



**Experiment title:**  
**High-pressure and high-temperature X-ray diffraction study of (Mg,Fe)SiO<sub>3</sub> compounds**

**Experiment number:**  
HS133

**Beamline:**  
ID30-BL27

**Date of experiment:**  
from: 28/08/96 to: 04/09/96

**Date of report:**  
19/02/97

**Shifts:**  
18

**Local contact(s):**  
D. Häusermann / M. Kunz

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

**G. Fiquet, A. Dewaele**

Laboratoire de Sciences de la Terre, ENS Lyon, 46 Allée d'Italie, 69364 Lyon cedex

**D. Andrault, T. Charpin**

Département des Géomatériaux, IPG Paris, 4 Place Jussieu, 75252 Paris cedex 05

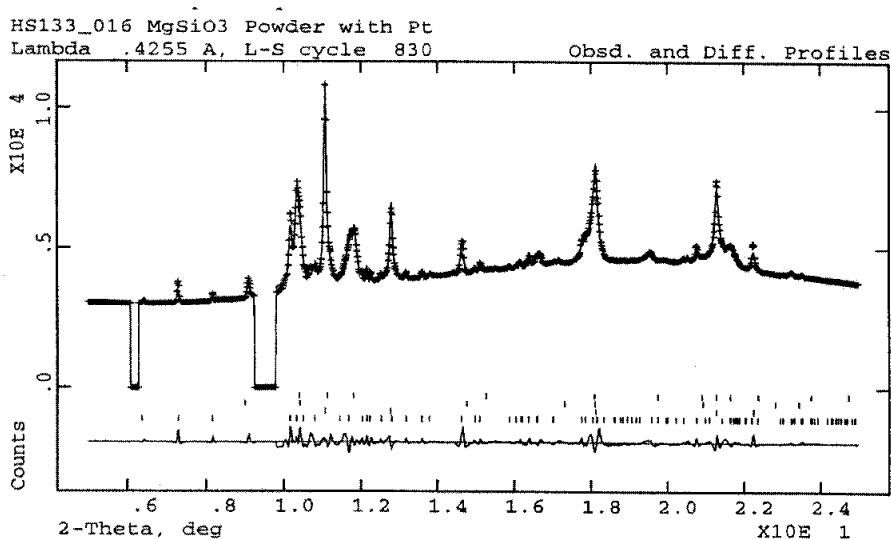
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### **Report:**

Following experiments started at LUKE, DWll (Orsay, France) on MgO (Fiquet et al., 1996) and continued on SiO<sub>2</sub> and Mg<sub>2</sub>SiO<sub>4</sub> polymorphs on ID9, ESRF (Andrault et al., in press), it has been possible to develop an angle-dispersive in situ X-ray diffraction study of MgSiO<sub>3</sub> perovskite in a laser-heated diamond anvil cell. PVT measurements on MgSiO<sub>3</sub> perovskite, currently accepted as the dominant phase of the Earth's lower mantle, have been performed at pressures between 26 and 57 GPa and temperatures up to 2700 K, thus extending the pressure and temperature conditions investigated in only two studies conducted so far in the stability field of the perovskite (Funamori and Yagi, 1993; Funamori et al., 1996) up to 36 Gpa and 2000 K.

In these experiments, we used a CO<sub>2</sub> laser-heating system, well suited to the investigation of the properties of MgSiO<sub>3</sub> samples. Before the tests performed on ID30 in July 1996, all diffraction studies of laser-heated materials under high-pressure were carried out using energy-dispersive diffraction technique, which suffers from an intrinsic detector limited low resolution of about 10<sup>-2</sup> and from very poor crystallite statistics due to the very small volume of reciprocal space covered. For these experiments, a water-cooled channel-cm Si (111) monochromator was used to produce a bright monochromatic X-ray beam at 29 keV from two phased undulators. A monochromatic X-ray focal spot of 10 μm x 20 μm (FWHM) was obtained at the sample location with two single-electrode bimorph mirrors at a wavelength of 0.4255 Å and used in association with image plates to collect data over a 2θ interval from 4 to 25°, thus taking advantage of a diamond anvil cell with a large optical aperture, allowing for in *situ* pressure and temperature measurements and full 4θ angle dispersive data collection.

A series of diffraction pattern (see Fig. 1 for example) could be recorded and analysed with a LeBail refinement procedure using the program package GSAS, thus giving a reliable determination of  $\text{MgSiO}_3$  cell parameters at these pressure and temperature conditions.



**Figure 2** - LeBail profile refinements of a diffraction spectrum of  $\text{MgSiO}_3$  at 30 GPa and 2500 K integrated from an image plate exposed for 15 mn using a monochromatic undulator beam of 29 keV focused to  $10 \times 20 \mu\text{m}^2$ . Sample reflections are mixed with reflections from argon, the pressure transmitting medium, and platinum, the internal pressure calibrant.

The PVT data were analysed in various way, and a set of thermoelastic parameters compatible with previous measurements has been identified within a generalized inversion procedure, in order to obtain new constraints on the compositional model of the Earth's lower mantle. Assuming that the thermoelastic parameters of  $\text{MgSiO}_3$  perovskite are applicable to perovskites with moderate iron content, the comparison of the calculated density profiles for  $(\text{Mg}_{0.9}\text{Fe}_{0.1})\text{SiO}_3$  composition with the PREM density distribution of the lower mantle indicates that a pyrolite composition with a relatively low amount of magnesiowüstite may satisfy the density of a PREM model as well as a pure perovskite composition (Fiquet et al., submitted).

### References

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