ESRF	**Experiment title:** **Crystal structure of the superconductor LiFeAs under high pressure**	**Experiment number**: HS-3814
Beamline: ID09a	**Date of experiment**: from: 18/7/2009 to: 21/7/2009	**Date of report**: 21/03/2011
Shifts: 6	**Local contact(s)**: Michael Hanfland/Gaston Garbarino	*Received at ESRF:*

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Report:

We investigated the evolution of the crystal structures of LiFeAs and the newly-discovered and isostructural compound NaFeAs with pressure at ambient temperature. This experiment was augmented by preliminary experiments on ID27 on LiFeAs up to 17 GPa and magnetometry measurements up to 2 GPa [1].

The results show the following:

1. LiFeAs is highly compressible and the $FeAs_4$ tetrahedra become even more distorted from regular on the application of hydrostatic pressure. From finite strain analysis we estimated a bulk modulus of 56.7 GPa and identified a positive-sloping strain-normalized pressure behavior, indicating that a fit to a third-order Birch-Murnaghan Equation of State. Rietveld refinement of the structural parameters showed that compression of the Li-As slab of the structure dominates the behaviour. Measurements up to 35 GPa on ID09a showed that there is a phase transition at 29 GPa, but further measurements are required to determine the structure of the high pressure phase.

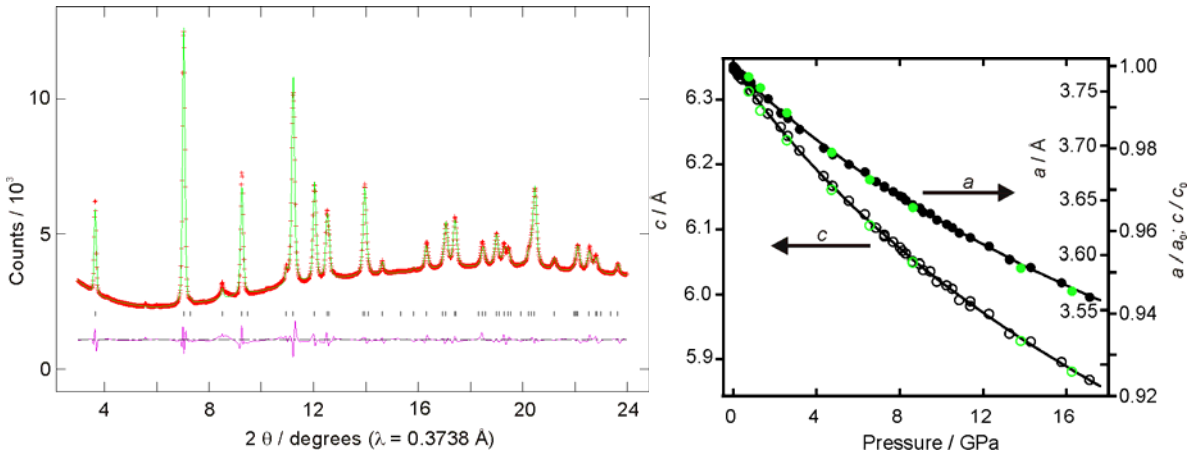

Figure 1. Left: Rietveld refinement against LiFeAs at 17 GPa (ID27 data) and the behaviour of the lattice parameters with pressure.

