# Experimental report

14/02/2018

**Proposal:** **TEST-2731** **Council:** 4/2016

**Title:** SrEr2O4 single crystal extinction coefficient measurement and structure determination

**Research area:**

**This proposal is a new proposal**

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**Local contacts:** Oscar Ramon FABELO ROSA

**Samples:** SrEr2O4

| Instrument | Requested days | Allocated days | From | To |
|---|---|---|---|---|
| D9 | 4 | 4 | 02/12/2016 | 07/12/2016 |

**Abstract:**

**Experimental report: D9** (Exp. No.5-41-913) Detailed crystal structure of $SrEr_2O_4$.

The measurement was performed on a small high quality single crystal of $SrEr_2O_4$ of dimension equal to 1.09, 3.73 and 2.89 mm along *a b* and *c* respectively. The sample was glued on an aluminum pine with *c* aligned parallel to the pin axis. The measurement was performed on D9 in 4-cycle mode. The temperature was set to 20 K and the neutron beam to 0.8 Å. A set of 544 independent reflections was measured considering a large reciprocal space coverage. The dataset was then corrected for absorption with the software Datap. The refinement of the data was then performed with the FullProf suite software giving a good agreement between the structural model obtained and the data (R Bragg = 3.57). In addition to the precise determination of the nuclear structure of $SrEr_2O_4$, the extinctions parameters of the single crystal sample were determined to a high precision. The second part of the experiment was dedicated to a measure of the fully polarised magnetic phase of $SrEr_2O_4$ using a cryomagnet. The measurement was performed at 1.5 K under a magnetic field of 2T applied along the Er chains (*b*), the wave length was set at 0.5 Å. In order to isolate the magnetic signal a 1.5 K background measured with no field applied is subtracted from the data. The scale factor is calculated from this data set collected in zero field.

From the irreducible representation performed with Basireps, we have obtained 8 IRs.

| Allows for : | Γ1 | Γ2 | Γ3 | Γ4 | Γ5 | Γ6 | Γ7 | Γ8 |
|---|---|---|---|---|---|---|---|---|
| Antiferromagnetic component within ac-plane | Yes | | | Yes | yes | | | yes |
| Allows for ferromagnetism along b | | | | | | yes | | |
| Allows for antiferromagnetism along b | | yes | yes | | | | yes | |
| Chi square | | 39.67 | 38.50 | | | 14 | 39.7 | |
| $Chi^2$ combination with Γ6 | unstable | | | 14.02 | unstable | | | unstable |

With a 20.0 kOe magnetic field applied along b we are expecting a significant ferromagnetically ordered component of the magnetic structure along this direction. Only Γ6 allows for this specificity and returns the best refinement. The model gives 5.56 $\mu_B$ and 2.0 $\mu_B$ on site one and two respectively (3.78 $\mu_B$ per $Er^{3+}$ ions on average), see fig.1.

RF2 -factor : 26.1; RF2w-factor : 25.3; RF -factor : 22.8; Chi2(Intens): 14.0

We have then tried to improve the refinement by combining Γ6 with models allowing for antiferromagnetic component within the ac-plane. This gives us the possibility to combine Γ6 with Γ1, Γ4, Γ5 and Γ8. However, none of these combinations returns an improvement to the fits obtained with Γ6 only (the fit does not go directly toward a stable state and keep oscillating between several configurations). In addition, the values obtained from those models for the x and z components of the magnetic moments are close to 0 $\mu_B$ and are within the range of the calculation uncertainties.

**Conclusion**: From the refinements performed on the data, it is clear that Gamma 6 is the dominant configuration for the magnetic structure. This model is consistent with the fact that we have applied a magnetic field along the b direction and forced the establishment of ferromagnetic order on both sites. Then from our refinements, we have established that allowing for a small antiferromagnetic component within the ac-plane was not improving the fits. The result of this analysis is consistent with the magnetisation measurement performed at 1.5 K and published in (PHYSICAL REVIEW B **78**, 184410 _2008). Interestingly the different site anisotropy is conserved even in the paramagnetic phase, as an application of a magnetic field leads to different sublattice magnetizations. This perfectly agrees with the short-range order and diffuse scattering above TN.

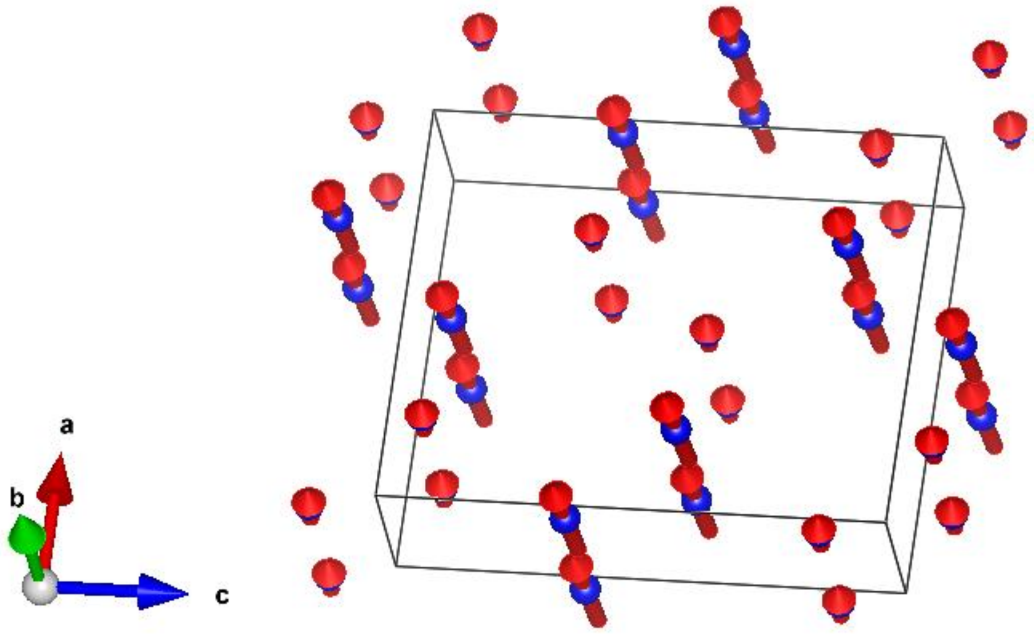


*Figure 1: Field induced magnetic structure of $SrEr_2O_4$ stabilised at 1.5 K under magnetic field of 20.0 kOe.*