ESRF	**Experiment title:** Structural study of dense water and dense fluid oxygen in a diamond anvil cell	**Experiment number**: HS1842
Beamline: ID09	**Date of experiment**: from: 13/06/02 to: 18/06/02	**Date of report**: 20/08/02
Shifts: 15	**Local contact(s)**: M. Hamfland	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

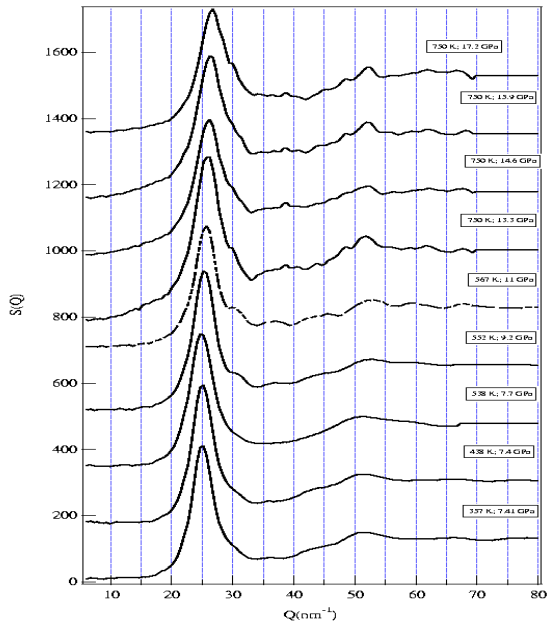
Weck Gunnar, CEA/DAM Bruyères-le-Chatel, France.
Benedetti Laura, CEA/DAM Bruyères-le-Chatel, France.
Sihachakr Davina, CEA/DAM Bruyères-le-Chatel, France.
Eggert Jon, Lawrence Livermore National Laboratory, Livermore, California.

Report:

The structure factor of fluid oxygen under high pressure and high temperature has been measured by X-ray diffraction on the ID09 beamline. The aim of the experiment was to obtain pair correlation functions of fluid oxygen for pressures and temperatures above the ε–β-fluid triple point (16.6 GPa, 640 K). It was also to show that we could provide accurate S(Q) for light elements in a pressure and temperature range of 30 GPa and 1000 K respectively.

Experimental method
Three samples of liquid oxygen have been loaded in membrane diamond anvil cells with large X-ray aperture ($2\theta_{max}$ = +/-37°, φ = 360°). Local heating onto the sample chamber was obtained by using a resistive gasket. Finally, the cell was inserted into a vacuum chamber in order to prevent any damage of the diamond anvil. Pressure was measured by using several pressure scales (ruby, $SrB_4O_7:Sm^{2+}$, gold) [1,2]. We performed angle dispersive diffraction with a monochromatic beam of energy E = 33 keV. This energy, combined to the X-ray aperture of the cell, allowed us to reach the maximum momentum transfer of $Q_{max} = 4\ \pi\ \sin\theta/\lambda\ \sim 100\ nm^{-1}$. The X-ray spectra were collected with an on-line image-plate detector (MAR3450). The beam was focused to 20 μm in diameter.

Results
Diffraction measurements were performed for different pressures along two isotherms at 550 K and 750 K. For both isotherms we reached the solid phase, at respectively 12 GPa and 25 GPa, in order to take a reference spectra. The X-ray data are analysed using an iterative procedure developed by our group during previous experiments on liquids [3]. Despite the signal weakness, we can obtain good quality structure factors of dense oxygen fluid for the data at 550 K (see fig. 1). At 750 K, the signal degrades rapidly with pressure due to the decrease of the sample thickness.



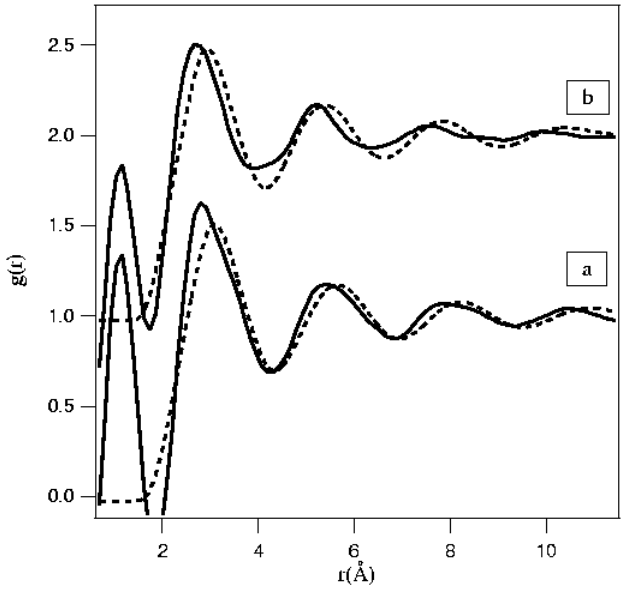


Figure 1 (left): Structure factors S(Q)) for oxygen fluid at several pressures and temperatures.

Figure 2 (right) : Comparison between experimental (continuous line) and theoritical g(r) (dashed line); (a): P = 9.2 GPa, T = 550 K; (b): P = 17.2 GPa, T = 750 K

We also performed classical molecular dynamic simulation using an exp-6 pair potential adjusted to the shock waves data [4]. The comparison between experimental and simulated g(r) show that the first neighbour distance is smaller in the case of the experiment (see fig. 2 and fig. 3). The approximation of a spherical potential is then no more valid to reproduce the structural data at high density. This highlights the anisotropy of the intermolecular interaction. Finally no evidence of the formation of O_4 molecule is observed in the fluid.

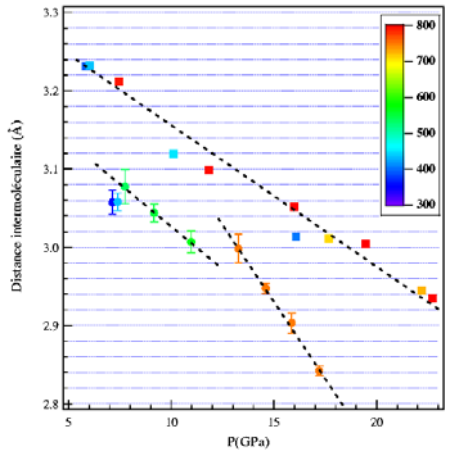


Figure 3: Evolution of the first neighboor distance with pressure; circle: experiment; square: simulation. The dashed line is a guide for the eyes.

Reference

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[4] M. Ross, F. H. Ree, J. Chem. Phys., **73**, 6146 (1980)