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## Thermal Expansion of Iron-Rich Alloys and Implications for the Earth's Core

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*Understanding the thermal-chemical state of the Earth's core requires knowledge of the thermal expansion of iron-rich alloys at megabar pressures and high temperatures. We have determined the unit-cell parameters and thermal expansivity of the iron-sulfur compound Fe<sub>3</sub>S by using synchrotron x-ray diffraction techniques and externally heated diamond-anvil cells at pressures up to 42.5 GPa and temperatures up to 900 K. Our data at 42.5 GPa and 900 K suggest that 2.1 atom % sulfur produces 1% density deficit in iron. We have also carried out energy-dispersive x-ray diffraction measurements on pure iron and Fe-Si alloy samples that were placed symmetrically in the same multi-anvil cell assemblies, using the SPring-8 synchrotron facility in Japan. Based on direct comparison of unit cell volumes under presumably identical pressures and temperatures, our data suggest that at most 3.2 atom % silicon is needed to produce 1% density deficit with respect to pure iron.*

The Earth's core makes up nearly one-third of the planet's mass. Its composition, properties, and dynamics are fundamental issues in the study of the Earth's interior. Deeply buried in the center of the planet, the core has kept its chemical composition a long-standing mystery. Cosmochemical studies of meteorites and geochemical analysis of samples from shallower portions of the Earth suggest that the core is made of iron(Fe)-rich alloys containing Ni and one or more lighter elements such as S, Si, C, O, or H. A critical test for any candidate core composition model is that it must be able to reproduce the physical properties of the core. On the basis of observing seismic rays penetrating the deep interior of the Earth and the orbital dynamics of the Earth as a planet in the solar system, models have been constructed to describe the physical state, density profile, and velocity profiles of the Earth's interior. One of the most widely used models is the Preliminary Reference Earth Model (PREM).

To perform the test of consistency between a composition model and the PREM model, we must know the thermal state of the core and the equation-of-state (EOS) of various Fe-rich alloys at the pressure and temperature conditions of the core. A survey of literature revealed a significant lack of thermal expansion data on Fe-rich alloys under static high pressure. In this study, we have determined thermal expansion of Fe<sub>3</sub>S, Fe, and Fe-Si alloys using in-situ synchrotron techniques.

**Figure 1**, left shows an externally heated diamond-anvil cell used to generate high pressures and temperatures. X-ray diffraction data were collected in several compression-heating-quench cycles covering pressures up to 42.5 GPa at 300, 600, and 900 K (**Figure 1b**). The experimental data are fitted by a modified Birch-Murnaghan equation of state for diverse temperatures such that thermoelastic parameters of can be completely derived (**Figure 1, right**). Given 6-10% deficit between the outer core and solid Fe, and 1-3% deficit between the inner core and solid Fe, we estimated 12.5-20.7 atom % S in the outer core and 2.2-6.2 atom % S in the inner core based on our data at the highest experiment pressure and temperature.

We have carried out energy-dispersive x-ray diffraction measurements on pure iron and Fe-Si alloy samples, using the SPring-8 synchrotron facility in Japan. **Figure 2** shows the scanning electron microscope images of

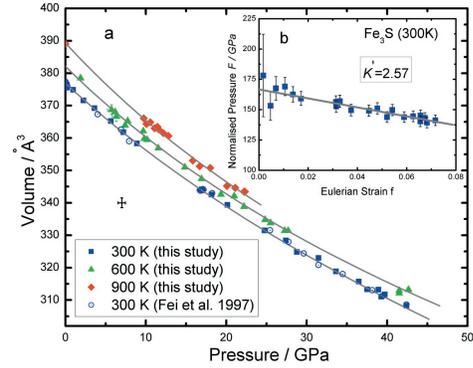
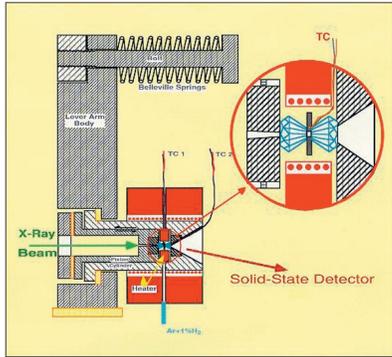


