

Raman Spectroscopic, Structural and Thermal studies of Barium Nitrate crystals grown by Slow Evaporation Technique

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Abstract: In this study Barium Nitrate crystal was grown by slow evaporation Technique. High Raman Gain Coefficient Barium Nitrate crystal was characterized by Laser Raman Spectra shows three Stokes and one AntiStokes lines. The crystals obtained were structurally characterized by X-ray diffraction (XRD). Crystallite size was measured by the data obtained from XRD spectra. Compositional reaction was studied by the Thermo Gravimetric Analysis. The graph of thermal behavior shows that titled compound was thermally stable up to temperature 480°C.

Keywords: Laser Raman Spectra, X-Ray Diffraction, Thermogravimetry Analysis.

1. INTRODUCTION:

Barium Nitrate (BN) crystal was also known as Raman crystal. Raman active crystals have the good physical and optical features and possess high Raman gain coefficient. [1]. The Stimulated Raman Scattering (SRS) conversion in the BN crystal is efficient. Eremenko et al 1980. BN crystals were grown by slow evaporation technique. Grown crystals were crystallizes in the cubic system. [2]. X-Ray diffraction able to give detailed information about crystal structure of titled compound. The temperature of decomposition reaction that are the most suitable for the identification and quantitative determination of compound is, however highly sensitive to both the materials properties and the conditions of the analysis. In present study we have to characterize BN crystals by Laser Raman Spectroscopy (LRS), X-Ray diffraction (XRD) and Thermogravimetry analysis (TGA).

2. MATERIALS:

Ba(NO₃)₂ Crystals were grown with taking salt with purity maximum up to 99% of Barium Nitrate in double distilled water. Saturated solution was kept for slow evaporation. Good quality transparent crystals were obtained after 5 weeks.

3. METHOD:

Grown crystals were characterized by SRS, XRD and TGA. Raman Spectra of BN crystals were obtained by the Renishaw Raman Microscope pumped at 532 nm wavelength. 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. TGA was examined by the Pyris -6 TGA heat from 25.00°C to 910.00°C at 10.00°C/min.

4. RESULT AND DISCUSSION:

LRS of BN crystals are at 300K temperature shown in Fig-1. This process is known as the Raman effect: the incoming photon excites the scattering matter from its electronic ground state into a virtual state, from which it relaxes under the emission of a Raman scattered photon of smaller or higher energy (Stokes or anti-Stokes scattering) depending on the initial and final vibrational levels.[3]. The figure shows a spectrum of the forced Raman Scattering of molecular Ba(NO₃)₂ crystal. The dominating line is 1047 cm⁻¹ what are YAG:Nd laser, generating radiation at 532 nm and interaction with this medium, at room temperature gives wavelength of 563 nm (1st Stokes), 587 nm (2nd Stokes), 591 nm (3rd Stokes) and also 507 nm (1st AntiStokes). The Raman spectra of BN crystal are dominated by strong narrow (0.4 cm⁻¹) peak at 1047 cm⁻¹, which correspond to a symmetric breathing mode vibration of the NO₃ molecular group. [5] BN crystal has become a key SRS material, owing to possessing the highest Raman gain coefficient among the artificial crystals known so far, which is 47 cm/GW at 532 nm.[5-6]

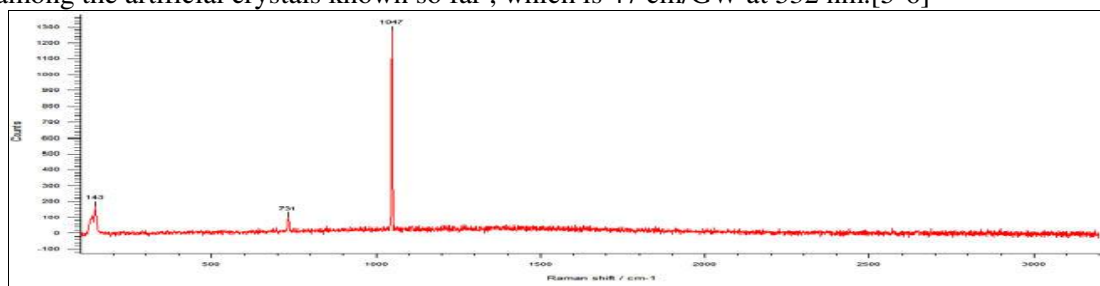


Figure 1: LRS of BN crystal

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. XRD spectra of BN crystals are shown in Fig.2. 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.

