Indian Journal of Pure and Applied Physics (IJPAP)
Vol.1.No.1 2013 pp 7-11
available at: www.goniv.com
Paper Received :10-04-2013
Paper Published:26-04-2013
Paper Reviewed by: 1. Dr.S.Selvakumar 2. Hendry Goyal
Editor : Prof. P.Muthukumar

GROWTH, OPTICAL AND STRUCTURAL CHARACTERIZATION OF SEMI ORGANIC NON LINEAR OPTICAL THIOSEMICARBAZIDE BORATE (TSCB) SINGLE CRYSTALS

[1]R.ARIVUSELVI and [2]M.SELVAPANDIYAN
[1,2]Sri Vidya Mandir Arts and Science college
[1,2]Katteri, Uthangarai,Tamilnadu, India.
E-mail address:lingesh.arivu@gmail.com

ABSTRACT

Non linear optical crystals of thiosemicarbazide borate (TSCB) single crystals were grown by slow evaporation solution growth technique using water as a solvent at room temperature. The grown TSCB crystals have been characterized by UV-Visible analysis, non linear optical test and powder X-ray diffraction studies. The optical behaviours including absorption spectrum and second harmonic generation were investigated to study its linear and non linear optical properties of the sample. Powder X-ray diffraction data reveals that the grown TSCB crystals belong to the orthorhombic crystal system.

Keywords: Growth from solution, Semiorganic, Nonlinear optical crystal

1. INTRODUCTION

Today, crystals are the pillars of modern technology. Without crystals, there would be no electronic industry, no photonic industry, no fibre optic communication, very little modern equipment and some very important gaps in conventional production engineering [1]. Progress in crystal growth and epitaxy technology is highly demanded in view of its essential role for the development of several important areas such as production of high efficiency photovoltaic cells, detectors for alternative energy and medicine, fabrication of bright long life time light emitting diodes and for saving energy by wide use in illumination and traffic lights. Single crystal of suitable size and perfection are required for fundamental data acquisition and for practical devices like detectors, integrated circuits and for other millions and millions of applications. To increasing the applications of semiconductor based electronics creates an enormous demand for high quality semiconducting, ferroelectric, piezoelectric & oxide single crystals [1, 2]. NLO crystals are used for harmonic generation including frequency doubling (SHG), frequency tripling (THG), frequency mixing; Optical parametric oscillator (OPO) & optical parametric amplifier (OPA) [3].

Among the class of NLO materials, the inorganic material possesses high melting point, high mechanical strength and high degree of chemical inertness. But, their optical nonlinearity is poor. Whereas, organic compounds are having high nonlinearity due to the weak Vander Waals and hydrogen bonds and possess high degree of delocalization. However, the difficulty is to grow the large and optically good quality single crystals for device applications. These drawbacks of organic and inorganic crystals may be overcome by semi-organic materials, which share both the properties of inorganic and organic materials [4].

Single crystals of thiosemicarbazide complexes have more attention in the last few years due to their non linear optical properties [5-8]. Thiosemicarbazide is a centrosymmetric in nature but when combined with inorganic material it produces complexes that are non-centrosymmetric [9].

In the present investigation, we report semiorganic non linear optical material of thiosemicarbazide borate (TSCB) crystal by solvent evaporation technique. The title compound was characterized by using various studies such as UV-visible analysis, second harmonic generation test and powder X-ray diffraction analysis.

2. EXPERIMENTAL

Analytic grade thiosemicarbazide (NH_2- NH-CS-NH_2) and boric acid (H_3BO_3) are taken in equal molar ratio was used to grow thiosemicarbazide borate (TSCB) crystal. The calculated amount of thiosemicarbazide and boric acid were thoroughly dissolved in double distilled with a magnetic stirrer in a tightly closed beaker about 3 hour under room temperature.

