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GROWTH, OPTICAL AND STRUCTURAL CHARACTERIZATION OF NON LINEAR OPTICAL GLYCINE THIOUREA (GTU) SINGLE CRYSTALS

R.ARIVUSELVI* and M.SELVAPANDIYAN
Sri Vidya Mandir Arts and Science college
Katteri, Uthangarai,Tamilnadu, India.
*Corresponding author. Tel: +91 9865588355.
E-mail address:lingesh.arivu@gmail.com

ABSTRACT
Organic non linear optical crystal of Glycine Thiourea (GTU) was grown successfully by slow evaporation solution growth technique. The powder X-ray diffraction (PXRD) confirms that it crystallizes in orthorhombic crystal system with space group Pnma. The UV-Visible transmittance spectrum shows that the crystal has a good optical transmittance in the entire visible region with lower cut off wavelength 271 nm. The existence of second harmonic generation signal was evidenced using Kurtz Perry powder test and the efficiency of the crystal was found to be 1.11 times that of the standard KDP crystal. The morphological structure of GTU crystal was found by SEM analysis. The presence of elements within the compound was determined by EDAX studies.

Keywords: Nonlinear optical crystal, powder X-ray diffraction, UV-Visible, Kurtz Perry powder test.

1. INTRODUCTION

The search for new materials with high optical nonlinearity is an important area due to their practical applications such as optical communication, optical computing, optical information processing, optical disk data storage, laser fusion reactions, laser remote sensing, colour display, medical diagnostics, and so forth [1–4]. Organic NLO materials are often superior to inorganic in terms of their response speed, optical clarity, and the magnitude of their third order susceptibility and for a material to exhibit NLO activity it should be noncentro symmetric. Organic materials with aromatic rings having high non linear optical coefficient, higher laser damage threshold, fast response, low mobility, and large band gap find many applications [5–8]. In the present work, we report the growth of Glycine thiourea single crystals and various optical, structural, elemental and morphological studies were discussed.

2. EXPERIMENTAL

Slow evaporation technique was employed for the growth of GTU crystals. The AR grade Glycine [NH_2-CH_2-COOH] and Thiourea [CS $(NH_2)_2$] were mixed in molar ratio 1:1 in 50 ml of double distilled water.

The solution was stirred at room temperature 30˚C for about 1 hour. The solutions was filtered and transferred into a beaker and then kept into an undisturbed condition to initiate the nucleation and then after 25 days the transparent and colourless crystals were obtain the dimensions of 4 x 3 x 2 mm³. The photograph of grown crystal is shown in Fig.1

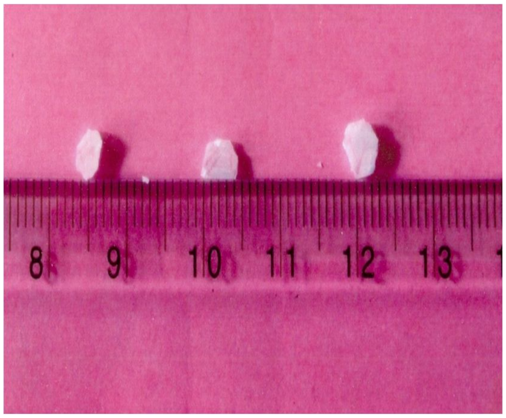

Fig.1. As a photograph of grown GTU crystal

3. CHARACTERIZATION

The grown crystals have been subjected to various characterization studies like powder crystal XRD, UV-Visible, SHG, EDAX and SEM. The UV-Visible spectrum of the grown crystal was recorded between 190 nm and 800 nm using Lamda 35 UV-Visible spectrophotometer. The powdered form of GTU crystal was subjected to Kurtz second harmonic generation test by using Nd:YAG Q switched laser beam with input pulse of 0.68J for the non linear optical property. The grown crystals have also been characterized by X-ray powder diffraction technique using Rich Seifert X-ray powder diffractometer with Cu - Kα radiation of 1.5406 Å. The 2θ range was analyzed from 10° to 80° by employing the reflection mode for scanning. The morphology of the grown crystal was found by GEOL-SEM model instrument.

4. RESULT AND DISCUSSION

4.1 UV-Visible Study

The optical behavior of the material based on the interaction of light radiation over the range of the electromagnetic spectrum. The ultraviolet light absorbed by the sample gives the information about the cut off wavelength and transparency window which are very important in optoelectronic applications.

The optical absorption spectrum of good quality of title compound was measured between the wavelength ranges of 190 – 1100 nm using Lamda 35 UV-Visible spectrometer as shown in fig.2. From the spectrum it is evident that the grown crystal has a lower cut - off wavelength of 271 nm.

