Effect of Sulfur on Partitioning between Metallic Fe and MgO

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Introduction

The Earth's core consists of a liquid outer core and a solid inner core,[1] which are believed to be made predominantly of iron (Fe).[2,3] Certain amounts of light elements are believed to exist in the outer core because its density is about 10% less than that of pure Fe under corresponding pressure (P) and temperature (T) conditions.[4] Sulfur (S) is one of the candidates for the light element dissolved into the Earth's core.[5]

Partitioning of Fe and Mg between perovskite and magnesiowüstite has been examined intensively.[6-8] However, the effect of light elements on the partitioning of Fe and Mg has not been examined. We carried out some experiments in the Mg-Fe-O-S system to determine the reaction of metallic Fe with MgO in the presence of S.

Methods and Materials

High P and T *in situ* x-ray diffraction experiments were performed using the 250-ton press installed at the GeoSoilEnviroCARS (GSECARS) 13-BM-D beamline at the Advanced Photon Source (APS), with a double-stage split-cylinder "T-cup" multi-anvil apparatus. *In situ* measurements were carried out based on the energy dispersive method with an energy range of 20-100 keV. Incident x-ray beam size was 100 × 100 μm and diffracted x-rays were detected by a Ge solid-state detector at a fixed diffraction angle of 5.5°.

Figure 1 shows a schematic of the cell assembly, together with a typical X-ray projection. The sample chamber is separated into two layers by a $W_{0.94}Re_{0.06}$-$W_{0.75}Re_{0.25}$ thermocouple. One side is filled with pure Fe as a standard and the other side with a mixture of Fe and FeS. Sulfur contents are controlled by changing FeS to Fe ratio. Both pure and S-containing Fe samples were mixed with MgO to inhibit grain growth. Samples were simultaneously heated by a pair of resistance heaters, which are made of TiC and diamond. Pressure is estimated from the diffraction peaks of MgO using the equation of state.[9]

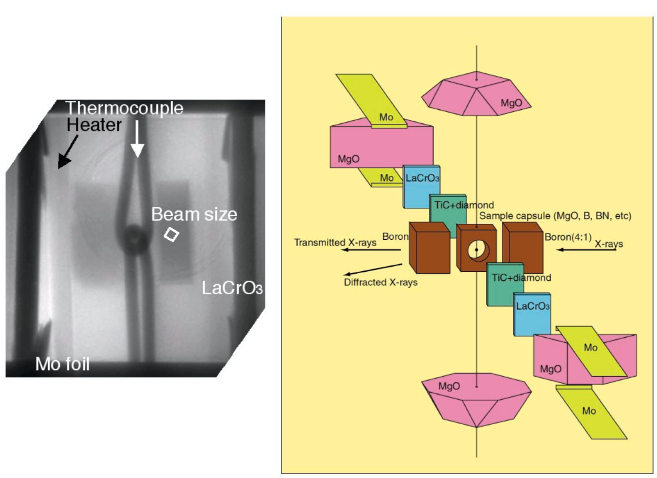

FIG. 1. Schematic sample assembly. Sample capsule is interchangeable depending on sample. A mixture of boron and epoxy resin, and MgO capsules are employed in the present study to examine whether the partitioning is affected by the surrounding capsule materials.

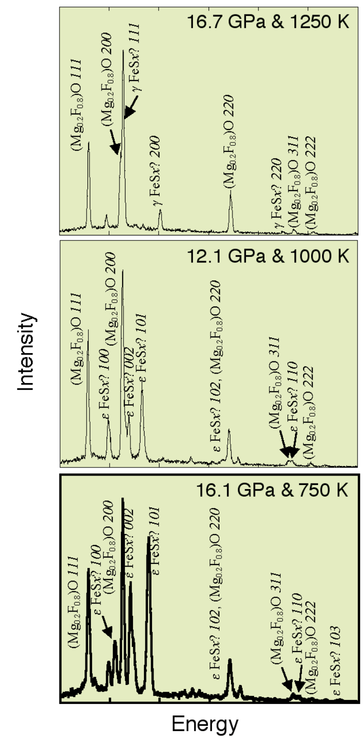

FIG. 2. X-ray diffraction change in the system containing S.

Results and Discussion

Figure 2 shows the x-ray diffraction patterns for the system containing S as a function of P and T. During room-temperature compression, both systems (with and without S) show basically the same pattern because the S content is low and the FeS is mechanically mixed with Fe, without any chemical treatment. At the temperature of 750K, most of Fe peaks start shifting toward lower energy, meaning the lattice parameters are becoming larger due to the reaction between Fe and FeS. At the same time, all of the MgO peaks also start shifting toward lower energy. At around 1000K, the reaction between Fe and FeS is complete and x-ray diffraction shows a simple pattern similar to ε-Fe, but with larger lattice constants. Further heating caused another phase transformation of the sample, showing a pattern similar to γ-Fe. Figure 3 shows the comparison of x-ray diffraction patterns before and after the experiment. On quench, the system containing S shows a similar pattern to the pure Fe system, but all of the peaks have shifted toward a lower energy. Assuming MgO transformed into magnesiowüstite $(Fe_x,Mg_{1-x})O$, we are able to estimate the Fe content x by interpolating the lattice parameter in the linear plot of

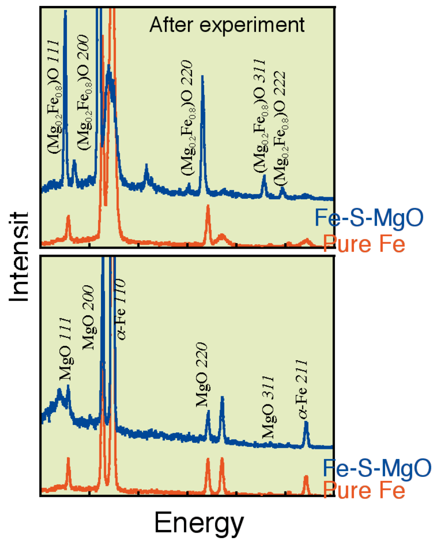

FIG. 3. X-ray diffraction patterns before and after experiment. Dotted lines indicate the position of MgO diffraction peaks for comparison.

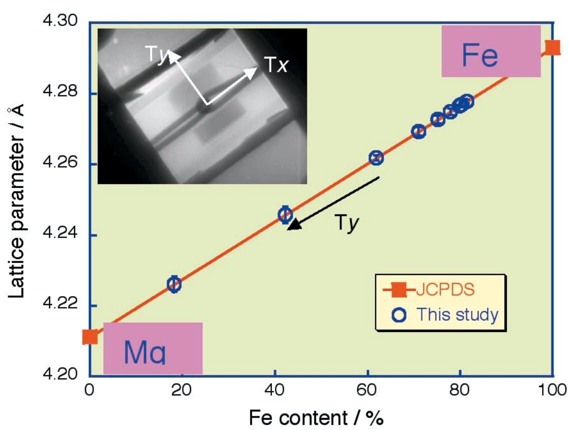

FIG. 4. Lattice parameter of magnesiowüstite as a function of Fe content. Scattering in Fe content is due to the x-ray beam position. At the optimistic beam position, Fe content is estimated to be 80%.

end-member lattice parameters (Fig. 4). The Fe content x was estimated from the plot to be 0.8.

These results suggest that S affects the partitioning between Fe (core) and MgO (mantle), resulting in a decrease in the diameter of the core and an increase in Fe content in the lower mantle.

Acknowledgments

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