Experimental report

30/10/2023

Proposal: 5-41-1215 **Council:** 4/2023

Title: Determination of the magnetic structure of the superconducting Fe spin-ladder BaFe2Se3 as a function of the magnetic field

Research area: Physics

This proposal is a new proposal

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Samples: BaFe2Se3

Instrument	Requested days	Allocated days	From	To
D23	4	0		
ORIENTEXPRESS	1	2	28/05/2023	29/05/2023
			03/09/2023	04/09/2023
D9	5	5	18/09/2023	01/10/2023

Abstract:

The Iron-based spin ladder BaFe2Se3 with multiferroic properties at high temperature becomes superconducting under pressure. Under a pressure close to the superconducting dome, its block-like magnetic order is replaced by the same stripe-like magnetic structure as those of the emblematic parent compound BaFe2S3. In order to understand the mechanism of superconductivity, we plane to perform single crystal X-ray diffraction under magnetic field. We aim at driving the block magnetic order to the stripe-like one, favorable for superconductivity

Determination of the magnetic structure of the superconducting Fe spin-ladder BaFe2S3 as a function of the magnetic field

- Objective & expected results : -

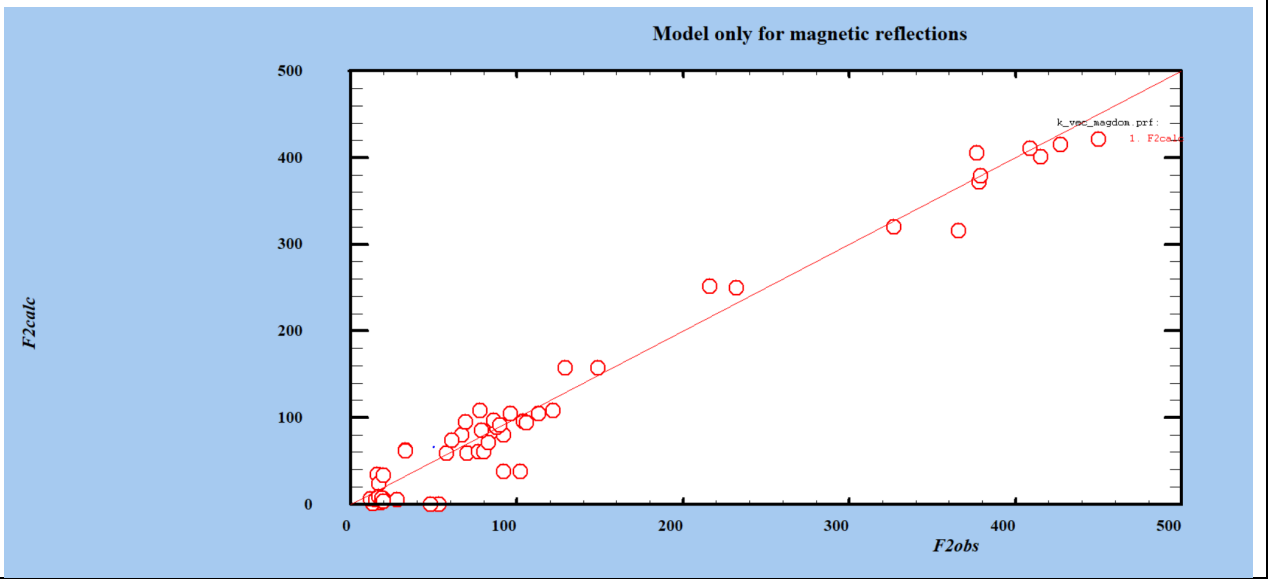
The Iron-based spin ladder BaFe2Se3 becomes superconducting under pressure. Under a pressure close to the superconducting dome, its block-like magnetic order is replaced by the same stripe-like magnetic structure as those of the emblematic parent compound BaFe2S3. This indicates that block and stripe magnetic instabilities are of similar energy. In order to understand the competition between the magnetic phases and the superconducting one, we plane to perform single crystal X-ray diffraction under magnetic field. We aim at driving the stripe-like into the block magnetic order in $BaFe_2S_3$.

- Results and the conclusions of the study (main part): **-**

We first aligned the crystal using orientexpress. We decided to align the b axis along the magnet as b is neither the easy axis nor the direction of the AFM ladder. After 12h of measurement in D9, the experiment was interrupted for 3 days due to troubles with the ILL reactor. We continued the experiment the week after and had enough time to: i) measure the effect of the magnetic field on the magnetic order ii) collect the reflections to refine the magnetic structure at 0T iii) accurately determine the critical temperature of the structural and magnetic transitions.

i) We measured about 30 magnetic reflections and 40 nuclear reflections at 2K as a function of magnetic field from 0 to 5.5 T. The nuclear reflections measured were standard reflections of the Cmcm space group as well as forbidden reflections of the C and c operations. Indeed, previous X-ray diffraction measurements showed that a symmetry breaking from Cmcm to Pbnm occurs at a temperature close to the Neel order (TN~100K). We found no variation of intensity for any reflection. This can be explained by a too strong anisotropy energy for the moments.

ii) We collected approximately 300 reflections at 2K and 0T. We were able to refine the magnetic structure in the $Pa2_1/m$ magnetic space group. Preliminary results give good reliability factors Rmagn~6 (see figure). It corresponds to the magnetic structure already published after powder neutron experiment but with a canting of the spin of about 20°.



iii) We were able to follow the (0.5 -0.5 1) magnetic reflection and the 1 -8 0 reflection forbidden in the Cmcm space group. We obtained a thermal variation of their intensity very different. This shows that the structural transition appears at high temperature (120K) than the magnetic one (95K). This result is of importance to understand the mechanism of stabilization of the magnetic order and thus to understand the superconducting phase.