Rietveld refinement for yttrium aluminium borates from neutron- and X-ray diffraction

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Abstract

Yttrium aluminium borate YAl\textsubscript{3}(BO\textsubscript{3})\textsubscript{4} (YAB) single crystals have excellent non-linear optical properties, and doped YAB crystals have important applications in laser engineering. Neutron- and X-ray powder diffraction measurements were performed on pure YAB and doped YAl\textsubscript{1.5}Ga\textsubscript{1.5}(BO\textsubscript{3})\textsubscript{4} (YAB : Ga\textsubscript{1.5}) specimens to analyse the crystallographic parameters. The Rietveld refinement showed that no lattice distortion is caused by Ga doping, while the lattice parameters increased by about 1\% on Ga doping. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Yttrium aluminium borate YAl\textsubscript{3}(BO\textsubscript{3})\textsubscript{4} (YAB) single crystals have excellent non-linear optical properties, and doped YAB crystals have important applications in laser engineering [1]. Recently, the preparation and characterisation of doped YAB crystals are in the focus of interest [2,3]. YAB crystals have suitable sites for some rare-earth elements at the Y\textsuperscript{3+} site (Nd\textsuperscript{3+}, Yb\textsuperscript{3+}, La\textsuperscript{3+}) or other doping ions at Al\textsuperscript{3+} site (Cr\textsuperscript{3+}, Ga\textsuperscript{3+}). The knowledge of the crystallographic parameters is important when characterising the optical properties of YAB crystals.

The space group of YAB is hexagonal R3\textsuperscript{2} (No. 155) with trigonal symmetry [4,5]. Most of the crystallographic studies originate from X-ray diffraction works, where the scattering of the relatively large yttrium (or other rare-earth) atoms predominates over that of the smaller atoms. However, in neutron diffraction the scattering of smaller atoms is comparable with those of rare-earth elements; therefore the combined application of X-ray and neutron diffraction could be expected as a helpful tool.

In this work we present the results on YAl\textsubscript{3}(BO\textsubscript{3})\textsubscript{4} and YAl\textsubscript{1.5}Ga\textsubscript{1.5}(BO\textsubscript{3})\textsubscript{4} (YAB : Ga\textsubscript{1.5}) samples studied by neutron and X-ray diffraction.

2. Experimental

YAB single crystal was grown by top-seeded high-temperature solution (flux) method [2]. The single crystal was powdered into fine grains to obtain good powder spectrum suitable for Rietveld refinement. YAB : Ga\textsubscript{1.5} sample was prepared by solid-state reactions [3].

The neutron diffraction measurements were performed at the 10 MW Budapest research reactor using the PSD neutron diffractometer [6] with monochromatic wavelength of \( \lambda = 1.0577 \) Å. The absorption of boron for neutrons is extremely high; therefore thin sample holder was used with a diameter of 5 mm, resulting in a transmission of about 50\%. The X-ray spectra were measured by a Philips X-ray diffractometer with monochromatic Cu K\textsubscript{α1} (\( \lambda = 1.5406 \) Å) radiation.

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3. Results

The intensity contrast between the corresponding Bragg reflections in the neutron and X-ray diffraction spectra is large, because of the different scattering amplitudes of the constituent elements with respect to the applied radiation. The difference between YAB and YAB:Ga1.5 spectra is also pregnant for both the neutron and X-ray cases.

For data treatment the FullProf’98 Rietveld refinement program was applied [7]. The space group of YAB is hexagonal R32, and the starting values for the atomic position parameters were taken from Ref. [5]. The refinement resulted in a reasonable agreement between measured and calculated pattern as it is shown for the YAB:Ga1.5 sample in Fig. 1. The characteristic crystallographic data are collected in Table 1.

As an important result we can conclude that the atomic position parameters have the same values — within limits of error — for YAB and YAB:Ga1.5 specimens. This means that no crystal distortion occurred although 50% of Al³⁺ ions were substituted by Ga³⁺ ions having larger atomic radius. The lattice parameters are also included in Table 1, they show an increase of about 1% on Ga doping.

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References