Authors (from left) Bin Chen and Lili Gao

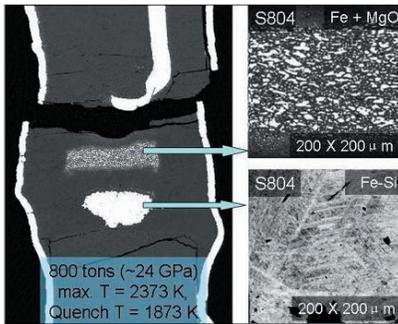
the quenched samples that were placed symmetrically in the same multi-anvil cell assemblies. Our pressure-temperature range covers 21–27 GPa and 300 to 2000 K. Within this pressure range and between 300 and 1,273 K, Fe adopts the hexagonal close-packed (hcp) structure. The starting Fe-Si alloy breaks down to a mixture of

a Si-enriched body-centered cubic phase and a Si-depleted hcp phase, which have been proposed to be the stable forms of Fe-Si alloys in the Earth's inner core. We have derived lattice parameters of pure iron and the Fe-Si alloys. Given 6–10% deficit between the outer core and solid Fe, and 1–3% deficit between the inner core and

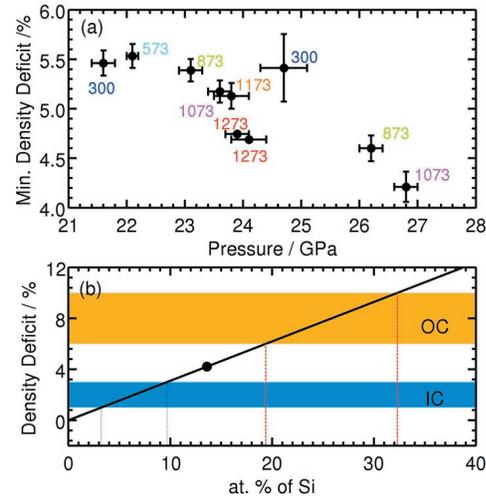
solid Fe, based on a direct comparison of unit cell volumes under presumably identical pressures and temperatures, our experimental data suggest an upper limit of 19–32 atom % Si in the outer core, and an upper limit of 3.2–9.6 atom % Si in the inner core.



**Figure 1.** Left: Experimental setups of an externally heated diamond-anvil cell using in-situ x-ray techniques. Right: Isothermal compression data of  $\text{Fe}_3\text{S}$  at 300, 600, and 900 K. (a) The three lines are the third-order Birch-Murnaghan EOS fits to the compression data. (b)  $f$ - $F$  plot of the compression data at 300 K. The data can be fitted by an inclined straight line, suggesting that the compression of  $\text{Fe}_3\text{S}$  can be adequately described by a third-order Birch-Murnaghan EOS.



**Figure 2.** Scanning Electron Microscopy (SEM) image of the cross-section of the quenched sample from the experimental run S804



**Figure 3.** (a) Minimum density deficit between  $\text{hcp-Fe}_{0.864}\text{Si}_{0.136}$  and  $\text{hcp-Fe}$  under different experimental conditions. Density deficit is defined as the absolute density difference divided by the density of pure iron. Numbers next to symbols denote temperatures in Kelvin. (b) Density deficit versus maximum Si content in Fe-Si alloy with hcp structure. Yellow and blue regions labeled "OC" and "IC" indicate density deficit of the outer and inner core compared with pure Fe, respectively. The filled circle represents the minimum density deficit produced by 13.6 atom % Si, based on data in (a). The solid line represents a linear relationship between density deficit and Si content; dotted and dashed lines enclose the ranges of maximum Si content in the IC and OC, respectively.