EUROPEAN SYNCHROTRON RADIATION FACILITY

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ESRF

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

http://193.49.43.2:8080/smis/servlet/UserUtils?start

Reports supporting requests for additional beam time

Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title: Studies of Structural, Magnetic, and Electronic States of Mott Insulators at High Pressures**	**Experiment number**: HS1212
Beamline: ID30	**Date of experiment**: from: 26.04.00 to: 1.05.00	**Date of report**:
Shifts: 15	**Local contact(s)**: T. Le Bihan	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

G. Kh. Rozenberg, L. S. Dubrovinsky, M. P. Pasternak, O. Naaman, T. Le Bihan, and R. Ahuja, High Pressure Structural Studies of Hematite (Fe_2O_3), submitted to Phys. Rev. B

ABSTRACT

Structural studies and full-profile refinement of the high-pressure phases of hematite (Fe_2O_3) were carried out to 76 GPa using X-ray synchrotron powder diffraction. It was found that pressure induces a progressive distortion of the corundum-like hematite structure (HP1) culminating into a structural phase transition (HP2) at ~50 GPa. At first sight the powder diffraction data obtained for HP2 could be equally explained in terms of either an orthorhombic perovskite or a Rh_2O_3(II)-type structure but recent Mössbauer spectroscopy results, comparative analysis of the O-O bond length for both structures, and *ab initio* calculations allowed for the unambiguous assignment of the HP2 phase to the Rh_2O_3(II)-type structure. As a result of the phase transition the following changes are observed: *i*) a

substantial decrease in the Fe-O distances with a slight increase in Fe-Fe distances which led to a reduced cell-volume, *ii*) a diminution of the Fe-O-Fe bond distortion, and, *iii*) reduction in the distortion of the FeO_6 octahedron. The structural transition coincides with a previously reported insulator-metal transition due to a *Mott* transition. It is suggested that the unusual volume reduction of 10% is accounted by the combined crystallographic *and* electronic (*Mott*) phase transition, the latter resulting into a substantial reduction in the ionic radii due to electron delocalization. The mechanism of the combined transition is discussed.

W. M. Xu, O. Naaman, G. Kh. Rozenberg, M. P. Pasternak, and R. D. Taylor, Pressure-Induced Breakdown of a Correlated System; the Progressive Collapse of the *Mott-Hubbard* State in *R*FeO$_3$, submitted to Phys. Rev. B

Abstract

Mössbauer spectroscopy (MS), Resistance, and XRD methods and using diamond anvil cells were combined to study the pressure-induced breakdown of the correlated perovskite systems $RFe^{3+}O_3$ (*R*=La, Pr). Following a 3% volume contraction at ~30 GPa in both oxides, an orthorhombic → tetragonal transformation is observed for the $LaFeO_3$ whereas the high pressure (HP) Pr oxide remains orthorhombic. The EOS of both HP and low-pressure (LP) phases were determined from which it was concluded that the compressibility of the $LaFeO_3$ HP phase is considerably larger than that of $PrFeO_3$. The HP phases at $P < 60$ GPa are characterized by the coexistence with equal abundance of *high*-spin ($S = 5/2$) and *low* spin ($S = 1/2$) sublattices of Fe^{3+} moments. With pressure increase a gradual *high* to *low*-spin transition is observed, fully converting to a $S=1/2$ state at ~60 and ~70 GPa for the La and Pr cases, respectively. For $PrFeO_3$up to 90 GPa, the highest pressure reached with MS, and for $LaFeO_3$ between 70 -120 GPa a *magnetic spin relaxation* spectra prevail suggesting that a magnetic exchange regime is still present, coinciding with a drastic decrease in the resistance. The presence of *paramagnetic relaxation* between 120 - 170 GPa in $LaFeO_3$ concur with the onset of a “metal with moments” as evidenced by R(P,T) studies. Detailed analysis of the magnetic interactions is presented.