



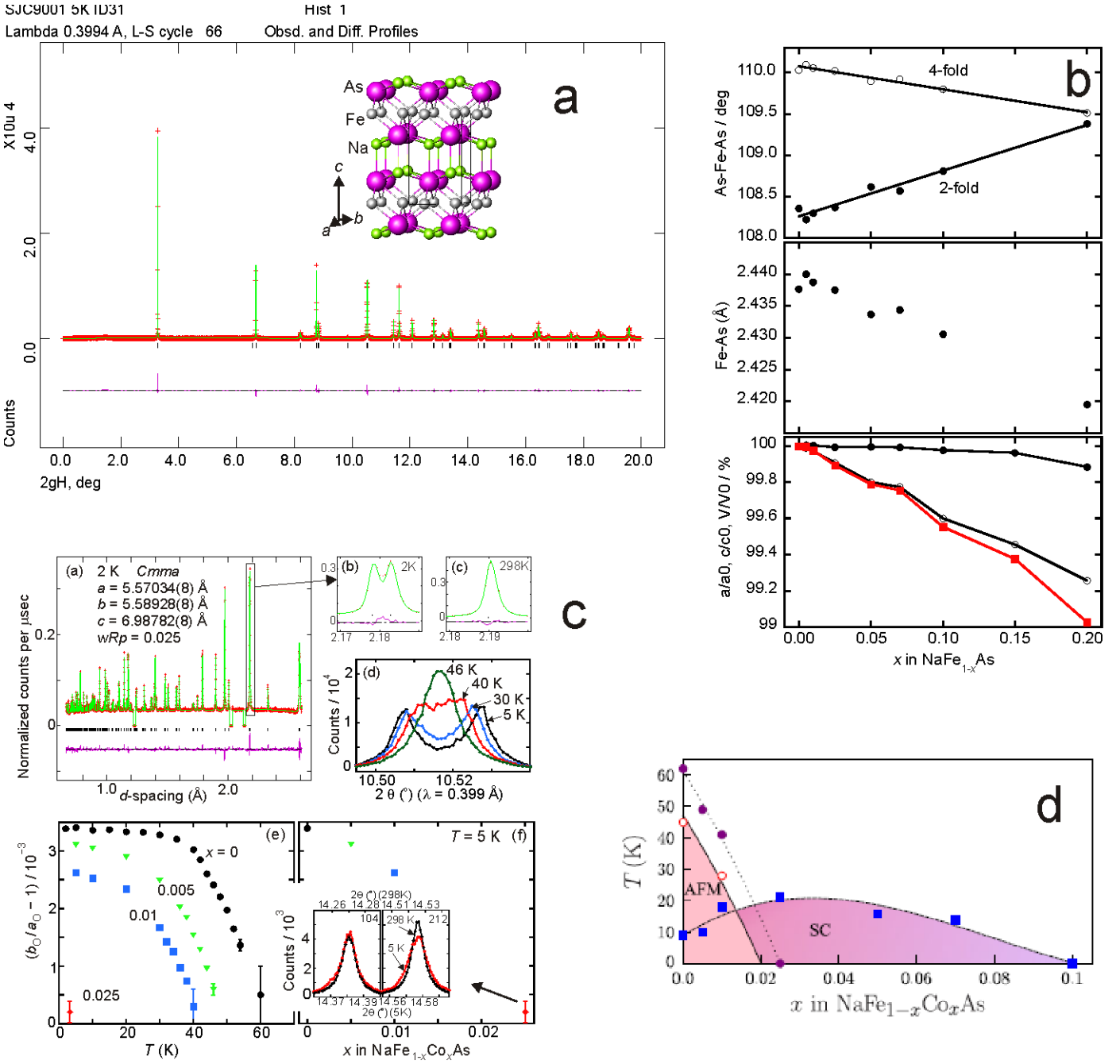
	Experiment title: Crystal structures of layered arsenide superconductors LiFeAs & NaFeAs	Experiment number: HS-3891
Beamline: ID31	Date of experiment: from: 1/7/2009 to: 3/7/2009	Date of report: 23/03/2010
Shifts: 6	Local contact(s): Irene Margiolaki	<i>Received at ESRF:</i>
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Report:

We investigated the evolution of the crystal structures of NaFeAs and NaFe_{1-x}Co_xAs with temperature and composition. The results show the following:
NaFeAs and compounds NaFe_{1-x}Co_xAs with $x < 0.01$ undergo a tetragonal-to-orthorhombic structural distortion driven by antiferromagnetic ordering on the Fe sublattice. This is in accord with other investigations of other members of the class of superconducting iron pnictides. The high resolution of ID31 is key to determining the distortion in these compounds because the extent of the distortion is proportional to the ordered moment on Fe and this is estimated from MuSR studies to be only about $0.1 \mu_B$ in NaFeAs. The high resolution also enables the onset temperature of the distortion to be determined and our results show that the structural distortion onset is above the onset of long range magnetic order probed by MuSR. For $x = 0.025$ in NaFe_{1-x}Co_xAs where the physical properties show 100 % superconductivity there is no obvious structural distortion evident even on ID31 although there is some peak broadening suggesting the intriguing possibility that the distortion may persist even into the superconducting regime.
Our results have enabled a phase diagram to be established for the NaFe_{1-x}Co_xAs series. A future experiment will probe further compositions in the range $0.01 < x < 0.025$.

This work has now been published (along with neutron diffraction, MuSR and magnetic susceptibility measurements): Control of the Competition between a Magnetic Phase and a superconducting Phase in Cobalt-Doped and Nickel-Doped NaFeAs Using Electron Count
Parker, D. R.; Smith, M. J. P.; Lancaster, T.; Steele, A. J.; Franke, I.; Baker, P. J.; Pratt, F. L.; Pitcher, M. J.; Blundell, S. J.; Clarke, S. J. *Phys. Rev. Lett.* **2010**, *104*, 057007.

Figures:



(a). Refinement of the structure of $\text{NaFe}_{0.99}\text{Co}_{0.01}\text{As}$ against ID31 data at 5 K.

(b). Evolution of the lattice and structural parameters of $\text{NaFe}_{1-x}\text{Co}_x\text{As}$ with x

(c). The evolution of the size of the structural distortion in $\text{NaFe}_{1-x}\text{Co}_x\text{As}$ with composition and temperature (the distortion is given by the ratio of the orthorhombic lattice parameters)

(d). The phase diagram for $\text{NaFe}_{1-x}\text{Co}_x\text{As}$ showing the competition between the antiferromagnetic and superconducting regions (T_c : blue squares, T_N : open circles, $T_{\text{structural}}$: closed circles). A further experiment will probe in more detail the region of coexistence between antiferromagnetism and superconductivity.