The crystallite size was calculated from XRD spectrum using the well-known Debye –Scherre formula.[7]

$$D = (0.9\lambda / \beta \cos\theta)$$

Average crystallite size was found 96.94 nm.

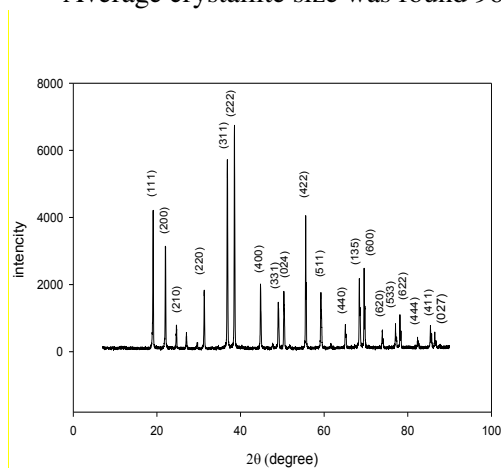


Figure 2: XRD pattern of BN crystals powder form.

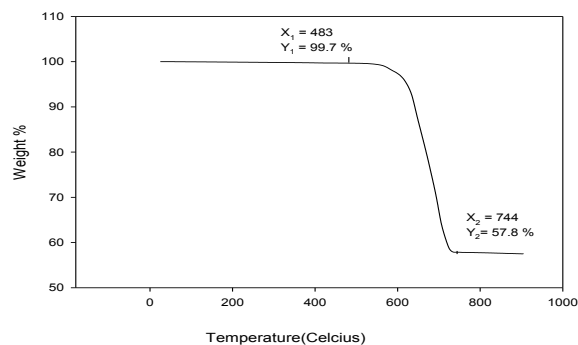


Figure 3: TGA thermogram of BN crystals.

Thermal properties of Barium Nitrate crystals were studied out by Thermogravimetry analysis (TGA), which were carried out between 25°C and 910°C with heating rate $10.00^\circ\text{C}/\text{min}$. The corresponding curves are presented in Fig.3. From the TGA analysis curves that the grown Barium Nitrate material decomposed about from 482.59°C to 744.42°C , and 57% of the compound gets decomposed completely. The grown Barium Nitrate crystals thermally stable up to approx. 480°C .

5. CONCLUSION:

Our study of the Barium Nitrate crystal made it confirmed that grown crystal was matched with standard stokes line peak 1047 cm^{-1} . Ba-n crystal has Highest Raman Gain coefficient among the artificial crystals was $47 \text{ cm}/\text{GW}$ at 532 nm pumped wave length of source. Ba-N crystal possesses cubic crystal structure, with lattice parameters $a=b=c=8.1184 \text{ \AA}$ and average crystallite size was 96.94 nm shows good quality crystal. Grown BN crystal thermally stable has endothermic reaction with its surrounding.

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REFERENCES:

1. Shuanghong Ding, Xingyu Zhang, Qingpu Wang, Peng Jia, Chen Zhang, Buo Liu, (2006) Science Direct, Optic Communications 267, 480-486.
2. Vanish.H.Tandel, I.B.Patel, Hitesh Patel,IJSART, Vol.2, Issue.9, September 2016, pp.128-130.
3. Gerhard Mestl, Journal of Molecular catalysis A: Chemical 158(2000), 45-65.
4. P.G.Zverev, T.T Basiv, V.V Osiko, A.M.Kulkov, V.N.Voitesk hovskii, V.E.Yakoboson, Opt. Matter.11 (1993) 315.
5. J.Simons,H.Pask,P.Dekker,J.Piper, Opt. Commun. 2-29 (2004) 305.
6. J.T.Murray, R.C.Powell, N.Peyghambarian, D.Smith, W.Austin, R.A.Stolzenberger, Opt.Lett.20 (1995)1017.
7. R.M.Almeida and E.E.J.Christensen, Sol-Gel Sci. Tech. 8 (1997) 409-413.