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Alkaline earth yttrium borates: synthesis, characterization and calculation of unit cell parameters

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ABSTRACT

Purpose: Purpose of this paper, our object is solid state synthesis and investigation of structural and chemical characterization properties of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$ as members of alkaline earth yttrium borates.

Design/methodology/approach: In the synthesis procedure; barium carbonate, strontium carbonate, yttrium oxide and boric acid weighed an appropriate molar ratio and homogenized in an agate mortar. The mixture placed into a porcelain crucible to heat in high temperature oven at 900°C for 4 hours. After intermediate grindings, samples were cooled down to room temperature. Homogenized powders were characterized by Powder X-ray Diffractometer (XRD) to determine crystal structures. FTIR spectrum was taken to support the functional groups. Morphological properties and semi-quantitative analyse of the sample was performed by Scanning Electron Microscope/Energy dispersive (SEM/EDX).

Findings: The XRD patterns of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$ compounds indicate that crystallization procedure were completed successfully. The unit cell parameters of the compounds was calculated by Rietveld refinement method. In FTIR spectrum the vibrations of B-O bonds are determined via comparison to literature

Research limitations/implications: Implication the synthesis method has some disadvantages such as low homogeneity, non-uniform product etc. We tried to minimize these negative aspects in our research and succeeded.

Practical implications: Alkaline earth yttrium borates $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$ compounds were synthesized by solid state technique at 900°C. Unit cell parameters of the compounds were calculated by Rietveld refinement method and vibrations of functional group was indicated in FTIR spectrum.

Originality/value: Value of the paper is first time conventional synthesis of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$ compounds, calculation of unit cell parameters, and investigation of morphological and thermal properties

Keywords: $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$; Powder X-ray diffraction; Alkaline earth yttrium borates; Solid state chemist

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MATERIALS

1. Introduction

The In the past decades, much research interest has been focused on the synthesis and characterization of borate compounds of alkaline earth and rare earth elements for the exploration of nonlinear optical materials [1]. Several new rare earth (RE) and alkaline earth borates, such as $RECa_4O(BO_3)_3$, $REBaB_9O_{16}$, $REBa_3(BO_3)_3$ and $REBa_3B_9O_{18}$ have been synthesized [2]. RE and alkaline earth borates have attracted so much attention because many of these compounds not only have been explored as new kinds of nonlinear optical materials themselves but also they have been widely used as hosts in preparation of self-frequency-doubling lasers and PDP phosphors [3].

The inorganic compounds $Sr_3Y_2(BO_3)_4$ (SYB) has a orthorhombic structure with Pc21*n* space group. The structure of $Sr_3Y_2(BO_3)_4$ is formed by isolated BO_3 triangles, strontium-oxygen polyhedra, and yttrium-oxygen polyhedra [5]. The structure information of $Sr_3Y_2(BO_3)_4$ indicated that longer distance between the rare earth ions in the crystal structure of $Sr_3Y_2(BO_3)_4$ can predict to result in higher doping concentration [4].

In 1999, Khamaganova et al. [5] have reported the compounds $Ba_3Ln(BO_3)_3$ (Ln=La-Lu,Y), α- $Ba_3YB_3O_9$ being one of them but the β-phase of $Ba_3YB_3O_9$ was not reported in his work. Also, Li et al. [1] have reported the crystal structure of β-$Ba_3YB_3O_9$.

In this paper $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$ were prepared by standard solid-state reaction and crystal structure of this compounds analysed by Rietveld refinement method by X-ray powder diffraction data.

2. Material and method

The samples of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$ were prepared by high temperature solid-state reaction. The starting materials MCO_3 (M: Ba; Sr), H_3BO_3 and Y_2O_3 were analytical-grade. Stoichiometric amounts of the reactants were weighed separately on an analytical balance and thoroughly mixed in an agate mortar, and then fired in air at 900°C for 4h in a covered porcelain crucible. After these steps the furnace was slowly cooled down to room temperature. The final samples were homogenized again to complete the characterization process.

PANanalytical X'Pert PRO Diffractometer (XRD) with Cu Kα (1.5406 Å, 45 kV and 30 mA) radiation was used to determine X-ray powder diffraction (XRD) pattern and data. Perkin Elmer Spectrum 100 FTIR Spectrometer was used to take Fourier transform infrared spectrum (FTIR) in the range 4000 to 650 cm^{-1}. Scanning electron micrographs were achieved in SEM JEOL 6390-LV. Perkin Elmer thermogravimetric analyser was used to determine thermal behaviour of the compounds.

