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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 via the User Portal:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Reports supporting requests for additional beam time

Reports can 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:** **A new scenario of the Mott transition - two-stage correlation breakdown in $MFe^{3+}O_3$ (M = Fe, Al, B)**	**Experiment number**: **HC-1887**
Beamline: ID09A	**Date of experiment**: from: 25.06.2015 to: 29.06.2015	**Date of report**:
Shifts: 12	**Local contact(s)**: **Dr. Michael Hanfland**	*Received at ESRF:*

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Report:

A part of the obtained results related to the study of Fe_2O_3, hematite, has been submitted as a report to Phys. Rev. Lett.:

E. Greenberg, G. Kh. Rozenberg, E. Bykova, W. Xu, M. P. Pasternak, L. Dubrovinsky, Z. Konopkova, H.-P. Liermann, and M. Hanfland, *Multi-stage correlation breakdown in Fe_2O_3 – a new scenario of the Mott transition.*

ABSTRACT

Electronic and structural properties of Fe_2O_3 have been studied at pressures up to 100 GPa combining ^{57}Fe Mössbauer spectroscopy, single crystal and powder synchrotron x-ray diffraction. In contrast to the classical case of the MT, leading to an insulator to metal transition concurrent with a complete collapse of magnetism, in Fe_2O_3 we have discovered *a new scenario* of Mott transition (MT) characterized by a *multi-stage correlation breakdown.* At the first stage of the transition at ~50 GPa hematite transforms into a double-perovskite

(DPv) structure; immediately following, a correlation breakdown on the octahedral sites of the DPv phase results in an insulator to metal transition and a collapse of magnetic moments on only half of the Fe-sites. Above 60 GPa the abundance of Fe^{3+} in the high-spin state starts to decrease, indicating further propagation of the correlation breakdown process. Finally, another structural transition occurs at ~ 68 GPa into an orthorhombic phase with a single Fe site concurrent with complete collapse of magnetism signifying the concluding stage of the correlation breakdown. A similar scenario of MT could be expected for many structurally complex strongly correlated systems.

We have also performed powder XRD studies of $BFeO_3$ and $AlFeO_3$ up to 116 and 98 GPa, respectively. He or Ne were used as pressure medium. Based on a preliminary analysis of the obtained XRD data we have established that $BFeO_3$ does not change the space group ($R\bar{3}c$) up to 116 GPa, the highest pressure measured. Similar to previous observations [1], an isostructural volume decrease of ~8% was observed at around 55 GPa coinciding with the drastic change of the magnetic properties. It is noteworthy, that also above this isostructural transition, the structure of $BFeO_3$ is characterized by a single Fe site. Meanwhile, our low-temperature Mössbauer data reveals two electronic sites of Fe: one –HS with significantly reduced T_N and another one – with no sign of a magnetic interaction down to 5 K. Undoubtedely an analysis of the pressure evolution of interatomic distances and bond angles may help to resolve this controversy. Such information could be obtained from single crystal XRD data.

In contrast to $BFeO_3$, powder XRD studies of $AlFeO_3$ revealed two structural phase transitions at the pressure range 17-80 GPa (Fig. 1). The first one starts at ~23 GPa and is completed around 40 GPa. The main features of this transition is the splitting of the peaks of the low-pressure (LP) phase (e.g. the peak at $2\Theta \sim 10°$ splits and shoulders are present around some other peaks). This indicates a gradual distortion of the LP structure, as the symmetry seems to change from orthorhombic to monoclinic. The refinement of the cell edge is difficult due to the strong overlap of the peaks that causes a strong correlation between the cell edge parameters. At 47 GPa some new peaks appear in the diffraction patterns and the peaks of the previous phase decrease gradually in intensity and finally are no more present at

69 GPa indicating that the transformation is complete. The features of this transformation clearly suggest a first order phase transition, but since the peaks are quite broad it is not trivial to identify the structure of the HP polymorph, and requires further analysis, and perhaps single-crystal diffraction measurements.

We belive that an additional single-crystal XRD study may help to solve the problems described for both materials.

