



Experiment title: Pressure response of the local atomic coordination in the narrow band gap semiconductor FeGa₃ and its relation to the semiconductor metal transition.

Experiment number:
HC1990

Beamline: ID24	Date of experiment: from: 28/09/2017 to: 04/10/2017	Date of report: 2018/08/04
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Report:

In semiconducting intermetallic FeGa₃, our high pressure x-ray diffraction studies showed that the 15–20 GPa initiate a disruption of the tetragonal P4₂/mm structure. Around the same pressure there is an emergence of a high-pressure metallic phase. Ga K-edge XANES and EXAFS measurements carried out provided important information.

Up to ~19 GPa there is a continuous evolution of Ga K-edge near-edge (XANES) features. This is followed by a distinct change where a second group of XANES profiles could be distinguished (see Fig. 3 (a) of the below cited publication). Compared with the LP suite, HP XANES profiles at $P > 19$ GPa are characterized by a clear shift in edge position, reduction in intensity, and broadening of the main absorption feature at ~10370 eV.

Extended absorption fine structure (EXAFS) beyond 19 GPa also demonstrated stark changes occurring beyond 19 GPa. Above 19 GPa, there is a pronounced damping of the oscillation amplitudes. A comparison of the Fourier-transform magnitudes $FT|k^2\chi(k)|$ of representative LP and HP EXAFS clearly evidenced changes in the first-shell region $R \sim 2$ Å, suggestive of distinct Ga local environments for LP and HP phases.

Main results from the present study are recently published as a rapid communication in Phys. Rev. B. Details of the publication are given below.

[Pressure-induced disruption of the local environment of Fe-Fe dimers in FeGa₃ accompanied by metallization:](#)

Phys. Rev. B, 2018, **98**, 020101

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