3. Results and discussion

In Figure 1, the XRD patterns of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$ compounds are shown. When we compare XRD patterns to database, the diffractions are corresponded to $Ba_3Y(BO_3)_3$ (ICSD:09-9180)and $Sr_3Y_2(BO_3)_4$ (ICSD:05-4759) compounds which are marked by plus and point, respectively. The XRD patterns of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$ compounds indicate that crystallization procedure were completed successfully. Therefore, the unit cell parameters of two compounds were calculated by Rietveld refinement method using observed pattern (Table 1). $Ba_3Y(BO_3)_3$ is crystallized in hexagonal system with calculated unit cell parameters a=9.419 Å, c=17.595 Å and space group P63cm. $Sr_3Y_2(BO_3)_4$ is crystallized in orthorhombic system with calculated unit cell parameters a=7.391 Å, b=8.694 Å, c=15.971 Å and space group Pna21.

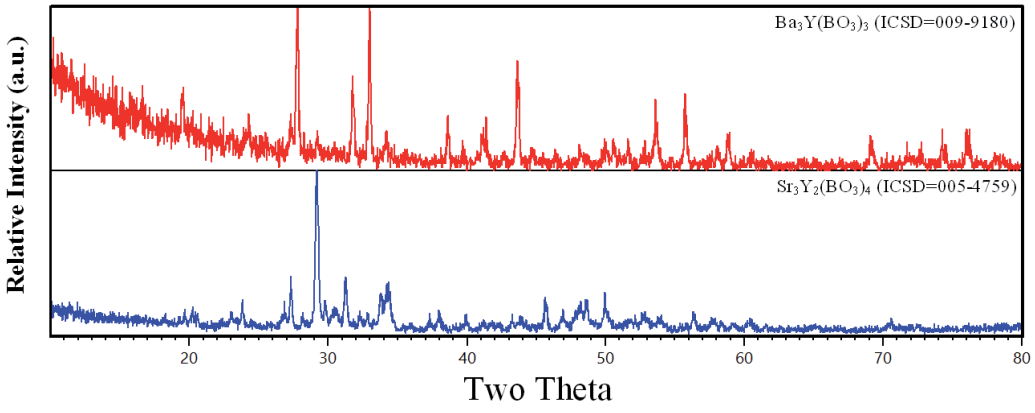

Fig. 1. The XRD patterns of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$

Table 1.
The observed and calculated XRD data of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$

$Ba_3Y(BO_3)_3$			$Sr_3Y_2(BO_3)_4$		
$d_{obs.}$ (Å)	$d_{calc.}$ (Å)	h k l	$d_{obs.}$ (Å)	$d_{calc.}$ (Å)	h k l
4.16864	4.15479	1 1 2	3.63987	3.62938	1 2 1
3.68799	3.67123	1 1 3	3.33487	3.34246	2 0 2
3.15824	3.21117	1 1 4	3.20850	-	-
3.03340	3.03737	1 2 1	3.08082	3.06180	1 2 3
2.91958	2.90912	1 2 2	3.01827	3.02780	0 1 5
2.81911	2.81403	1 1 5	2.90237	-	-
2.71786	2.71982	0 3 0	2.86426	2.86034	2 1 3
2.32810	2.33289	2 1 1	2.79726	2.79777	1 1 5
2.24507	2.24270	1 3 1	2.74880	2.73585	1 2 4
2.21185	2.12041	1 2 6	2.54117	2.54080	1 3 2
2.07967	2.07335	2 2 4	2.07422	2.08174	0 4 2
1.94070	1.95381	2 2 5	1.82470	1.81206	3 3 2
1.50053	1.49981	2 2 9	1.31581	1.31737	2 6 2

