

Structural and Optical Studies of Barium Nitrate (BN) Crystals Grown by Slow Evaporation(SE) Technique

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Abstract- *Inorganic Non Linear Optical Barium Nitrate (BN) crystals were grown by slow evaporation technique. Solubility of BN salt was 10.35 gm/100 ml. good transparent crystals were grown after 5-6 weeks at ambient temperature. Elements of BN crystals were confirmed by the EDX. Structural analysis of grown crystals from powder XRD studies with unit cell parameter and volume. SHG efficiency has been studied by Kurtz Perry method. Results are reported in this paper.*

Keywords- EDX, XRD, SHG.

I. INTRODUCTION

In order to grow good quality of crystals, it is essential to increase purity up to a respectable level. [1] Crystals of Barium Nitrate are Raman-active crystals have the good physical and optical features and possess high Raman gain co-efficient. [2] Ba(NO₃)₂ composite solid electrolytes exhibit high ionic conductivity and good mechanical properties and are found to be promising materials for solid state batteries, fuel cells, electrodes etc. [3] X-RAY mapping in electron microscopes with energy dispersive spectrometry (EDS) builds on the basics of qualitative X-ray microanalysis by providing a visual representation of the elements presents. [4] Nonlinear optical materials are expected to play a major role or prominent role in the technology of photonics including optical information processing and frequency conversion. [5-8]. Now days, frequency conversion is a common tool to create blue or infrared laser light in the laboratory, i.e. at frequencies where no alternatives laser sources are available. This experiment will explore the process of Second Harmonic Generation by studying the conversion of a high power infrared beam at a wavelength of 980 nm into blue light at wavelength of 490 nm. [9]

II. EXPERIMENTAL PROCEDURE

CRYSTAL GROWTH BY SLOW EVAPORATION TECHNIQUE

Barium Nitrate (BN) crystals were synthesized by GR grade salt of BN to make aqueous solution with double

distilled water. In this technique, stirrer mechanism was used to stir well the solution, the speed of stirrer was kept at 1200 rpm. The saturated solution was prepared 60-65 minutes. After making solution, its filtered and kept for slow evaporation at ambient temperature. The seed Crystals were grown after 5-6 weeks.

CHARACTERISATION METHODS

Energy Dispersive X-Ray Spectroscopy (EDX)

Presence of elements in powdered form of BN crystals was carried out with net counts and energy of beam 0-10 keV.

X-Ray diffraction (XRD)

The grown BN crystals were studied to single crystal X-Ray diffraction (XRD) using diffractometer with Cu K α radiation ($\lambda = 1.5418 \text{ \AA}$) radiation to confirmed the crystal structure.

Second Harmonic Generation (SHG)

SHG conversion efficiency of BN crystals were measured by the Kurtz and Perry method; Q-switched Nd:YAG laser using to measure first harmonics output of powdered crystalline sample.

III. RESULTS AND DISCUSSION

Slow evaporation technique is suitable for formation of BN crystals. The aqueous solution of BN salt was prepared with double distilled water. The solubility limit of BN was 10.35 gm./ 100 ml. Seed crystals of BN were seen after 4-5 days .Grown BN crystals were good quality and transparent. The aqueous solution and grown BN crystals are shown in fig.1 and fig.2.



Fig: 1 Grown BN crystals in solution



Fig: 2 Grown BN crystal

Elemental analysis of grown material was done by the Energy Dispersive X-Ray (EDX). Powder form of BN crystals were taken for the analysis.

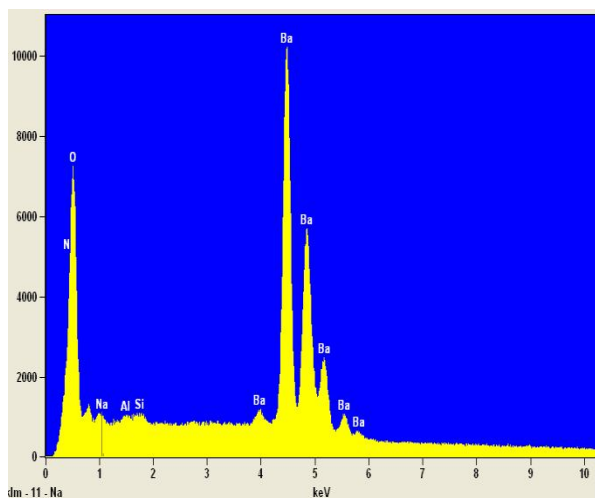


Figure: 3 EDX pattern of powder form of BN crystals

Table 1: Amount of elements present in BN crystals

Elements	Weight%	Atom%
<i>N</i>	12.13	32.74
<i>O</i>	20.02	47.32
<i>Na</i>	0.58	0.95
<i>Al</i>	0.13	0.19
<i>Si</i>	0.30	0.40
<i>Ba</i>	66.85	18.41
<i>Ba</i>	—	—
Total	100.00	100.00

