Hydrostatic Compression of Fe-Si Alloy

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Introduction

As major constituents of the Earth's core, iron (Fe) and its alloys have long been of great interest to geophysicists [1]. Information on their high-pressure behavior, such as phase relations and equations of state (EOSs), is essential for interpreting seismic and geomagnetic observations and for numerical modeling of the Earth's deep interior. Seismic observations coupled with laboratory research indicate that the density of the outer core and perhaps the inner core is lower than that of pure Fe, which has led to extensive research on possible lower-atomic-weight components in the Earth's core. Silicon (Si) has been suggested as a possible candidate for one of the light elements on the basis of geochemical evidence [2], and previous work has shown than the addition of a modest amount of Si (i.e., as little as 2-4 wt%) to Fe can have a profound effect on the Fe [3].

The EOSs of a number of Fe-Si alloys have been investigated recently [4]. However, the hydrostatic behavior of Fe-rich Fe-Si alloys had not been previously investigated. For the ε-phase, the axial (*c/a*) ratio is measure of configurational changes and is a good indicator of anisotropy. Accurate determination of the *c/a* ratio as a function of pressure is critical for investigating the possible origin of core anisotropy [5]. Hydrostatic measurements provide a better constraint on *c/a* for two reasons. Individual lines are sharper because of the reduced lattice strain, which results in a smaller *d*-spacing error. The effects of preferred orientation are also reduced, so the *00l* lines, which are normally lost in the presence of uniaxial stress, are retained. This allows for the direct determination of *c*. In this article, we report on the results of a study on the compression (to 50 GPa) of Fe with 7.9 wt% Si at room temperature.

Methods and Materials

Powdered samples of Fe with 7.9-wt% Si were loaded into a 200-μm hole that was drilled in a rhenium gasket. A small proportion of powdered platinum (Pt) was mixed with the sample as an internal standard [6]. Ruby chips were added for pressure calibration and to monitor the degree of hydrostaticity [7]. Helium (He) was loaded as the pressure-transmitting medium. Although it solidifies at 11.5 GPa, He remains very soft and is hydrostatic to at least 50 GPa [8].

Experiments were conducted in a symmetric diamond anvil cell. Monochromatic synchrotron x-radiation (λ = 0.3311 Å) focused to a 10 × 30-μm spot at GSECARS beamline station 13-BM-D at the APS was used for angle-dispersive diffraction measurements. Diffraction patterns were taken by using a Bruker charge-coupled device (CCD) detector with between 5- and 10-minute exposure times. Diffraction peaks were fit to Gaussian curves to determine *d*-spacings, which were used to calculate the unit cell parameters. Errors were calculated from the variation in the *d*-spacings. Pressure variation was determined by measuring the ruby pressure before and after each diffraction pattern.

Results

The pressure-volume data (Fig. 1) are shown for the bcc (α) phase and compared to Ref. 3.

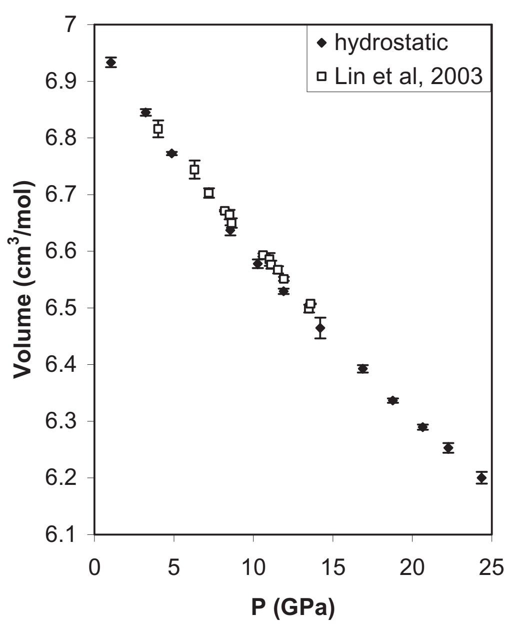

FIG. 1. Volume versus pressure plot for bcc phase of Fe-rich Fe-Si alloy. Hydrostatic results are shown for Fe with 7.9-wt% Si. For comparison, results from Ref. 4 for Fe with 15-wt% Si are shown.

Discussion

An Fe-rich Fe-Si alloy was studied at ambient temperature under hydrostatic conditions to 50 GPa by using *in-situ* x-ray diffraction upon both compression and decompression of the sample. The bcc (α) phase transformed into an hcp (ε) phase over a range of pressures. Hydrostatic measurements give precise determination of the dependence of the c/a ratio in the hcp phase with pressure, which has implications on core anisotropy. Previous studies under nonhydrostatic conditions suggested that Si is an important light element in both the outer and inner core. Extrapolation of our results to core conditions will show whether the density of the Fe-Si alloy studied is within the range of uncertainty in Earth model densities.

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