The resulting solution was filtered and transferred into a beaker and then kept undisturbed to initiate nucleation. After 33 days, a transparent and colourless crystals were collected of size about 5 X 2 X 2 mm^3. The photograph of grown crystal is shown in fig.1

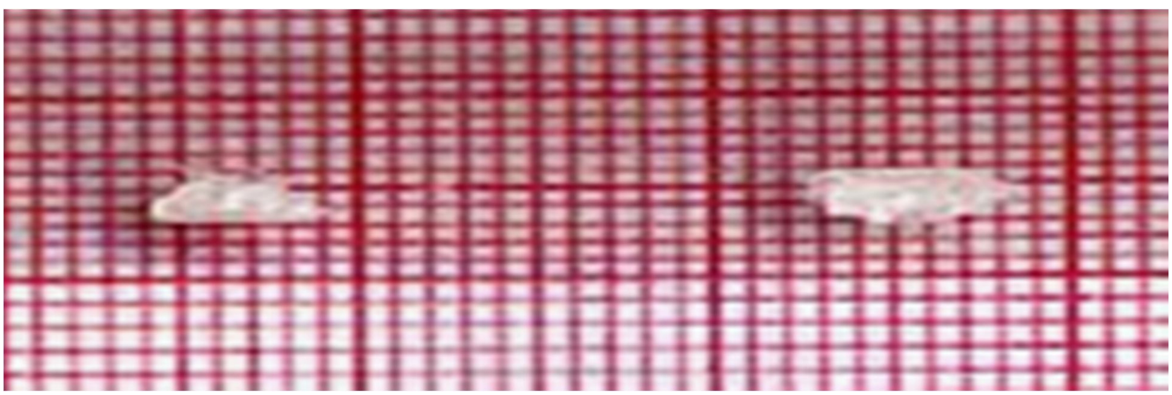

Figure.1.Photograph of TSCB Crystal

3. CHARACTERIZATION

The grown was subjected to powder crystal X-ray diffraction analysis using Shimadu XRD -6000 Diffractometer to determine the structural details. The optical absorption spectrum was measured in the range of 190 – 1100 nm using Lamda 35 UV- Visible spectrophotometer. The relative second harmonic generation was carried out by Kurtz powder technique in order to confirm nonlinearity of the crystal.

4. RESULT AND DISCUSSION

4.1 UV- Visible Analysis

The UV-Visible absorption and transmission spectrum of TSCB was recorded in the range of 190-1100 nm using LAMBDA 35 UV-Visible spectrophotometer. The figure 2 and 3 shows the UV -Visible absorption and transmission spectrum thiosemicarbazide borate crystal. From the spectrum it is seen that the crystal has a lower cut-off wave length of 221 nm. The percentage of transmission is about 98% .

The band gap or energy gap (E_g) of grown crystal is found by the following relation, $E_g = h\ c/\lambda$. Where, h- is the Planck constant (6.625×10^{-34} JS),c- is the velocity of light (3×10^{8}m/s) and λ- is the cut off wavelength of grown crystal (nm). The calculated value of energy gap for TSCB crystal is 5.620 eV. Hence the title compound was belongs to the category of insulating because the energy gap is 5.620 eV.

