EXPERIMENTAL REPORT
RAPPORT D'EXPERIENCE

Programme Committee Proposal Number
N° Projet Comité de Programme

PROJECT TITLE : *TITRE DU PROJET :*

Absorption and anomalous scattering of X-rays in levitated liquid yttria

LIGNE :	**D2AM**		**I F**	
INSTRUMENT :	PETITS ANGLES	☐	EXAFS	☐
	7 CERCLES	☒	G M	☐
	F I P	☐	S U V	☐

NUMBER OF RUNS USED
NOMBRE DE SESSIONS EFFECTUEES : **21**

STARTING DATE
DATE DE DEMARRAGE : **May, 10 2001**

AUTHORS : *AUTEURS :* **L. Hennet D. Thiaudière, C. Landron, M. L. Saboungi, J.F. Berar, D. L. Price**

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In a general study on the Al_2O_3-Y_2O_3 phase diagram, we have studied the structure of liquid Y_2O_3 at 2500°C using anomalous scattering near the yttrium K absorption edge (17036). The melting point was achieved using aerodynamic levitation and laser heating. The analysis chamber, designed for working on the 7-circle goniometer of the D2AM station, enables combined X-ray absorption and diffraction measurements. The first results obtained are in good agreement with molecular dynamics simulations and provide values for the different distances Y-O, O-O and Y-Y.

Yttrium and aluminum oxide mixtures produce some technologically important phases such as YAG (yttrium aluminum garnet : $Y_3Al_5O_{12}$), YAP (yttrium aluminum perovskite : $YAlO_3$) and YAM (yttrium aluminum monoclinic : $Y_4Al_2O_9$), with interesting mechanical and optical properties. In order to understand the structural properties of these compounds, it is necessary to study each side of the phase diagram Al_2O_3-Y_2O_3.
Different studies have been reported on the structure of liquid alumina using X-ray scattering[1], neutron scattering[2] and molecular dynamics simulations[3].
Yttrium oxide (Y_2O_3) is extremely refractory with a melting point of 2458°C, higher than aluminum oxide (2054°C) and there are only a few studies on the liquid state. Krishnan et al[4] have reported the first measurement of the total X-ray structure factor and the corresponding pair correlation function of liquid yttrium oxide and based on these results, molecular dynamics simulations have been performed[5].

In order to complete these studies, we have performed anomalous X-ray scattering on levitated yttria near the yttrium K absorption edge (17036eV).

A high temperature chamber was mounted on the center of the D2AM 7-circles goniometer. The working principle of this device is described detail elsewhere[6]. The spherical sample (with a diameter around 2.6mm) was situated on a levitator in the center of the chamber. This device contains a nozzle for diffusion of a gas jet below the sample. During the experiment, we have used a gas mixture argon/oxygen (3.5%). The gas flow was regulated with a microprocessor-controlled mass flow controller. This enables the sphere to remain in a stable position (to within 50µm), without any contact with the nozzle.
The heating system consisted of a continuous 125W CO_2 laser operating at a wavelength of 10.6µm. The primary laser beam with a diameter of approximately 5 mm was focused on the sample using mirrors in order to

obtain a final diameter of about 1mm at the sample position. Good optical alignment was ensured by the use of a red (diode) laser beam co-linear with the invisible CO2 laser beam.
X-rays scattering measurements were performed using a NaI detector and an analyzing crystal (graphite).
For each sample, we performed separate measurements on liquid Y_2O_3 (2500°C) at 16750eV (about 280eV below the yttrium absorption edge) and at 17010 (just below the edge). In this report, we present the first calculations performed on the data.