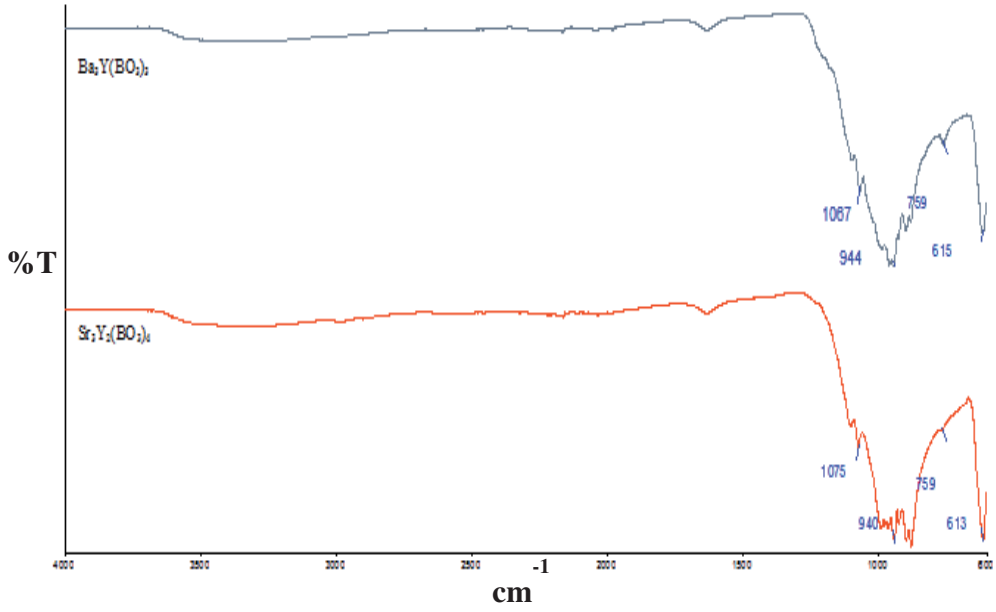

Fig. 2. FTIR spectrums of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$

Figure 2 displays Fourier transform infrared spectrums of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$. The vibrations at 610-615 cm^{-1}, 750-760 cm^{-1}, 940-950 and 1065-1075 cm^{-1} ranges are belongs to plane bending ν_4, out of plane bending ν_2, symmetric stretch ν_1 and antisymmetric stretch ν_3 of BO_3 group, respectively [6].

Figure 3 exhibits SEM micrographs of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$ compounds. Figure 4 presents EDS results. The distributions of the samples are seen homogeneous with particle size 2-5 μm.

The thermograms of the results of thermogravimetric analysis of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$ are given in Fig. 4.

