ESRF	**Experiment title:** Experimental Study of Some Geophysically Important Iron Based Alloys in the Molten State by in-situ X-ray diffraction at high pressure and high temperature in a large volume press	**Experiment number:** HS-496
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Shifts: 15	**Local contact(s):** Mohamed Mezouar	Received at ESRF:

Names and affiliations of applicants (*indicates experimentalists):

Guyot F!rancois Mineralogie, IPGP, 4 place Jussieu, 75252 Paris cedex 05

Sanloup Chrystèle Sciences de la Terre, ENSL, 46 allée d'Italie, 69364 Lyon cedex 07

Gillet Philippe idem.

Fiquet Guillaume idem.

Martinez Isabelle Isotopes stables, IPGP.

Mezouar Mohamed Experiment division, ESRF

Report:

Here we present *the second set of experiments we performed on metallic liquids* in *the Fe-S system which is appropriate at least to the terrestrial* outer-core and *the martian core. Using a large* volume *press apparatus (Paris-Edinbourg press), the P-T* range *0-5GPa/20-2150°C was explored while high energy X-ray absorption data were collected* in-situ *simultaneously with X-ray diffraction data.*
Equations of state of liquid Fe-S alloys are determined and **appear** *to be strongly dependant upon the sulfur content. Also, diffraction signal collected* in *the liquid state is strong enough to be interpreted in terms* of *interatomic positions (mean distance to the 1st and 2nd* nearest *neighbours).*

PRELIMINARY RESULTS

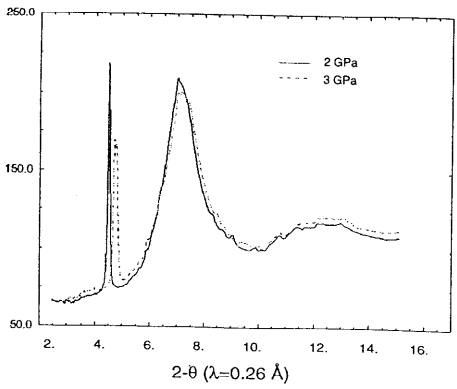
Using a large volume press apparatus (Paris-Edinbourg press), the P-T range O-5 GPa/20-2150°C was explored while high energy X-ray absorption data (λ=0.26Å) were collected in-situ, following the method developped by Katayama [l] for the study of liquid Tellurium; experiments were carried out at the ESRF ID30 synchrotron X-ray beamline..
The pressure and temperature conditions were determined by computing the intersections of the isochoric lines for hBN (hBN cylinder around the sample) and either MgO or Platinum inserted in the cell assembly.
Disappearance of crystalline diffraction peaks allowed a precise determination of the melting point of samples while their density was obtained from the X-ray absorption curve (fig. on the right side, Fe-lO%S, T=1600”C) as X-ray absorption obeys the Beer-Lambert law.

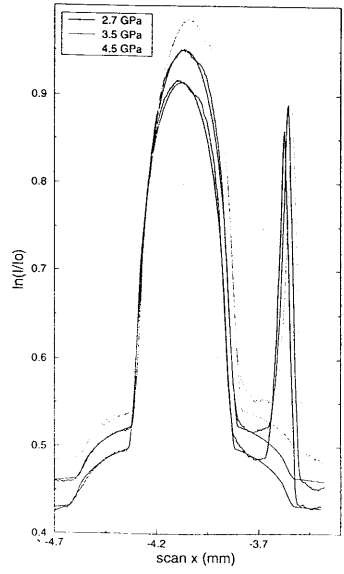
During our first set of experiments (HS-327), liquids were obtained in the Fe-S system by mixing Fe and FeS powders such as to have 25wt% S as expected for the martian core. It appeared that the presence of sulfur dramatically reduced the bulk modulus, K_0, as Nasch et al. [2] already noticed, while conducting an ultrasonic interferometry investigation of molten Fe-5%Ni-lO%S at ambient pressure. Indeed, they obtained a value of 63 GPa for Ko while it is 110 GPa for pure liquid iron, and the value we obtained in these experiments is as low as 36 GPa with 2.5 their amount of sulfur.

During this second set of experiments, liquids were obtained in the Fe-S system for various sulfur contents (lO%S, 2O%S, 27%S and also pure Fe) and at much higher temperatures (up to 2150°C), allowing experiments on pure Fe. The strong dependency of the bulk modulus, K_0, on the S content is confirmed as we measure : $Ko_{10\%S} = 52 \pm 5$GPa (2O%S data processing in progress). As for the Earth, this new result makes sulfur a very improbable candidate for the liquid outer core as its seismically measured bulk modulus is very close to this of pure iron. This is actually not so surprising as silicon is given to be the major light element in the terrestrial outer core by recent geochemical models (7.3wt% Si *vs* 2.3 wt% S in Allegre et al., 1995; 10.3% Si *vs* 2.6% S in Javoy, 1995). Indeed, sulfur is a very volatile element and its abundance in planetary liquid cores is expected to decrease with the distance from the planet to the sun. Sulfur may be the suited light element for more external planets (Mars, galilean satellites) whereas silicon would be the best candidate for the Earth's core. Experiments in the Fe-Si chemical system therefore appear to be the necessary next step.

As mentionned above, we collected simultaneously absorption and diffraction data; in addition to the disappearance of crystalline state, the diffraction data give a first order approximation of the radial distribution function (at least the mean 1st neighbour distance and also the 2nd neighbour distance in pure Fe melts; fig. on the left side). These interatomic mean distances are slightly increasing with temperature and decreasing with higher pressures, while the 1st order effect of sulfur in Fe melts is clearly to increase the structural disorder.

Since such structural informations from X-ray diffraction are quite promising, but require additional confirmation, we hope to explore soon the Fe-S system with a local probe as provided by EXAFS data.





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