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Studies on characteristics of Glycine barium nitrate crystal

M.B. Jessie Raj[1,]* and J. Joseph Prince[2]

[1]Department of Physics, Bishop Heber College, Trichy.

[2]Department of Physics, Anna University of Technology, Trichy.

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ABSTRACT

The title compound of C2H5NO2·Ba (NO3) Glycine Barium Nitrate (GBN), a semiorganic glycine additive material has been grown from slow evaporation solution growth technique at room temperature.. The grown single crystals have been analyzed by powder crystal X-ray diffraction. The title compound has good optical transmission in the entire visible region. The optical band gap has been estimated using Tauc's plot. Its relative SHG efficiency has been tested by Kurtz powder method and it quite interesting that it acts as poison, not favoring NLO efficiency. Thermal stability of the grown crystal was investigated by thermo gravimetric and differential thermal analyses.

Introduction

The demand for large-size type single crystals has increased sharply in recent years because these crystals have important piezoelectric, ferroelectric, electro-optic and nonlinear optical properties [Rajesh P et al., 2009]. It is substantially known that additives are one of the significant factors influencing the growth kinetics, morphology and quality of the crystals. In the recent past, many organic amino acids are mixed with the inorganic salts in order to enhance its physical and chemical properties. Previous reports shows that the amino acid group of glycine is mixed with H2SO4 [S.Hoshiono et al., 1957], CaNo3 [S. Natarajan et.al., 1984], SrCl2 [P. Narayan et al., 1975], CoBr2 [K.Ravi kumar et. al.1985] to form a single crystals. But none of these are reported to have nonlinear optical (NLO) property. In this paper, we report the growth of Glycine Barium Nitrate (GBN), C2H5NO2·Ba(NO3) single crystals by slow evaporation technique and its characterization.

Materials and Methods

Equimolar quantity of Glycine with additives namely, Glycine Barium Nitrate (GBN) were used for synthesis. The reaction taking place is given as follows:

$C_2H_5NO_2 + Ba_2\ (NO_3) \rightarrow C_2H_5NO_2.Ba_2\ (NO_3)$

In order to grow good quality crystals, it is essential to increase purity up to a respectable level. In the present study, the commercially available Analytical grade salt was dissolved in deionized water and the recrystallised material was used to prepare the saturated solution. The resulting aqueous solution was filtered and allowed to evaporate under optimized conditions to grow crystals by slow evaporation method at room temperature. Transparent good quality crystals were harvested after a particular period.

Characterisation

Powder XRD studies

The grown crystals are confirmed by Riagaku X-Ray diffractometer with Cu Kα (λ = 1.5418Å) radiation. The samples were scanned for 2θ values from 10˚ to 90˚ at a rate of 2˚/min. Figure 1 shows the Powder XRD pattern of the GBN crystal. The sharp peaks observed in the spectrum reveals that the purity and crystalinity of the grown material. The result obtained is good agreement with the reported values.[S.Dhanakodi et.al., 2002, T. Balakrishnan 2006]. Comparing the XRD pattern, the incorporation of the additives in glycine lattice is confirmed.[Figure. 1]

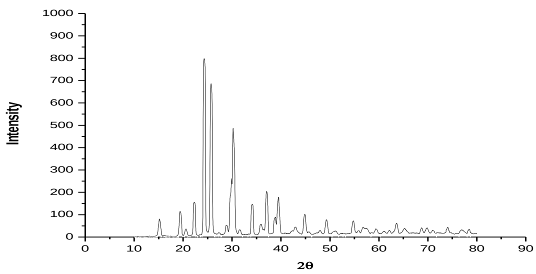

Figure 1: Powder XRD spectrum of GBN crystal

Linear optical studies:

Optical properties of the grown crystals were studied using Lamda-35 UV spectrometer. Optical transmittance and absorption were recorded for the crystals of thickness approximately around 2mm.

UV transmittance studies:

The optical property of the title compound has been assessed by using LAMBDA-35 UV spectrometer. As the crystal is colorless, there is a very low absorption in the entire visible region which is the most desirable property of the crystals used for NLO applications. It is observed from the spectrum that GBN has a wide optical transmission window (350–1100 nm). It has good transparency and the lower cutoff wavelength of the crystal is found to be 350 nm, and thus to ascertain the fact that the crystal can be used for laser applications. The recorded spectrum is shown in the Fig. 2. High

Tele:

E-mail addresses: mbjessie_phy@yahoo.co.in

transmittance % is observed from 350nm which clearly indicates the crystal possess good optical transparency for SHG of Nd:YAG laser.