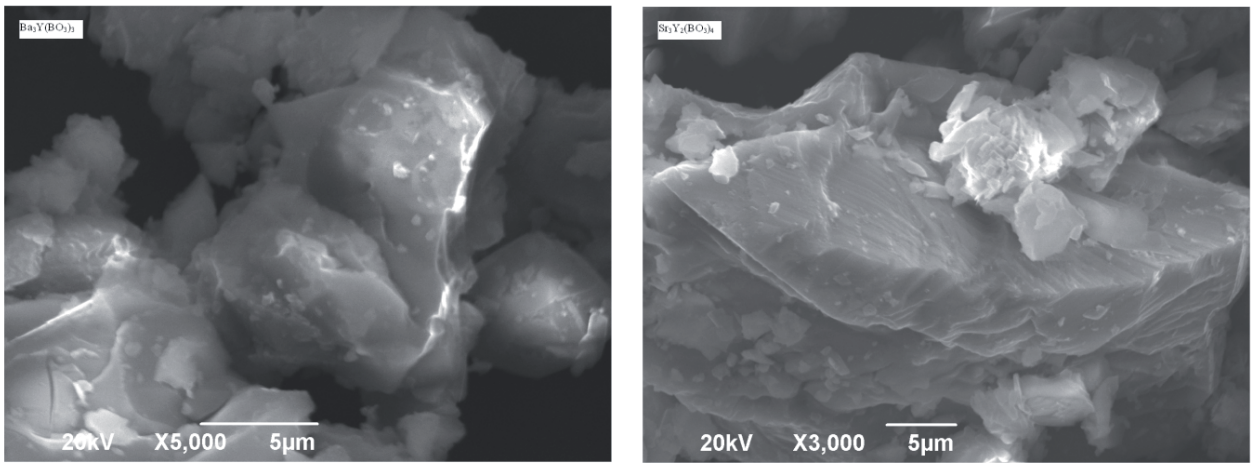

Fig. 3. SEM micrographs of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$

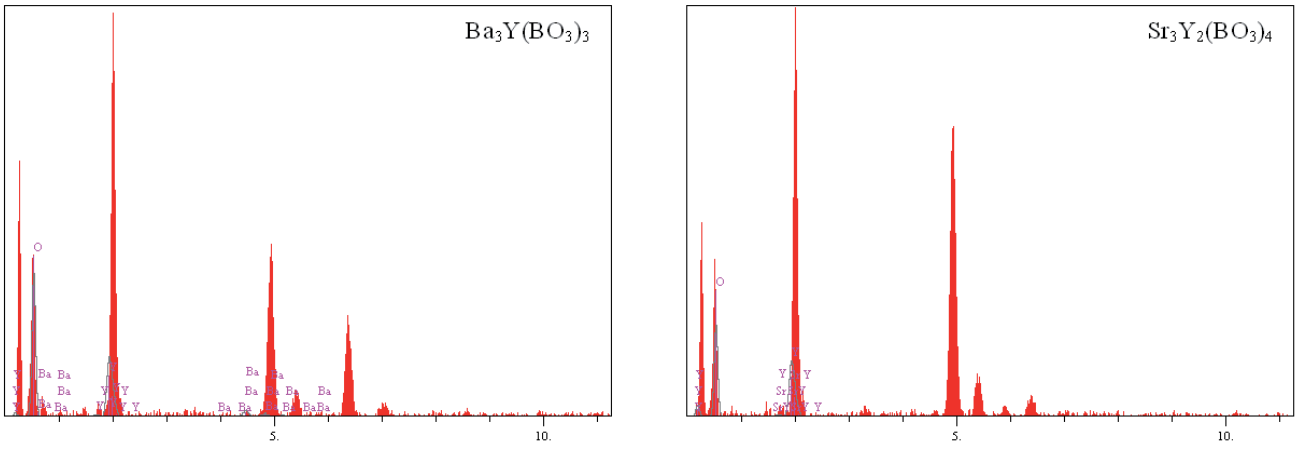

Fig. 4. EDS analysis of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$

There is only one mass loss (500-700°C range) in both thermograms which is related to decomposition of the yttrium borates in the range of room temperature to 1190°C.

4. Conclusions

Alkaline earth yttrium borates $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$ compounds were synthesized by solid state technique at 900°C. Unit cell parameters of the compounds were calculated by Rietveld refinement method and vibrations of functional group was indicated in FTIR spectrum. Morphological and thermal properties were supported the stable and homogeneous crystal structure of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$.

Acknowledgements

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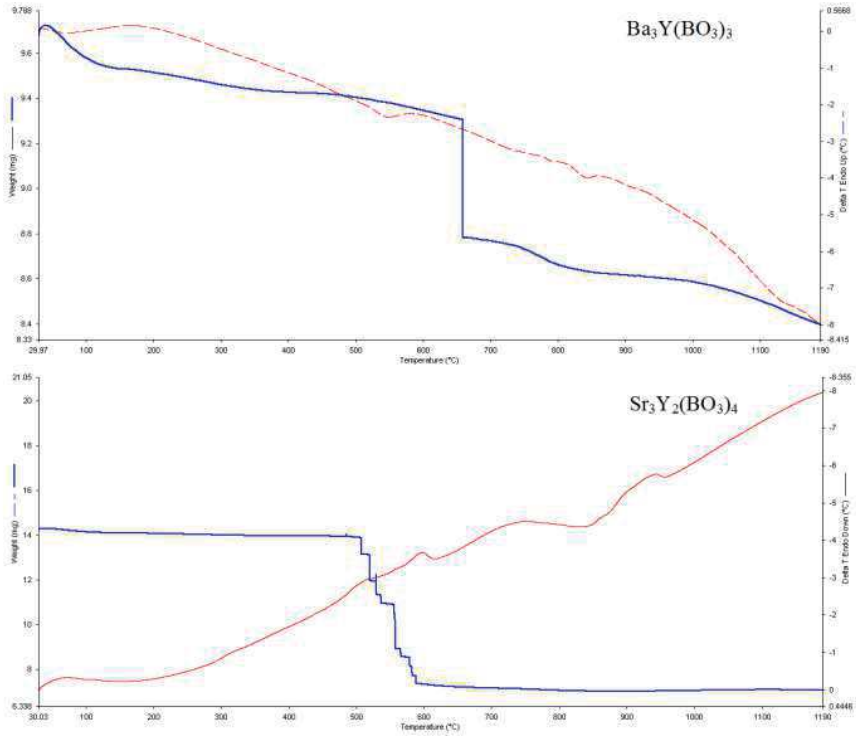

Fig. 5. Thermograms of $Ba_3Y(BO_3)_3$ and $Sr_3Y_2(BO_3)_4$

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