| | | |
|---|---|---|
| ESRF | **Experiment title:**<br>**Crystal structure of hematite (alpha-Fe2O3)** | **Experiment number**:<br>HC-1470 |
| **Beamline**:<br>ID-22 | **Date of experiment**:<br>from: 10.09. 2014 to: 12.09.2014 | **Date of report**:<br>08.09.2015 |
| **Shifts:**<br>6 | **Local contact(s)**: A. Fitch | *Received at ESRF:* |


**Names and affiliations of applicants** (* indicates experimentalists):

Radoslaw Przenioslo(*) , Michał Stękiel(*), Michał Duczmal(*), Dariusz Wardecki, Izabela Sosnowska
Faculty of Physics, University of Warsaw, Poland

Joey A. Lussier(*)
Faculty of Chemistry, University of Manitoba, Canada


## Report:

The crystal structure of $\alpha$-$Fe_2O_3$ (hematite) has been studied by SR powder diffraction at ID22. Several powder $\alpha$-$Fe_2O_3$ samples from different providers have been used in this study. The Bragg peaks positions observed at RT agree with those predicted with the rhombohedral crystal structure model based on the space group R-3c [1,2]. There is however a persistent effect of anisotropy of the peakwidths which is observed for all $\alpha$-$Fe_2O_3$ samples in this study. These observations can be described by using a crystal structure model based on the monoclinic space group C2/c [3,4]. The rhombohedral-to-monoclinic transformation implies relative changes of the unit cell parameters $\Delta a/a \approx 2\times10^{-4}$. The details of the $\alpha$-$Fe_2O_3$ monoclinic symmetry model observed at RT have been published recently [4].

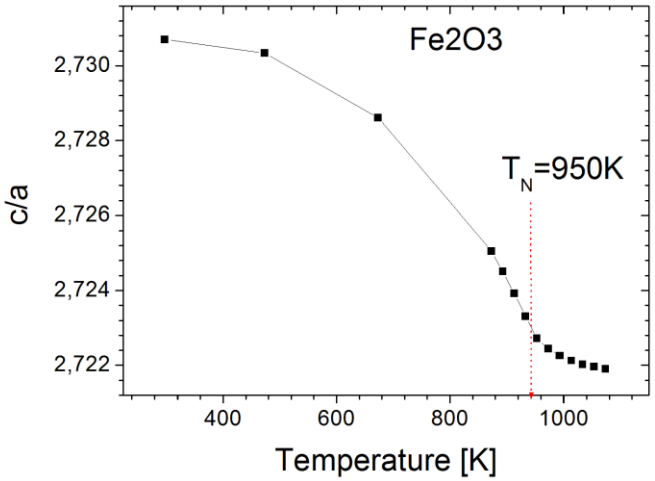


*Fig.1. Ratio of the hexagonal unit cell parameters c/a of $\alpha$-$Fe_2O_3$ determined from SR powder diffraction data. The dotted vertical line shows the Neel temperature $T_N$=950K.*

The crystal structure of $\alpha$-$Fe_2O_3$ have been also studied as a function of temperature in the region from the Neel temperature $T_N$=950K [5] down to the Morin transition $T_M$=250K [5]. In the first step, the SR powder diffraction patterns were refined by using the rhombohedral crystal structure model [2]. The Rietveld refinements converge to a satisfactory agreement in the temperature range between $T_N$=950K and $T_M$=250K[5]. There are clear indications of the spin-lattice coupling and in the vicinity of $T_N$=950K shown by anomalous behaviour of the hexagonal unit cell ratio. The hexagonal unit cell parameters are used for the rhombohedral $\alpha$-$Fe_2O_3$ structure model. The temperature dependence of the c/a ratio is shown in Fig.1.

A refinement of the $\alpha$-$Fe_2O_3$ SR diffraction patterns has been also performed by assuming the monoclinic structure model based on the space group C2/c. The refinement with the monoclinic model works well at RT but in the vicinity of $T_N$=950K the fit stability becomes problematic. Further analysis of the possible monoclinic distortions of the rhombohedral crystal structure of $\alpha$-$Fe_2O_3$ as a function of temperature are in progress.

## References


[1] L. Néel and R. Pauthenet, *Comptes Rendus*, **234**, 2172 (1952).

[2] E.N. Maslen, V.A. Streltsov, N.R. Streltsova and N. Ishizawa, *Acta Cryst* **B50**, 435 (1994).

[3] R. Przeniosło, I. Sosnowska, M. Stękiel, D. Wardecki, A. Fitch, *Physica* **B449**, 72 (2014).

[4] M. Stękiel, R. Przeniosło, I. Sosnowska, A. Fitch, J.B. Jasiński, J. Lussier and M. Bieringer, *Acta Cryst.* **B71**, 203 (2015).

[5] A. Morrish "Canted Antiferromagnetism: hematite" World Scientific, Singapore, 1994.