



	<b>Experiment title:</b> 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	<b>Experiment number:</b> HS-327
<b>Beamline:</b> ID30	<b>Date of Experiment:</b> from: 10-14-1997                      to: 10-21-1997	<b>Date of Report:</b> February, 24th. 1998
<b>Shifts:</b> 18	<b>Local contact(s):</b> Mohamed Mezouar	<i>Received at ESRF:</i> <b>- 3 MAR. 1998</b>

**Names and affiliations of applicants** (\*indicates experimentalists):

**Guyot François** Minéralogie, IPGP, 4 place Jussieu, 75252 Paris cedex 05

**Sanloup Chrystèle** Sciences de la Terre, ENSL, 46 all&e d'Italie, 69364 Lyon cedex 07

**Gillet Philippe** idem.

**Martinez Isabelle** Isotopes stables, IPGP.

---

**Report:**

*Physical properties of Fe-based liquids are of much interest to better understand both the current state of planetary cores and their formation during the differentiation of planets. Here we present the first experiments we performed on metallic liquids in the Fe-Ni-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 **0-4 GPa/20-1250°C** was explored while high energy X-ray absorption data were collected in-situ.*

*Equations of state of liquid iron alloys are therefore on the way to be determined along with accurate melting phase diagrams as a function of pressure and temperature relevant to geophysical conditions.*

PRELIMINARY RESULTS

Using a large volume press apparatus (Paris-Edinbourg cell), the P-T range 0-4 GPa/20-1250°C was explored while high energy X-ray absorption data ( $\lambda=0.21\text{\AA}$ ) were collected in-situ, following the method developed by Katayama [1] 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  $\gamma\text{Fe}$  just before melting; also, the temperature was calibrated against the power delivery system thanks to these isochoric lines which allowed us to measure an empiric law for T as a function of the input power, and then to extrapolate it to higher temperatures while iron is melted.

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 (figure 1) as X-ray absorption obeys the Beer-Lambert law.

During our first set of experiments, 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 appears that the presence of sulfur dramatically reduces the bulk modulus,  $K_0$ , as Nasch et al. [2] already noticed, while conducting an ultrasonic interferometry investigation of molten Fe-5%Ni-10%S at ambient pressure. Indeed, they obtained a value of 63 GPa for  $K_0$  while it is 110 GPa for pure liquid iron, and the value we obtained in these experiments is as low as 27 GPa with 2.5 their amount of sulfur. This result could be of considerable geophysical and astrophysical importance, if confirmed in our future studies.

As mentioned 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. The 1-D integrated diffraction pattern of liquid 73%Fe-27%S at 3.9 GPa and 1235°C (figure 2) displays a broad peak around 5.5 2- $\theta$  angle, which corresponds to an interatomic distance of 2.1Å for the first-neighbour shell, and we can also distinguish a second but weaker peak around the 10.5 2- $\theta$  angle.

Since these preliminary results are quite promising, we hope to explore soon the Fe-Ni-S system both at higher pressures (up to 8-10 GPa) and for various other compositions.

## References

Y. Katayama (1996) *High Pressure Research*, 14, 383-391.

P.M. Nash (1997) *Science*, 277, 219-221,

