Crystal structure and Mössbauer studies of gallium iron borate single crystals

I. Lyubutin[1], N. Snegirev[1], E. Smirnova[1], S. Starchikov[1], M. Lyubutina[1] , V. Artemov[1], S. Yagupov[2], M. Strugatsky[2], Yu. Mogilenec[2], O. Alekseeva[1]

[1] *Shubnikov Institute of Crystallography of FSRC "Crystallography and Photonics" RAS, 119333, Moscow, Russia*
[2] *Physics and Technology Institute, V.I. Vernadsky Crimean Federal University, 295007, Simferopol, Russia*
lyubutinig@mail.ru

Mössbauer spectroscopy is a very effective and in many cases a unique experimental method widely used to study the structural, magnetic, electronic, and phonon properties of various materials. The appearance of synchrotron methods based on Mössbauer resonance significantly expanded the range of tasks and led to the discovery of a number of new effects, for example, in the field of high pressure physics, superconductivity, magnetism of nano-objects, geophysics and others. In synchrotron installations, very high requirements are imposed on monochromatization of synchrotron radiation to ensure Mössbauer resonance conditions [1]. In the case of Mössbauer resonance on Fe-57 iron nuclei, the iron borate crystal $FeBO_3$ has the most optimal diffraction parameters appropriate for the final stage of monochromatization. Tuning to purely nuclear reflections in this crystal of the type (111) and (333), which are forbidden for X-ray diffraction, makes it possible to obtain an ideal Mössbauer radiation source.

However, very high requirements are imposed on the crystalline quality of such crystals, and their growth is a rather complicated technological task. Recently, we proposed a modernized method for growing single crystals based on iron borate $FeBO_3$ [2,3]. Meanwhile, for the required diffraction conditions, the $FeBO_3$ crystal should be heated to a temperature near the Néel point (about 348 K) [3,4]. In this case, deformations can occur in the crystal that distort or destroy the diffraction conditions. Therefore, an important task is the search and synthesis of crystals with similar diffraction properties, but with a Néel point near room temperature.

In this work we propose to apply the method of diamagnetic dilution and synthesized a series of single crystals with iron substitution by gallium in the series $Fe_{1-x}Ga_xBO_3$. The high quality $Fe_{1-x}Ga_xBO_3$ single crystals with wide range of diamagnetic doping $0 \leq x \leq 1$ were grown. The developed synthesis technique makes it possible to avoid cracks and imperfections of crystalline samples. The exact composition of the solid solutions was determined by energy-dispersive spectroscopy (EDS). Structural refinement of the $Fe_{1-x}Ga_xBO_3$ crystals was performed by single crystal X-ray analysis (XRD). Electronic and magnetic properties of the crystals were studied by conventional Mössbauer spectroscopy. It is established that diamagnetic impurity leads to a slight rearrangement of the crystal structure and effect on the hyperfine parameters of the samples. We found that the magnetic properties of these crystals change significantly even with a small substitution of iron ions by gallium ions. From the temperature behavior of the Mössbauer spectra (Fig. 1), the Néel temperatures of $Fe_{1-x}Ga_xBO_3$ crystals for various gallium concentrations were determined.

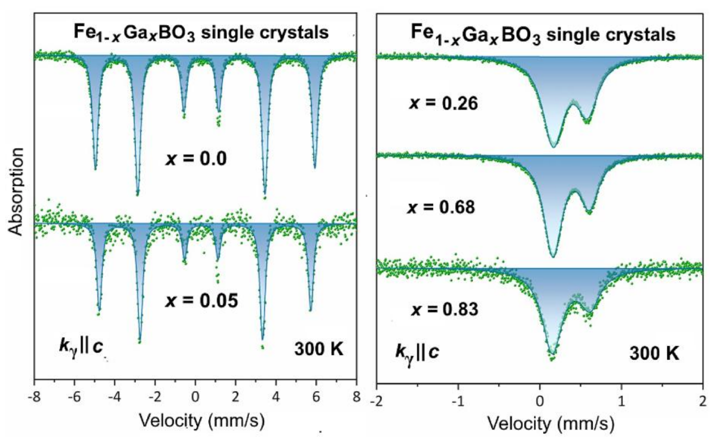

Figure 1. The room-temperature Mössbauer spectra of $FeBO_3$ single crystals diluted by diamagnetic gallium with various concentrations. The direction of the propagation vector of the Mössbauer radiation k_γ is normal to the basic plane (*ab*) of the crystals.

The obtained data on the quality and nuclear diffraction parameters of the crystals at various temperatures will show the way of introducing functional impurities into $FeBO_3$ crystals to optimize the parameters of their operation in synchrotron experiments. Such crystals will be widely in demand at all synchrotrons of the third and fourth generations.

This study was funded by RFBR, project number 19-29-12016-mk.

[1] Potapkin, V., Chumakov, A. I., Smirnov, G. V., Celse, J.-P., Rüffer, R., McCammon, (2012). *J. Synchrotron Radiat.*, **19,** 559
[2] Yagupov, S., Strugatsky, M., Seleznyova, K. et al. (2018). *Cryst. Growth Des.* **18**, 7435.
[3] Smirnova, E.S., Snegirev, N.I., Lyubutin I.S. et al. (2020). *Acta Cryst. B.* **76**, 1100.
[4] Snegirev, N., Mogilenec, Yu., Seleznyova, K. et al. (2019). *IOP Conf. Ser. Mater. Sci. Eng,* **525**, 012048.

Keywords: iron-gallium borate single crystals, flux growth, XRD analysis, Mössbauer spectroscopy