases of iron silicate and 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 FeSi and FeS were loaded into a 100 μm diameter holes that were drilled into a rhenium gasket. NaCl was used as pressure calibrant [1]. The samples were heated with a YAG 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 with a wavelength of about 0.42 angstrom 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 (Rigaku).

Results and Discussion

FeSi was compressed up to 67 GPa. A phase transition in FeSi to cubic was observed at 40 GPa after the laser-heating. Before the heating, a strain–broadening of the diffraction peaks of the sample was observed, because a large differential stress was induced in the diamond anvil cell experiments as pressure increased. Next, the sample was heated to about 1500-2000 K to relax the differential stress and to overcome potential kinetic effects on possible phase transitions. After the heating, some new peaks appeared in the diffraction pattern. This implies that the starting material transformed to a new high-pressure phase. The transition pressure could not been determined. The lattice parameters at 41 GPa and 300 K, for example, are a = 2.954(1) Å with a unit cell volume of 25.77(2) Å^3 for the cubic. A pressure-volume relation is shown in Fig. 1. The isothermal bulk modulus of cubic phase was determined to be about 230 GPa. This value is in generally agreement with that predicted by the theoretical calculations reported by previous study.

FeS was compressed up to 110 GPa. Some phase transitions in FeS were observed. Before the heating, a strain–broadening of the diffraction peaks of the sample was also observed. At about 55 GPa, a new orthorhombic phase was observed, after the laser-heating. Next, the sample was compressed to 100 GPa. Some new peaks appeared in the diffraction pattern after the heating. This implies that a new high-pressure phase was stable at pressures higher than 100 GPa. This new high-pressure phase has cubic symmetry.

According to our preliminary results, both iron silicide and iron sulfide have the cubic symmetry at the core-mantle boundary. These materials are likely to contribute to decrease seismic velocities of both Vp and Vs at the base of the lower matnle.

References

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* sono@jamstec.go.jp

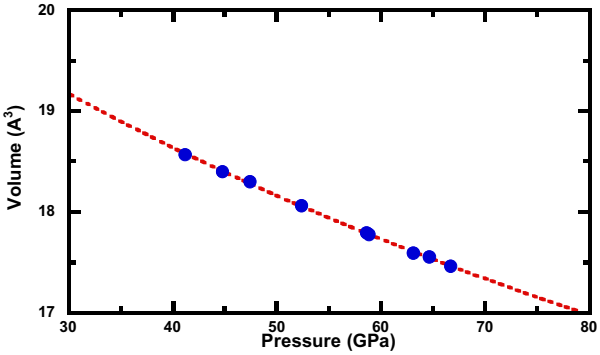

Figure 1. Pressure-volume data for high-pressure phase of iron silicide at 300 K. Circles are volume data of iron silicide. Dashed curves are Birch-Murnaghan equation fits.