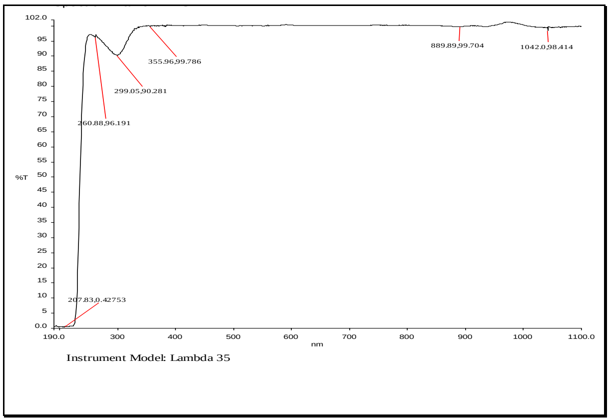

Figure 2: UV transmission spectra of GBN crystal

The dependence of optical absorption coefficient and the photon energy helps to study the band structure and the type of transmission of electrons [V.Ciupina et.al., 2004]. The optical band gap of the crystals was determined using Tauc's plot. The value of band gap energy were estimated from the graph between (hν) and $(\alpha h\nu)^2$ by extra plotting the linear portion of curve to zero absorption. Here α is the absorption coefficient and hν the photon energy. The band gap energy calculated is 5.4 ev for GBN crystals. As a consequence of wide band gap, the crystals under study have relatively longer in the visible region [A.J. Ekpunodi , 2006]. The internal efficiency of the device also depends upon the absorption coefficient. Hence by tailoring the absorption coefficient and tuning the band gap of the material, one can achieve devised material, which is suitable for fabricating various layers of the optoelectronic devices as per requirements [G.Bhagavannarayana et.al., 2009].

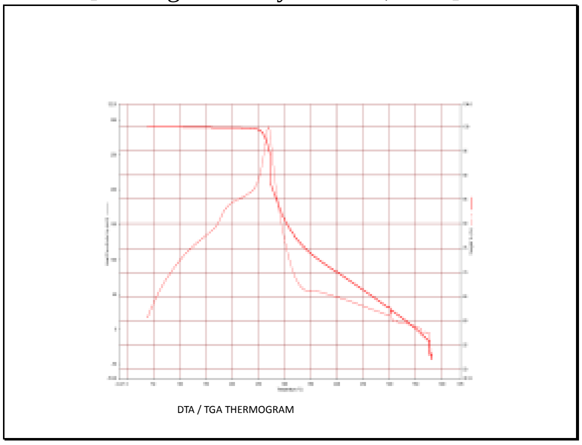

Figure 3: TGA/ DTA Thermogram of GBN crystal

TGA/ DTA Studies

The TGA reveals that the sample is thermally stable and has relatively higher melting point. TGA/DTA studies establishes the good thermal stability of the crystal up to the melting point 270 ºC suggesting the crystals to be a potential for laser application where crystal with stand high temperature. Since there is no decomposition observed up to the melting point, crystallization can be done by melt method also.

NLO Efficiency

The second harmonic generation (SHG) conversion efficiency of GBN was measured by powder Kurtz and Perry power technique.[S. K. Kurtz and T.T. Perry, 1968] The crystal was grounded into a fine powder and densely packed between two transparent glass slides. A Q switched Nd: YAG laser emitting a fundamental wavelength of 1064nm (pulse width 10 ns) was allowed to strike the sample cell normally. The SHG output 532nm (green light) was finally detected by the photomultiplier tube. A sample of potassium dihydrogen phosphate (KDP), also powdered was used for the same experiment as a reference material in the SHG measurement. It is surprising that glycine with additive barium nitrate is acting as poison to NLO property.

Conclusion:

In the present study, the crystals of GBN have been grown by solvent evaporation technique at room temperature. The crystals were harvested after 3 weeks. The crystals were transparent and their size and external shape are sensitive to the additive present in the solution during growth. Crystalline nature and incorporation of additives in the glycine lattice were confirmed by powder XRD pattern. UV spectra of the crystals are highly transparent, which is most desirable property for NLO applications. The crystals have wide optical band gap. The internal efficiency of the device also depends upon the absorption coefficient. Hence by tailoring the absorption coefficient and tuning the band gap of the material, one can achieve devised material, which is suitable for fabricating various layers of the optoelectronic devices as per requirements. Since there is no decomposition observed up to the melting point, crystallization can be done by melt method also. It is surprising that glycine with additive barium nitrate is acting as poison to NLO property.

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