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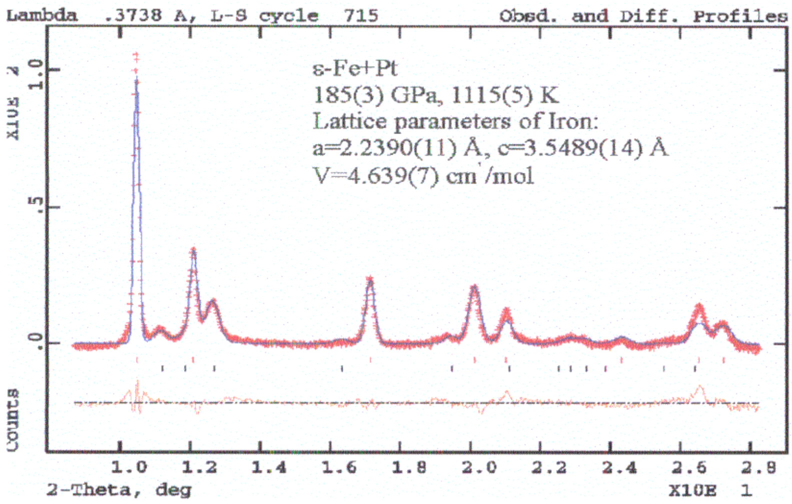
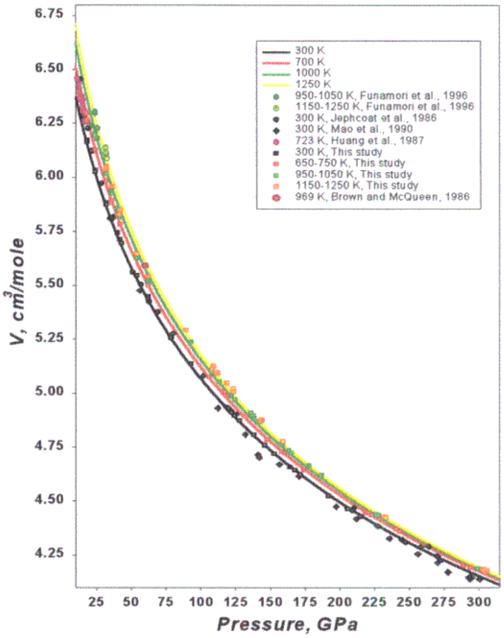
Here we present the results of experiments on X-ray studies of ε-Fe in externally heated diamond anvil cell (DAC) at pressure up to and over 300 GPa and temperatures above 1300 K. By combining the present results with our earlier data (1), we could obtain EOS for iron at multimegabar pressures, estimate density of iron at conditions of Earth's core, and demonstrate that β-Fe with dhcp structure could be synthesised at pressures up to 300 GPa.The experiments were performed on beamline ID 30 at the European Synchrotron Radiation Facility (Grenoble, France). The third generation synchrotrons permit the use of monochromatic radiation to study samples of very small size with area detectors. In our experiments powder diffraction data were collected with fine incident X-ray beam ($8*9\ \mu^2$ or less) of 0.3738 Å wavelength on the FastScan imaging plate.

In one of our experiments, we heated the samples externally in a Mao-Bell type DAC. Powdered samples (iron of 99.999% purity) were loaded into the 30-35 μ initial diameter hole in Re-gasket and then confined between beveled diamonds with 40 μ (50 μ in experiments with maximum pressure 240 GPa) culets. Pressure was determined with powdered platinum (99.999% purity) as an *in situ* X-ray standard mixed in small proportion with the iron sample. The thermal equation of state for platinum has been determined by a first-principles reduction of shock wave compression data to 660 GPa and 2000 K . There is a large body of evidence involving many different materials, both theoretical and experimental, that indicates that the reduction procedure is accurate. In fact, it is likely that platinum scale is accurate to a few percent and is preferable over the secondary ruby scale, which can not be used to measure *in situ* pressures at high temperatures. In our analysis of the integrated x-ray spectra, we used the program GSAS (20) and PeakFit 4.0 (Fig. 1). The lattice parameter of Pt was determined with an accuracy better than 0.002 Å in the whole pressure and temperature range studied in the present work with resulting uncertainty of 2 GPa at pressure up to 100 GPa and of 5 GPa up to 300 GPa according to the equation of state.





We reached a maximum temperature of 1370(5) K at a pressure of 305(5) GPa (Fig. 2). Diamonds failed on further increase in temperature at ~240 GPa in the first experiment, and on heating sample above 310 GPa in the second experiment, but the samples were saved for lattice parameters measurements of both α-Fe and Pt at room conditions.The lattice parameters matched their initial values before experiments within the experimental errors (0.0004 Å) indicating that there was no reaction between Pt and Fe in our experiments.

During heating at different pressures between 135 and 305 GPa, we observed the appearance of new spotty lines at temperature above 1325-1350 K. Such lines could not be due to chemical reaction, because after experiments we lowered temperature and pressure to ambient condition and did not find any diffraction lines except for the lines of α-Fe and Pt. Upon cooling at temperatures below 1250 K, the spotty lines disappeared and only lines of ε-Fe remained. This observation could be explained as due to a reversible transformation of ε to β iron with dhcp structure (1). Detection of β-Fe at pressure above 300 GPa and high temperature means that this phase could form the bulk of Earth's inner core (if no other new phases of iron is found at temperature above 1400 K at high pressure).

In all, 109 data points were collected over the pressure range of 80 to 305 GPa and at temperatures between 300 to 1300 K to determine EOS of ε-iron (data available from authors on request). When combined with our previous data (1) in the pressure range of 18-68 GPa and at temperatures up to 1700 K (79 data points), there is enough information to determine a thermal equation of state of ε-Fe at Earth's core conditions (Fig. 2).

1. S. K. Saxena, L. S. Dubrovinsky, P. Haggkvist, Y. Cerenius, G. Shen, H. K. Mao, *Science*, 269, 1703-1704 (1995); L. S. Dubrovinsky, S. K Saxena, P. Lazor, *Phys. Chem Minerals*, 25, 434-441 (1998); L. S. Dubrovinsky, S. K Saxena, P. Lazor, Geophys Res Lett, 24, 1835-1838 (1997); L. S. Dubrovinsky, S. K Saxena, P. Lazor, Eur. J. Mineral., 10, 43-47 (1998).
2. L. S. Dubrovinsky, S. K. Saxena, F. Tutti, S. Rekhi, T. LeBehan (1999) In situ X-ray Study of Thermal Expansion and Phase Transition of Iron at Multimegabar Pressure (submitted).
3. P. Lazor, S.K. Saxena, L.S. Dubrovinsky, T.Le Bihan, H.P. Weber (1999) Synchrotron X-ray Diffraction of Iron under High Pressure and Temperature (submitted).