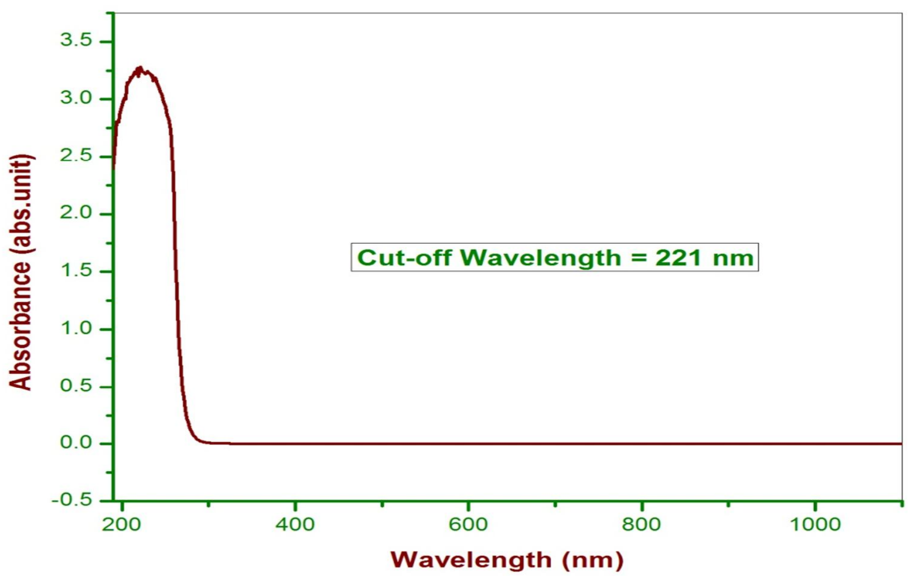

Figure.2.UV-Visible absorption spectrum of TSCB Crystal

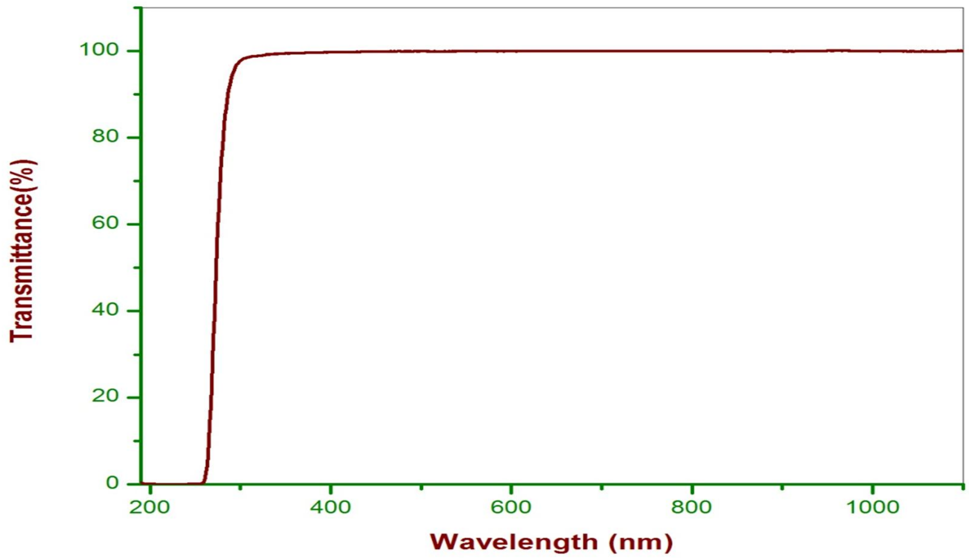

Figure.3.UV-Visible transmission spectrum of TSCB Crystal

4.2 Non linear optical test

The NLO conversion efficiency was tested using a modified setup of Kurtz and Perry [10]. The sample in fine powdered form was filled in a capillary which was exposed to anA Q-switched Nd:YAG laser beam of wavelength 1064 nm and input power of 0.68 J. The output from the Nd: YAG laser was used as source and it was illuminated to the crystal specimen. The generation of second harmonic was confirmed by the emission of green light. The SHG conversion efficiency of TSCB crystal was found to be about 0.67 times that of KDP.

4.3 Powder crystal X-ray analysis

The grown TSCB crystals have been crushed to a uniform fine powder and subjected to Shimadu XRD -6000 Diffractometer with Cu-Kα radiations (λ =1.5406 Å) from a copper target were used. The powdered sample was scanned over the range of 10^0-90^0 at a scan rate of 1^0/min. There are number of very sharp high intensity peaks were observed in the X-ray diffraction pattern, which are shown in fig.4. The calculated lattice parameter values of grown crystals are a = 7.66 Å, b = 11.00 Å, c = 11.92 Å and $\alpha = \beta = \gamma = 90^0$. From the X-ray diffraction analysis it was observed that the crystal belongs to the orthorhombic crystal system having the space group is Pbam.

