Hyperfine interactions of ^{57}Fe nuclei in a weak ferromagnet $FeBO_3$

N. Snegirev[1], S. Starchikov[1], I. Lyubutin[1], E.S. Smirnova[1], M. Chuev[2], S. Yagupov[3], M. Strugatsky[3] and O.A. Alekseeva[1]

[1]Shubnikov Institute of Crystallography of FSRC "Crystallography and Photonics" RAS, 119333, Moscow, Russia
[2]Valiev Institute of Physics and Technology RAS, 117218, Moscow, Russia
[3]Physics and Technology Institute, V.I. Vernadsky Crimean Federal University, 295007, Simferopol, Russia

niksnegir@yandex.ru

Iron borate $FeBO_3$ (space group $R\bar{3}c$) is a known crystal which exhibits specific magnetic, magnetoacoustic, magnetooptical, and resonance properties [1,2]. It was proposed to use such crystals for monochromatization of synchrotron radiation in nuclear resonance spectroscopy as the so-called synchrotron Mössbauer source (SMS) [1,2]. The spectra of reflected radiation strongly depend on the hyperfine interactions in this crystal, while the required radiation parameters are achieved near the Néel point ($T_N \sim 348{,}5$ K) [1]. In this case, precise studies of the magnetic, electronic, and structural properties of an iron borate single crystal, especially near the Néel point, are of a great importance.

Studies were carried out by means of conventional Mössbauer spectroscopy and single crystal X-ray diffraction analysis. The iron borate single crystals were previously synthesized using the flux-growth technique [1,2]. High structural perfection of the studied $FeBO_3$ and $^{57}FeBO_3$ crystals was confirmed by X-ray measurements.

The Mössbauer spectra were processed in the framework of the combined magnetic and electric hyperfine interactions taking into account the nonresonant background and the effective thickness of the absorber. At $T < T_N$, the magnetic moments of two sublattices $\mathbf{m_1}$ and $\mathbf{m_2}$ lie in the basal plane of the crystal and are oriented at an angle of $\vartheta \sim 179.17$ [3]. It was found that the main axis of an electric field gradient (Z') is orthogonal to the moments $\mathbf{m}_1$ and $\mathbf{m}_2$ and does not change the orientation over the entire investigated temperature range 10-400 K (Fig.1).

The maximum entropy method was used to analyze the anisotropy of electron density distribution in $FeBO_3$. There is no evident of local disordering near the Fe sites below and above the the Néel point, (Fig. 2) which is consistent with Mössbauer data.

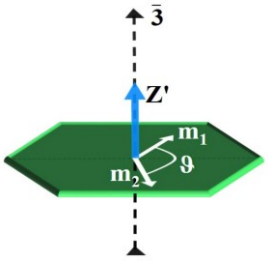

Figure 1. Schematic orientation of the magnetic moments and the principal axis of an electric field gradient in the $FeBO_3$ crystal.

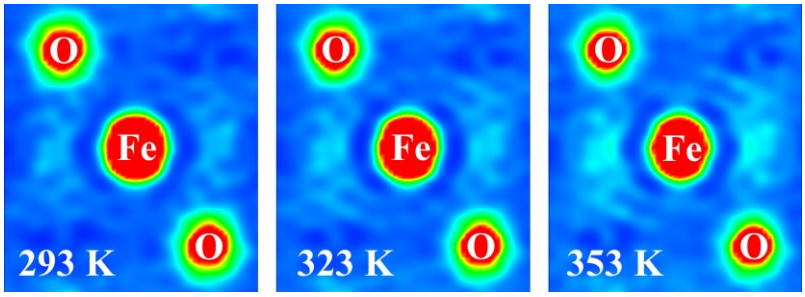

Figure 2. Electron density distribution in the $FeBO_3$ in the $(\bar{1}1\ 10\ 0)$ plane passes through Fe and O atoms, at temperatures 293 K (left), 323 K (middle) and 353 K (right). Distributions shown in red and blue colours correspond to maximum and minimum saturations, respectively.

In addition, for the $FeBO_3$ single crystal, the hyperfine parameters were determined and the crystal structure was refined in a wide temperature range. The data obtained could be very useful for tuning pure nuclear diffraction in SMS experiments.

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