Evolution of structure and local atomic environment upon pressure-induced metallization in intermetallic $FeGa_3$

Boby Joseph[1]*, S. Bhattacharjee[2], B. P. Doyle[2], M. A. M. Ahmed[2], P. Musyimi[2], E. Carleshi[2] and G. R. Hearne[2]

[1]*Elettra, Sincrotrone-Trieste, S. S. 14, Km 163.5, Basovizza, 34149, Trieste, Italy*
[2]*Dept. Physics, University of Johannesburg, P.O. Box 524, Auckland Park 2006, Johannesburg, South Africa*

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*e-mail: boby.joseph@elettra.eu

External pressure is applied to the hybridization-gapped semiconductor $FeGa_3$ to modify the Fe-3d/Ga-4p hybridization strength. This permits tuning its physical properties without introducing any chemical perturbation. Pressure is thus a preferred tool for perturbing such narrow band-gap intermetallic compounds and probing the response. This is primarily to tune the system to charge-gap closure, particularly from the effect of varying electron correlation strength, U/W, where U is the on-site repulsion and W the bandwidth.

Theoretical calculations of intermetallic $FeGa_3$ estimated the U/W ratio to be 0.6 with U about 3-4 eV [1], thus rendering the system as having moderate electron correlations. The calculations also indicate gap-closure occurs at 25 GPa, due to a strong rearrangement of Fe 3d and Ga 4p hybridization near the Fermi level.

Investigations of the lattice structure as a function of pressure in $FeGa_3$ is a first step in the comparison between calculations and experiments, which also helps to contrain free parameter values involved in the computational studies. The critical pressure to attain metallization is readily established from electrical-transport measurements.

To understand the effect of varying hybridization and electron correlations in $FeGa_3$, we have undertaken both x-ray powder diffraction (HP-XRPD) and variable temperature electrical resistivity measurements to high pressures [2]. These results were complimented by high pressure x-ray absorption spectroscopy (XAS) measurements [2] to provide site-specific local structural information.

Our HP-XRPD results evidence initiation of a structural phase transition in FeGa3 above 16 GPa, with a broad coexistence range involving the low pressure tetragonal phase and the nascent high pressure phase up to 30-35 GPa. Onset of metallic behavior occurs just beyond ~16 GPa, close to the critical pressure where the new high pressure phase starts to emerge. There is a square-root temperature dependence of the resisitivity below the resistivity minimum at ~10 K for data in the metallic state above 16 GPa. This is typical of disordered metallic alloys with enhanced electron-electron interactions. Ga K-edge XAS evidences significant atomic arrangements above 19 GPa indicative of differing Ga local environments of low and high pressure phases of $FeGa_3$.

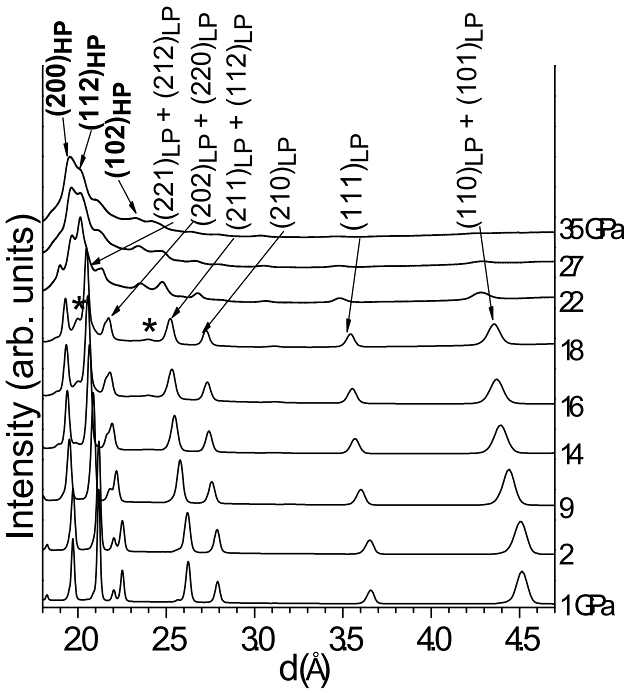

Figure 1. HP-XRPD data evidencing the evolution of the low-pressure (LP) phase to a new high pressure (HP) phase initiated at 16-18 GPa.

The interplay between structural aspects of the phase transition and "bad" metallic behavior subsequent to gap-closure from pressurization of the $FeGa_3$ intermetallic, will be discussed in further detail.

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