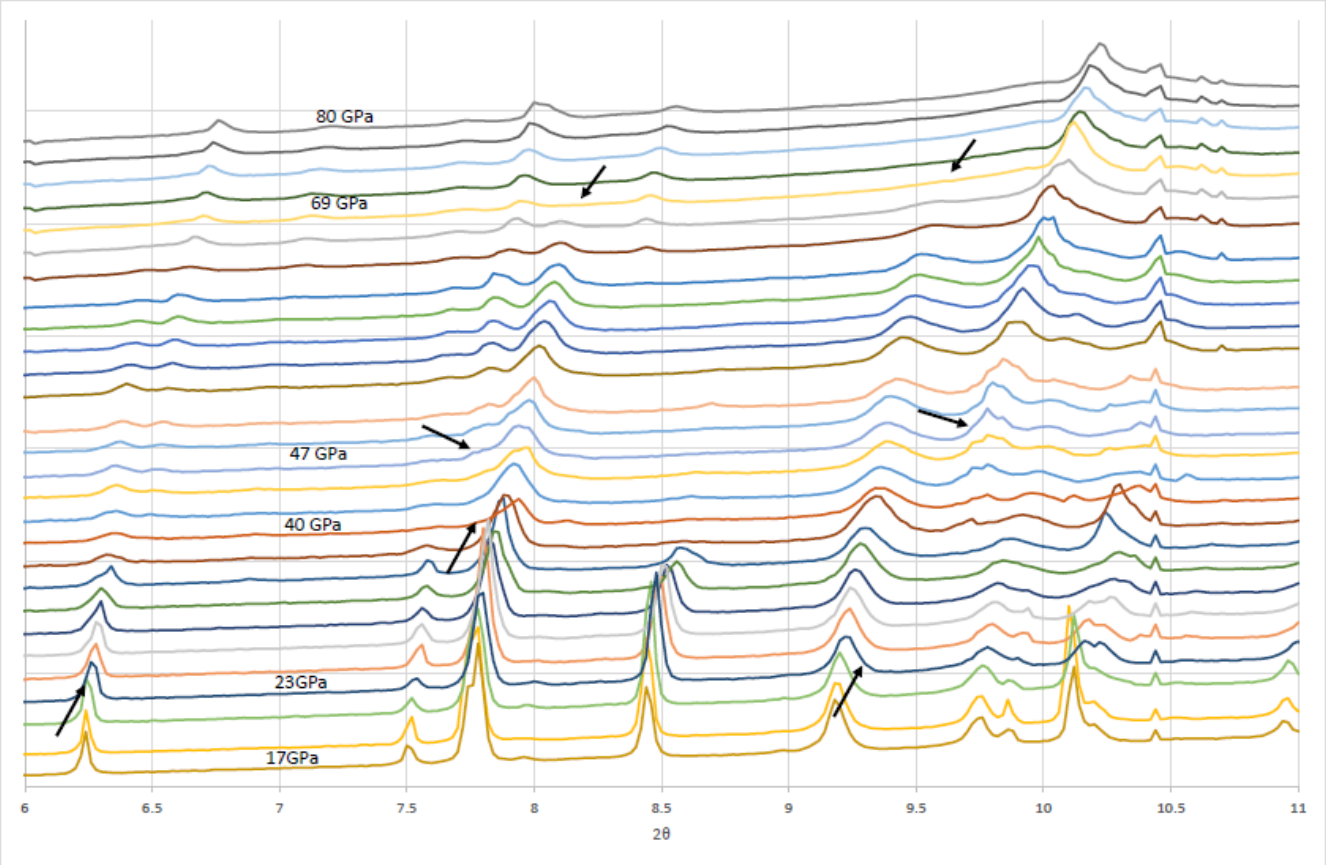

Fig.1 Evolution of the XRD pattern of $AlFeO_3$ at pressure range 17 – 80 GPa.

[1] A. G. Gavrilyuk, I. A. Troyan, R. Boehler et al., JETP Letters **75**, 23 (2002).

[2] E. Bykova, M. Bykov, V. Prakapenka et al., High Pressure Res. **33**, 534 (2013)