ESRF	**Experiment title:** X-ray resonant scattering investigation of the magnetic order in the superconducting parent compound $BaFe_2As_2$	**Experiment number**: HE-2777
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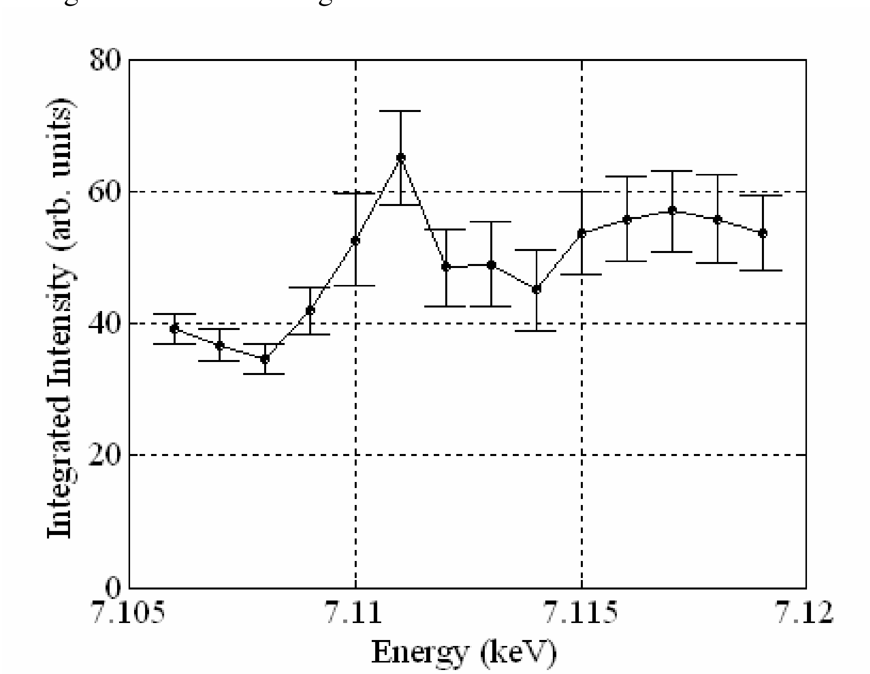
Report: The original subject of proposal HE 2777 was to investigate the phase diagram of the magnetoelectric multiferroic material $CuFe_2O_2$, but when we were given access to single crystal samples of $BaFe_2As_2$ we felt it would be more timely to attempt the first X-ray resonant scattering experiment on the new class of iron arsenide superconductors. We then arranged to make this sample change with both the ESRF director and the head of the X-ray Absorption and Magnetic Scattering Group – Dr Brookes.

The discovery of the iron arsenide based superconductors has provided new impetus to the field of high-T_C superconductivity [1, 2], with a maximum reported superconducting transition temperature at ambient pressure of 55 K in fluoride doped SmFeAsO [3]. The crystal structure of the so-called 1111-type superconductors is tetragonal with alternating layers of edge-sharing RE-O and Fe-As tetrahedra, where the superconductivity emerges in the Fe-As layers on adding or removing electrons, reminiscent of the Cu-O layers in the cuprate superconductors. More recently, another family of 122-type superconductors have been discovered, with a transition temperature of 38 K in potassium doped $BaFe_2As_2$ [4]. These 122 superconductors are also tetragonal with Fe-As layers separated by rare earth ions. The non-superconducting parent compounds LaFeAsO and $BaFe_2As_2$ show remarkably similar properties: both are poor metals, are weakly magnetic and display a spin density wave anomaly that appears to be associated with a structural phase transition into an orthorhombic structure. In addition, the structural transition appears to be related to the devlopment of an antiferromagnetic structure. In the superconductors the SDW anomaly, structural transition and antiferromagnetic ordering are suppressed, suggesting that spin fluctuations may play an important role in the superconducting mechanism, and as such a deeper understanding of the phase diagram in the parent compounds will be important in helping to understand the superconductivity in the iron arsenides.

Single crystal samples of $BaFe_2As_2$ were cut with a c-face and mounted in the displex cryostat on ID20. Unfortunately the sample is very thin in cross-section, and strains from the way the sample was attached led to bowing of the sample. The position of the X-ray beam incident on the sample was therefore very carefully optimised. At low temperatures, below the structural transition, we see clear evidence of twinning due to the orthorhombic distortion, but the domain populations are unbalanced and the splitting between the two twins is very small <1%, indicating that the difference between a_O and b_O is of the order of 0.01 Å.

In order to investigate the magnetic ordering, we mounted an MgO (222) crystal, which whilst it is a good energy match for working at the iron K-edge, is unfortunately a poor match for the large mosaicity of the sample, making it difficult to find peaks. We searched for peaks in σπ of the type (101) in the stronger domain. Very weak broad peaks were seen at (1 0 9) and (1 0 11). To determine the energy dependence of the scattering at (1 0 11) theta-2theta scans were measured as a function of energy. Fitting a lorentzian line-shape to the individual rocking curves the following result was obtained:



There is possibly a very weak resonance at 7.111 keV, but this is on top of a sizeable non-resonant background. The combination of such a weak resonance and the mosaic of the sample leading to any scattering intensity being smeared out over a considerable width made it very difficult to perform these measurements and until sample quality has improved any further, measurements using a technique with such high wavelength resolution will prove to be very challenging.

References:

[1] Y. Kamihara et al., J. Am. Chem. Soc., 130, 3296 (2008).
[2] D. Johrendt and R. Pöttgen. Angew. Chem. Int. Ed., 47, 4782 (2008).
[3] Z. Ren, et al., Chin. Phys. Lett., 25, 2215 (2008).
[4] M. Rotter et al., arXiv:0805.4630 (2008).