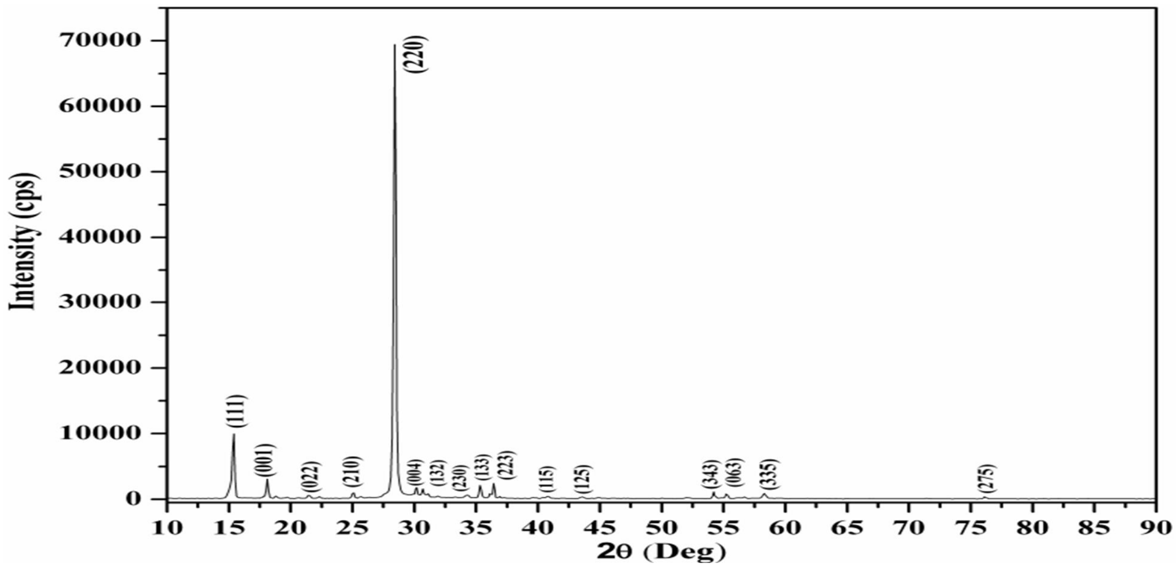

Figure.4.Powder XRD pattern of TSCB Crystal

5.CONCLUSION

Thiosemicarbazide borate (TSCB) crystals were grown by slow solvent evaporation technique. The optical quality of the grown crystal was justified using UV- Visible absorption and transmission studies. The lower cut off wavelength was found to be 221 nm. The crystallinity of the grown crystal was confirmed by powder crystal X-ray diffraction analysis and the lattice parameter values are calculated. The property of the SHG measurements of the crystal confirms the non-linear nature and the SHG efficiency is found to be 0.67 times that of KDP. The study reveals that TSCB crystal is a potential material for frequency conversion applications.

REFERENCES

[1] P.Santhanaraghavan, P.Ramasamy, Crystal growth process and methods, Kru Publications,Kubakonam.

[2] V.Raghavan, Material science & engineering, Printice Hall of india private limlted, New Delhi, India.

[3] V.Sivashankar, R.Siddeswaran,T.Bharathasarathi, P.Murugakoothan, J. Cryst. Growth 311 (2009) 2709-2713.

[4] K. Kirubakaran, K. Selvaraju, R. Valluvan, N. Vijayan, S. Kumararaman Spect. Chem. Act., A, 69 (2008), pp. 1283–1286

[5] M.H.Jiang, D.Xu, G,C.Xing, Z.S.Shao, Synth.Cryst.1 (1985) 14.

[6] W.B.Hou, M.H.Jiang, D.R.Ruan, D.Xu, N.Zhang, M.G.Liu, X.T.Tao, Mater.Res.Bull.645 (1993) 28.

[7] S.G.Bhat, S.M.Dharmaprakash, J. Cryst. Growth 181 (1997) 390.

[8] W.B.Hou, D.Xu, D.R.Yuan, M.G.Liu, N.Zhang, Xu-Tang Tao, Suo-Xing Sun, Min-Hua Jiang, Cryst.Res.Technol 29 (1994) 939.

[9] V.Venkataramanan, G.Dhanaraj, V.K.Wadhawan, J.N.Sherwood, H.L.Bhat. J. Cryst. Growth 154 (1995) 92.

[10] S.K. Kurtz, T.T.Perry. J. Appl. Phys.39 (1968) 3798.