



	Experiment title: Acoustic phonons and optical modes in iron at high-pressure	Experiment number: HS1502
Beamline: ID28	Date of experiment: from: 28/04/01 to: 09/05/01	Date of report: 18/07/2001
Shifts: 30	Local contact(s): H. Requardt	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): G. Fiquet* Laboratoire de Minéralogie et Cristallographie J. Badro* Université Pierre et Marie Curie – UMR CNRS 7590 F. Guyot* 4 Place Jussieu 75252 Paris cedex 05 cedex France H. Requardt* A. Mermet* ID28 ESRF BP220 38043 Grenoble cedex France M. Krisch*		

Report:

Physical properties of iron are needed to better understand both the current state of planetary cores and their formation during the differentiation of planets. The knowledge of the elastic constants of the different phases of iron, which makes up 70-90 wt% of planetary cores, is essential for comparison with global seismic models of the Earth, which provide acoustic wave velocity profiles. In this proposal, we were planning to extend measurements previously carried out on the dispersion of longitudinal acoustic phonons of iron at high pressure [1] to transverse acoustic modes as well as optical modes. The integration of these dispersion curves over all Q -space would have provided the phonon density of states (DOS), from which thermodynamic parameters such as vibrational kinetic energy, heat capacities and Debye temperature of hcp iron can be derived as a function of pressure.

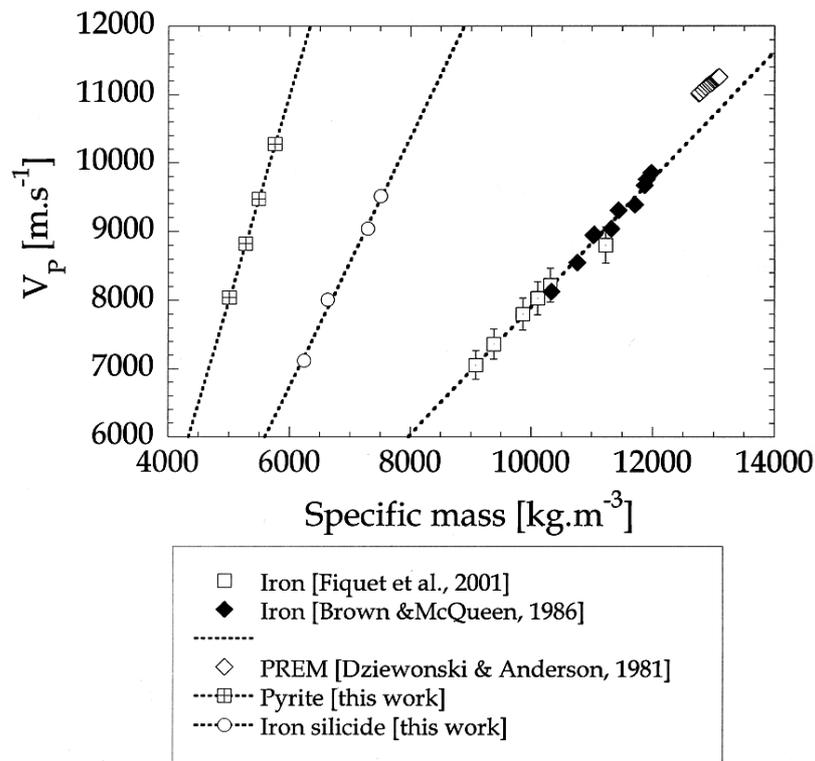
Unfortunately, these expectations could not be met:

(1) in addition to the (LA) phonon branch that could be clearly observed over the whole momentum and pressure range explored, additional features were detected between the quasi-elastic line and the (LA) phonon of iron. Wave velocities derived from the energy position of these excitations strongly suggest that they correspond to the transverse acoustic (TA) phonon of iron. The (TA) phonons, however, have been detected at 2 or 3 momentum transfers at two pressures only, precluding any further attempt to derive the pressure dependence of shear velocities. These excitations appear to be weaker than the ones related to transverse phonons, which makes their analysis difficult.

(2) attempts to map optical modes have been unsuccessful: signal associated with such excitations is indeed one order of magnitude smaller than that of acoustic modes. When detected at large Q values (close to the

edge of the first Brillouin zone), these excitations are close to the longitudinal acoustic ones which makes interpretation even more complicated.

As a backup experiment, we decided to carry out an inelastic x-ray scattering study on different iron alloys at high pressure. For the past forty years, there has been considerable debate about which light element among sulfur, silicon, oxygen, carbon or hydrogen is in the Earth's core [2]. In this report, we bring new constraints on the behaviour of sulfur and silicon alloyed with iron. Samples of iron silicide (FeSi) and pyrite (FeS₂) have been compressed in a diamond anvil cell and IXS pattern have been recorded as pressure was increased to about 50 GPa. In the meantime, X-ray diffraction patterns were recorded at each pressure step to derive the molar volume, hence the sample density. As shown in the figure below, the Birch's law (*i.e.* a linear dependence of longitudinal acoustic velocity as a function of density) seems to hold for these compounds as it is the case for iron.



These preliminary measurements represent the first direct determination of sound velocities for these compounds at high-pressure. It is obvious from the figure above that elements such as silicon or sulfur drastically change the elastic behaviour compared to that of pure hcp iron. Assuming an ideal solid solutions between pure iron and FeSi, or FeS₂, such data can bring strong constraints on the inner core composition. The confidence in the extrapolation to higher pressure however relies on the Birch's relationship validity at higher densities. These measurements have thus to be extended to higher pressures, to verify if the Birch law is still valid and if no structural changes can be detected.

[1] G. Fiquet, J. Badro, F. Guyot, H. Requardt, M. Krisch, Sound velocities in iron to megabar pressures, *Science* **291**, 468-471 (2001)
 [2] J.P. Poirier, Light element in the outer core – a critical review, *Phys. Earth Planet. Int.* **85**, 319-337 (1994)