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Synthesis and characterization of a novel nonlinear optical material $Mg_2Na_2ZnB_4O_{10}$

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Abstract

A novel borate compound with the chemical formula $Mg_2Na_2ZnB_4O_{10}$ (MNZB) has been synthesized first time from the 2MgO-Na_2O-ZnO-$2B_2O_3$ system via solid-state reaction. The obtained polycrystalline borate material MNZB was characterized by powder X-ray diffraction, Fourier transform infrared (FT-IR) spectroscopy, and second harmonic generation (SHG) measurement. Ultraviolet-visible spectroscopy has been carried out to analyze transmission of the MNZB crystals grown by slow cooling method. The optical band gap has been estimated. The functional groups were identified by using the FT-IR data. The SHG efficiency of the crystal was obtained by the Kurtz powder technique and it is found to be 2.78 times that of potassium dihydrogen phosphate. The results are presented and discussed.

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Keywords: Nonlinear optical material, X-ray powder diffraction, Fourier transforms infrared spectroscopy, ultraviolet-visible spectroscopy, second harmonic generation;

1. Introduction

Now a day, research in nonlinear optics (NLO) is being flourished because NLO materials have played an important role in laser science and related technology [1]. They are playing main part in generating laser beams in the ultraviolet and visible regions and applications like signal processing, medical surgeries, optical data storage

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devices, optical data communication, colour displays, entertainment purposes and many more [2-5]. Borates are presently receiving great attention from material scientists due to their excellent nonlinear and linear optical, piezoelectric, luminescent and other useful physical properties for technical applications [6]. In recent few years, several novel NLO crystals have been developed for efficient second-harmonic generation (SHG) and other parametric processes. The requirements for the excellent NLO crystal includes high NLO coefficient, moderate birefringence for phase matching, high transparency at the wavelength of interest, non-hygroscopic nature, high-laser-damage threshold, good mechanical and thermal properties [7-9]. In the inorganic family crystals, borate crystals have attracted much attention due to their intrinsic favorable properties. The borate based NLO crystals like lithium borate LiB_3O_5 (LBO) [10], β-$Ba_2B_2O_4$ (BBO) [11], $CsLiB_5O_{10}$ (CLBO) [12], $SrBe_2B_2O_7$ (SBBO) [13], $KBe_2BO_3F_2$ (KBBF) [14], $K_2Al_2B_2O_7$ (KAB) [15], $Re_2CaB_{10}O_{19}$ (ReCB) [16], $K_3YB_6O_{12}$ (KYB) [17], $La_2CaB_{10}O_{19}$ (LCB) [18], and $Li_2Pb_2CuB_4O_{10}$ [19] have excellent transmission properties in combination with NLO behavior. Therefore, intense work has begun in developing new materials for NLO applications and expanding the frequency range provided by the conventional laser sources [4, 20].

In the present investigation, the synthesis of novel magnesium sodium zinc borate (MNZB) polycrystalline material and its optical study has been reported. The crystal of it was grown by melt slow cooling technique. In the search of new compound material, we have tried new system $2MgO$-Na_2O-ZnO-$2B_2O_3$ to synthesize MNZB. Powder X-ray diffraction (XRD) was used to analyze crystal structure. The ultraviolet visible (UV-vis) spectroscopy study was carried out to study transmission and determine optical energy band gap. Functional groups were studied by Fourier transform infrared (FT-IR) spectroscopy. Second-harmonic generation (SHG) efficiency of polycrystalline MNZB in comparison with potassium dihydrogen phosphate (KDP) was measured by using analogues setup as proposed by Kurtz and Perry in 1968 [21].

2. Experimental

2.1. Material and methods

Sodium carbonate (Na_2CO_3) and zinc oxide (ZnO) were purchased from Fisher Scientific, India. Magnesium oxide (MgO) was obtained from CDH, India. Boron trioxide (B_2O_3) was purchased from sd Fine chemicals, India. All the chemicals used for synthesis were of analytical reagent grade and used as received without further purification.

2.2. Solid-state synthesis of MNZB

The polycrystalline material was synthesized by solid-state reaction technique in programmable high-temperature resistive heating furnace. The chemicals MgO, Na_2CO_3, ZnO and B_2O_3 of 99.99% purity with appropriate amount were crushed with the help of mortar and pestle to make the homogeneous mixture. Then the homogeneous mixture was transferred to a platinum crucible and kept it in muffle furnace. Initially, the prepared material was heated at 450 ^oC for 6 h to make the mixture miscible. The mixture was further heated at 850 ^oC continuously for 10 h to decompose B_2O_3. The temperature was then increased up to 1000 °C to melt a charge and maintained constant for another 24 h. After that, muffle furnace was turned towards slow cooling with a rate of 3 $^oC/h$ to reach 650 ^oC and finally cooled to room temperature at a rate of 10 $^oC/h$. As the MNZB compound decomposes at high temperatures, the reaction temperature was carefully controlled. A polycrystalline material and few crystals were obtained and used for further study.

The expected reaction-taking place during synthesis is given below.

$$2MgO + Na_2CO_3 + ZnO + 2B_2O_3 \rightarrow Mg_2\,Na_2\,Zn\,B_4O_{10} + CO_2\uparrow$$

The crystallanity and phase formation of the polycrystalline sample was confirmed by powder XRD data recorded on a Rigaku’s MiniFlex-II X-ray Diffractometer. UV-vis transmission data was recorded using UV-vis spectrophotometer (Black-C-SR, Stellarnet, USA). The FT-IR spectrum was obtained at a room temperature with the help of Agilent Technologies FT-IR spectrometer.