Before the geometrical constraints for X-Ray interference are derived the interactions between X-Rays and matter have to be considered. There are three different types of interaction in the relevant energy range. In the first, electrons may be liberated from their bound atomic states in the process of photoionization. Since energy and momentum are transferred from the incoming radiation to the excited electron, photoionization falls into the group of inelastic scattering process. In addition, there exists a second kind of inelastic scattering that the incoming X-Ray beams may undergo, which is termed Compton scattering. Also in this process energy is transferred to an electron, which proceeds, however without releasing the electron from the atom. Finally, X-Rays may be scattered elastically by electrons, which is named Thomson scattering. [10]

Powder XRD is useful to structural study of BN crystals. XRD data of BN crystals were collected from a single crystal X-Ray diffractometer with Cu α radiation. The unit cell parameter are $a=b=c=8.1184 \text{ \AA}$. The values of $\alpha=\beta=\gamma=90^\circ$. Volume of the unit cell is 535.0709 \AA^3 . Grown BN crystals were crystallize in cubic system with the space group $P2_13$ with the number of molecules per unit cell (Z) for BN crystal is found to be 4.

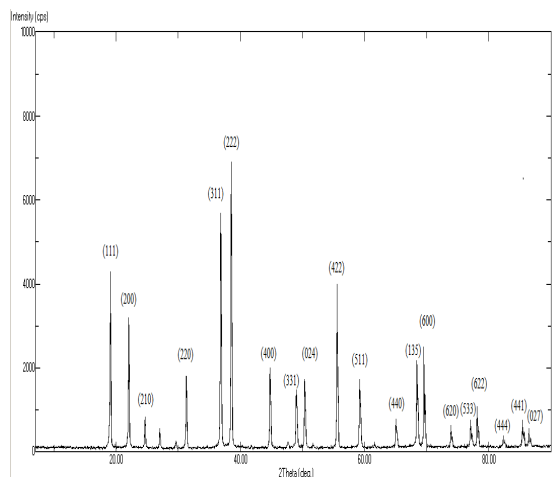


Fig: 4 XRD pattern of powder of BN crystals

Figure-4 shows the powder XRD pattern with well-defined peaks at specific 2θ values of the powder of synthesized BN crystals. XRD performed with range (2θ) 10° to 90° ; at a scan speed $2^\circ/\text{min}$ using Cu $K\alpha$ radiation of 0.154nm wavelength. The analysis of XRD data of BN crystals powder confirms the phase formation of the material in cubic crystal structure and matched well with standard JCPDS data (card no: 76-0378, 76-0920). The sharp peak observed in the spectrum reveals the purity and crystallinity of the grown materials.

Second Harmonic Generation (SHG) test was done by the Kurtz and Perry method to measure the NLO efficiency of the grown BN crystals. The power of fundamental beam was monitored by a split beam technique, in one channel of the power meter. The sample was ground in the form of fine powder of known grain size and passed between two glass plates. The sample size was kept larger than the beam cross section. The generated harmonic was passed through a 1064nm narrow pass filter and fed to other channel of the power meter. The ratio of the fundamental and harmonic intensities determines the efficiency of the sample. [11] The input power of the laser beam was measured to be 1 mJ/pulse .

First harmonics output of powdered crystalline sample was 1064 nm with pulse width of 10 ns and repetition rate of 10 Hz , Method found that the SHG of the compound is 52 mv .

IV. CONCLUSION

In the present study, the BN crystals have been successfully grown by slow evaporation technique at ambient temperature. Good quality and transparent crystals are formed after 5-6 weeks. The average size is $6\text{mm} \times 5\text{mm} \times 2\text{mm}$. Element confirmed by the EDX pattern. Nature of crystals and lattice parameter were studied by the XRD spectrum. Sharp peaks give information of the crystallographic planes to determine lattice parameters and crystal structure. Grown BN crystals were formed in cubic system. High transparency of BN crystals is very important for NLO applications. The value of SHG efficiency of BN crystals was good compared to the KDP crystals.

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