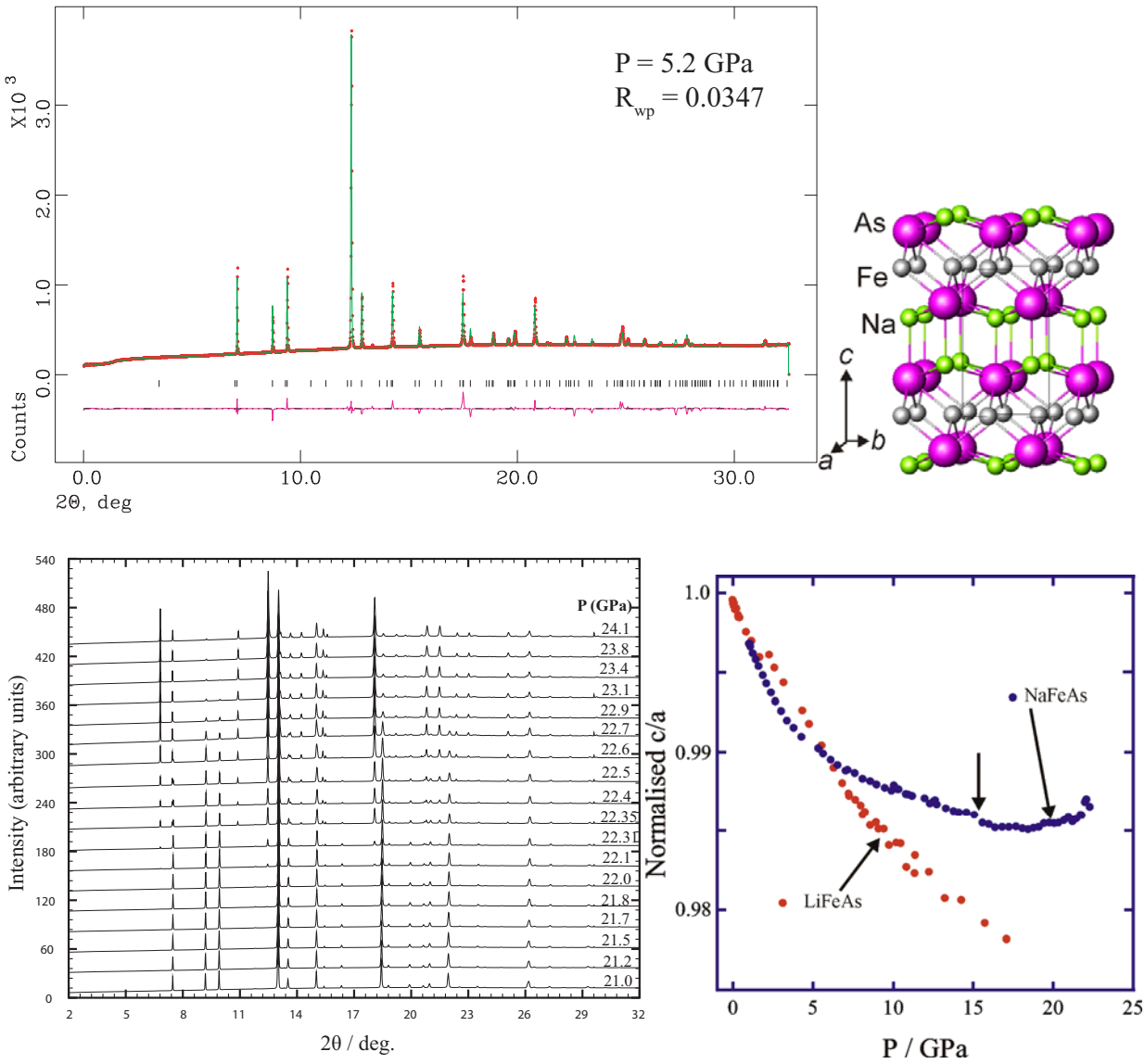

Figure 2. Behaviour of NaFeAs as a function of pressure and comparison woth LiFeAs.

2. NaFeAs also shows a high pressure phase transition and the suggestion of structural anomalies at high pressures. The figures show a Rietveld refinement against ID09a data at 5 GPa, the appearance of the new phase of NaFeAs above 22 GPa and the rather different evolution of the *c*/*a* ratio in NaFeAs and LiFeAs.

Refinement of the internal coordinates of NaFeAs was somewhat hampered by preferred orientation , but there is the suggestion of anomalies at high pressure at the approach to the phase transition.

Now that single crystals of these materials are available, further measurements are propsed to determine the high pressure structures and the detained response of the structure of NaFeAs to applied pressure.

[1] Mito, M.; Pitcher, M. J.; Crichton, W.; Garbarino, G.; Baker, P. J.; Blundell, S. J.; Adamson, P.; Parker, D. R.; Clarke, S. J. *Journal of the American Chemical Society* **2009**, *131*, 2986-2992.