

Fig. 2. The phase diagram of magnetite. The $T_V(P)$ curve in the 0 - 70 Kbar range (Rozenberg et al [3]) corresponds to the 1st order insulating-metal transition and the 70 - 125 Kbar to 2nd order transition in which magnetite below this curve is quasi-metallic. The T_V curve measured by Mori et al [4] does not include this 2nd transition. The " \leftrightarrow " line shows a typical mode of operation. The sample is first cooled the desired T and P is increased and decreased, accordingly. The \triangle and ∇ symbols correspond to "cubic" and "orthorhombic-distorted" phases, respectively.



Fig. 1. Typical XRD patterns measured at 82.5 K at different pressures. 85.3 Kbar corresponds to a pressure in which magnetite is metallic, 65.6 Kbar insulator, and 78.5 Kbar at the border line. The arrow in Fig. 2 describes the experimental mode (increase and decrease of P).

References:

^{1 -} M. P. Pasternak, W. M. Xu, G. Kh. Rozenberg, R. D. Taylor, and R. Jeanloz, JMMM 265 L107, (2003).

^{2 -} Z. Szotek et al. Phys. Rev. B 68, 054415, (2003).

^{3 -} G. K. Rozenberg, G. R. Hearne, M. P.Pasternak, P. A. Metcalf, and J. M. Honing, Phys. Rev. B 53, (1996) 6482.

^{4 -} J. Môri, J. App. Phys. 89, (2001) 7347

	Experiment title: STRUCTURAL PROPERTIES OF THE PRESSURE-INDUCED COORDINATION CROSSOVER TRANSITION IN MAGNETITE	Experiment number : HS2288
ESKF Beamline:	Date of experiment:	Date of report:
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Shifts: 12	Local contact(s): Dr. Michael Hanfland	Received at ESRF:
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Report:

XRD data were collected using ESRF's DAC with membrane and loading the sample with He pressure medium. The search for the coordination crossover in magnetite was carried out at temperatures close to the Verwey transition ($T_V(P) \sim 80 - 120$ K), in the 80 - 150 K range and 3 - 12 GPa.

It turned out that the low-temperature choice was wrong; despite the He medium lines were relatively broad to such an extent that the expected fine and *delicate* structural transition could not be detected.

Instead we have by chance, luckily, and serendipitously discovered an extremely and most fundamental property concerning the "origin" of the metal > insulator phase transition (the Verwey transition) in magnetite.

Our careful and detailed experiments resulted in successfully mapping regions within the (T,P) phase in which the structural cubic distortion of the spinel phase takes place.

The resulted structural results at various pressures scanned at 82.5 K (\leftrightarrow) is shown in Fig. 1. The orthorhombic distorted phase (\bigtriangledown symbols) is clearly contained inside the T_V(P) region, clearly depicted by the experimental curve of Mori [2] whereas cubic phase (\triangle symbols) are outside.

These results clearly establish the source of the Verwey transition. It's not the Mott-Verwey mechanism based on the *d*-*d* correlation gap opening (as shown experimentally by Pasternak et al. [1] and theoretically deduced by Szotek et al. [2]) but it arises from a crystallographic cubic distortion of the spinel.

We are now in the process of submitting a manuscript to PRL.