| ESRF | **Experiment title:** Crystal structures of charge-ordered superstructures of highly stoichiometric $SmBaFe_2O_5$, $EuBaFe_2O_5$ and $GdBaFe_2O_5$ | **Experiment number:** CH-1534 |
|---|---|---|
| **Beamline:** ID31 | **Date of experiment:** from: 23.06.2004 to: 28.06.2004 | **Date of report:** 30.07.2004 |
| **Shifts:** 15 | **Local contact(s):** Dr. François Fauth | *Received at ESRF:* |

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Report:

Prior the measurements, the title phases were annealed for several weeks at 700 K in closed silica ampoules in presence of a small amount of Zr getter, with subsequent slow cooling down to the room temperature. This was done in order to ensure high homogeneity of the oxygen content across the sample and the best possible starting point for the charge ordering. Diffraction scans at ID31 over the h00, 0k0, 00l peaks confirmed that this procedure was successful in bringing the most symmetrical Bragg peaks seen to date on $RBaFe_2O_5$ samples. High-sensitivity diffraction data in radiation of 0.4 Å wavelength were collected over a wide angular range for the title phases at both 100 K and 300 K. In addition, several short isothermal scans were obtained between these two temperatures, as well as finely paced scans across the Verwey-transition temperature range.

Owing to the new highly linear detectors installed at the powder diffractometer at ID31, as well as the new very well designed sample mounting/rotation, the collected patterns are now almost flawless. After the appropriate care is taken of the so called "cross-talks", actually residuals of the sample-diffracted Bragg beams passing via the Si detectors, Rietveld refinements of the charge-ordering superstructure are very straightforward. This is not surprising, since visual inspection shows about 30 nicely resolved superstructure peaks above the background in the collected pattern of the charge-ordered phase, as compared with the maximum of some 5 observable only several years ago.

It is now possible to register the charge ordering at the Verwey transition in $RBaFe_2O_5$ even in rather quick isothermal scans. While without ambitions for structural refinements of the superstructure, these patterns clearly show that the charge-ordering and disordering proceed sharply within the temperature range the Verwey transition characterized by the two-phase region at the transition.

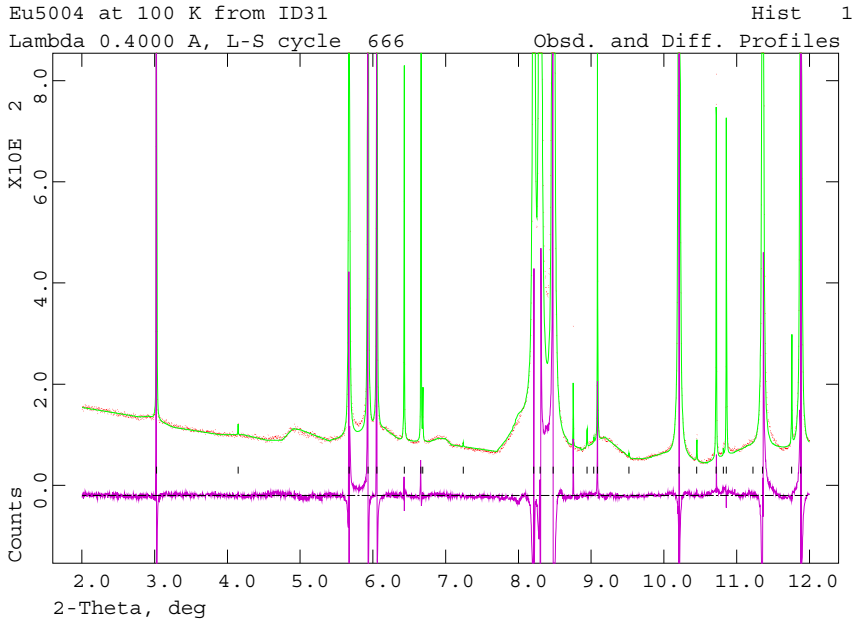


Fig. 1: Detail of the first quarter of the refined pattern (1/100 of the intensity range) for charge-ordered $EuBaFe_2O_{5.004}$ at 100 K. Note the good fit to the charge-ordering superstructure Bragg reflections, the strongest of which is 102 with intensity of ~100 counts at 6.687° of the angle two theta where it is barely resolved (but sufficiently for the refinement) from a 1000-counts line 011 at 6.661°.

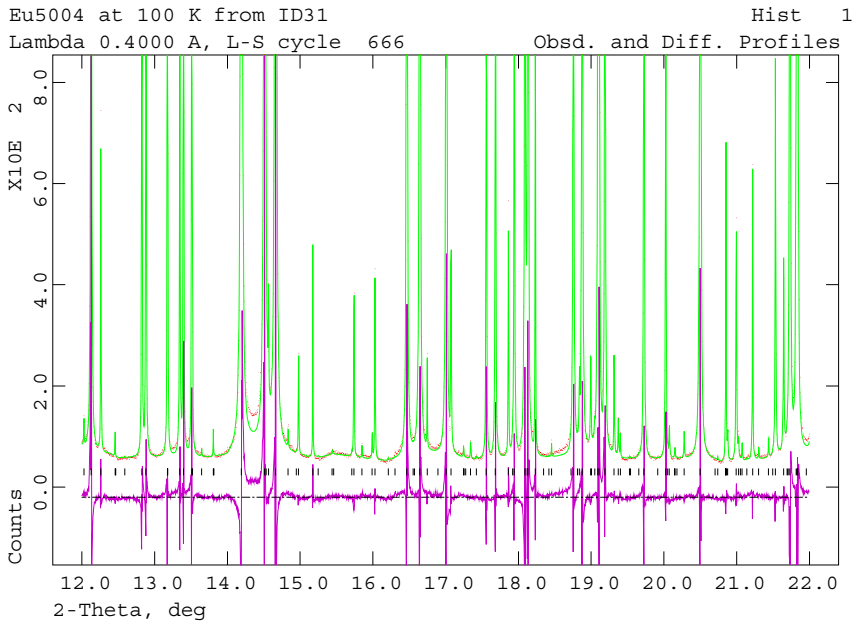


Fig. 2: Detail of the second quarter of the refined pattern (1/100 of the intensity range) for charge-ordered $EuBaFe_2O_{5.004}$ at 100 K.