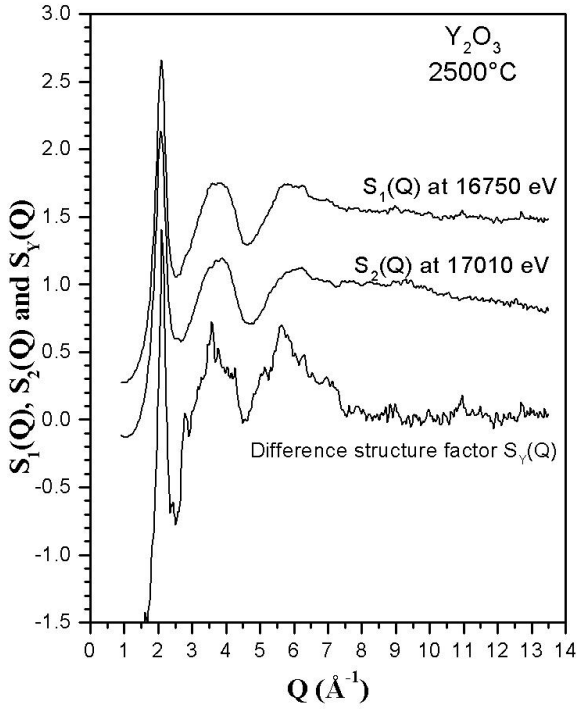

Figure 1
X-ray structure factor of Y_2O_3 measured at 16750 (S_1) and 17010 eV (S_2) and difference structure factor (S_Y)

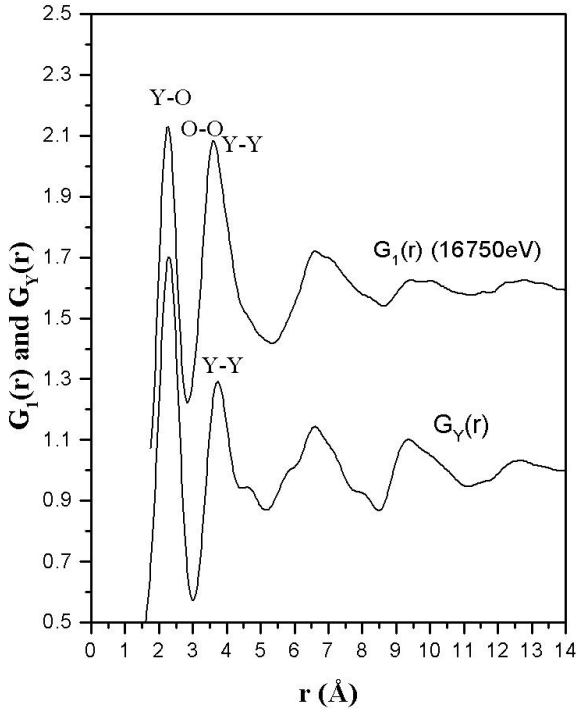

Figure 2
Pair correlation function of Y_2O_3 at 16750 (G_1)and yttrium difference pair correlation function (G_Y)

In Figure 1, we show the total x-ray structure factors $S_1(Q)$ and $S_2(Q)$ obtained at the two energies (respectively at 16750 and 17010eV) and the resulting difference structure factor $S_Y(Q)$.
The total pair correlation function $G_1(r)$ at 16750eV and the difference pair correlation function, $G_Y(r)$, are shown in figure 2. Putting the appropriate weighting factors we get for $G_1(r)$ and $G_Y(r)$:

$$G_1(Q) = 0.557G_{Y\text{-}Y} + 0.379G_{Y\text{-}O} + 0.064G_{O\text{-}O}$$
$$G_Y(Q)= 0.735G_{Y\text{-}Y} + 0.265G_{Y\text{-}O}$$

The major peaks in $G_1(r)$ occur at about 2.26Å, 3.67Å, 6.77Å, 9.75Å and 12.9Å. these results are in a good agreement with the molecular dynamics simulations[5]
The first peak in the liquid $G_1(r)$ arises from Y–O nearest-neighbour pairs, while the second peak at 3.67Å is a combination of O-O and Y-Y correlations. In $G_Y(r)$ the second peak is only due to Y-Y pairs and is position is around 3.74Å. Combining these results, we find a distance O-O around 3.06Å.
More results, especially on the coordination numbers, will be obtained with a precise analysis of all the data and by comparing with our recent neutron diffraction experiments on liquid Y_2O_3.

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