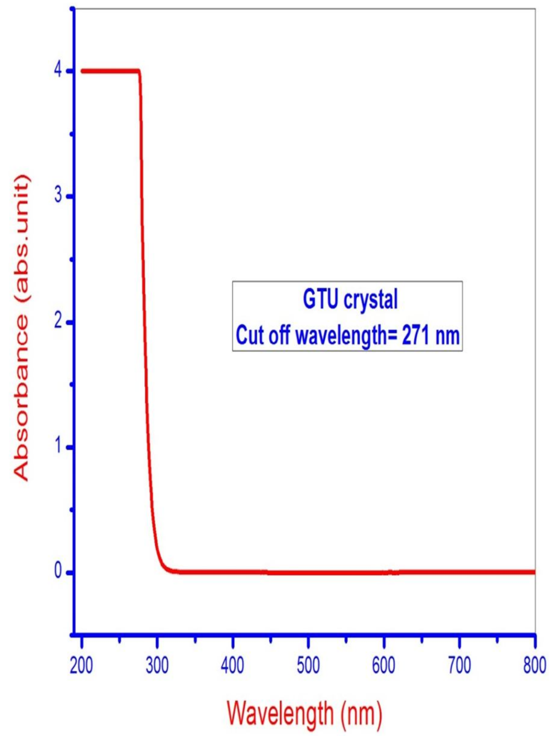

Fig.2.UV-Visible absorption spectrum of GTU crystal

4.2 NLO property Analysis

In order to confirm the NLO property, the grown specimen was subjected to NLO test using high intensity Nd: YAG laser. It emits fundamental wavelength at 1064nm and its power is about 0.68 J. The output of Q-switched Nd: YAG laser was used as a source and it was illuminated to the crystal specimen. The output could be seen as a green flash emission from the sample.

Potassium Dihydrogen phosphate was used as a standard material for comparison purpose. An output Second harmonic generation signals of GTU was 9.8 mJ compared to 8.8 mJ of that of KDP resulted in second harmonic generation efficiency of GTU crystal was 1.11 times of that of KDP.

4.3 Powder X-ray diffraction Analysis

The powder X-Ray diffraction pattern of the title compound is shown in fig 4.3 The powder crystal X-Ray diffraction has been carried out using X-Ray diffractometer. The powder form of the specimen was scanned over the range of 10^0 – 80^0 scan rate of 1 degree/ min. Form this experiment the grown single crystal belongs to orthorhombic crystal system and has to Pnma space group and lattice dimension are listed in table .1

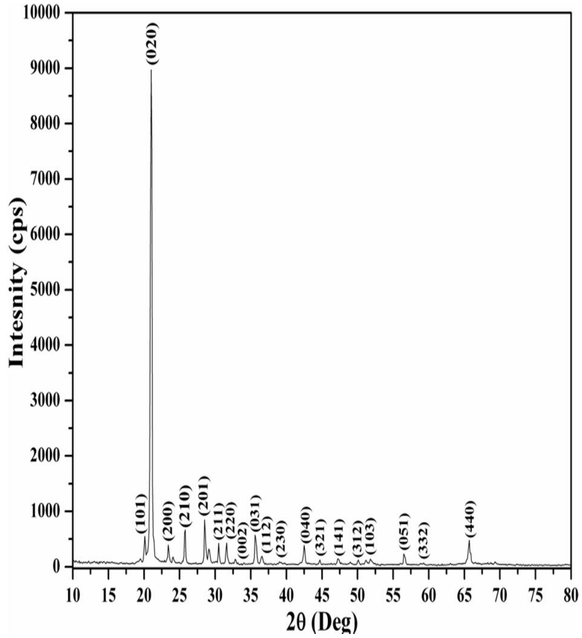

Fig.3.Powder XRD pattern of GTU Crystal

Table.1 Lattice dimension of GTU crystal

Lattice parameter	Values
a	7.657 Å
b	8.588 Å
c	5.486Å

4.4 Energy Dispersive X-Ray Analysis

The compositions of the constituent elements present in Glycine thiourea crystal were determined using energy dispersive X-Ray spectrometer. The EDAX spectrum of GTU single crystal having peaks attributed to carbon, nitrogen, oxygen and sulphur at different energies is depicted in fig .4. The results of corresponding elements present in the crystal in atomic and weight percentage are given in table 2.

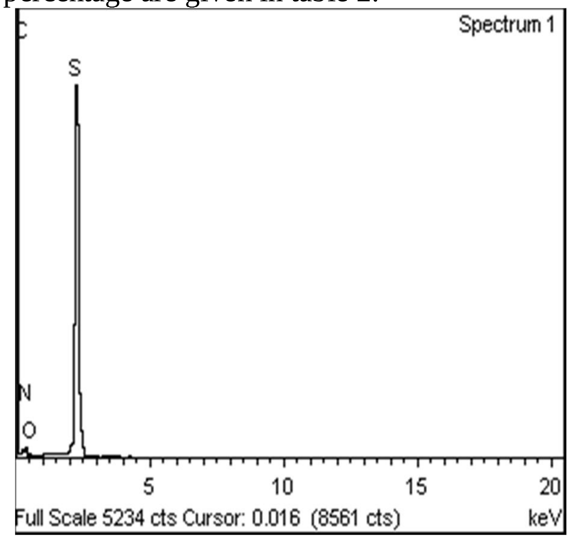

Fig.4.EDAX spectrum of GTU Crystal

Table.2 EDAX parameter of GTU crystal

Elements	Weight %	Atomic %
C	21.92	32.40
N	30.99	39.28
O	4.04	4.49
S	43.04	23.83
TOTAL	100.00	100.00

4.5 SEM analysis

The morphology of the grown crystal were observed by the Scanning Electron Microscope (SEM) which was carried out an a LEO 1530 SEM operated at an acceleration voltage of 10 K volt. The SEM micrograph of GTU crystal is shown in fig.4.5. It is evident from the photography that the crystal is considered of orthorhombic crystal system (Rectangular). The growth of such pattern is consistent in the entire portion under observation indicating the building black with step like pattern

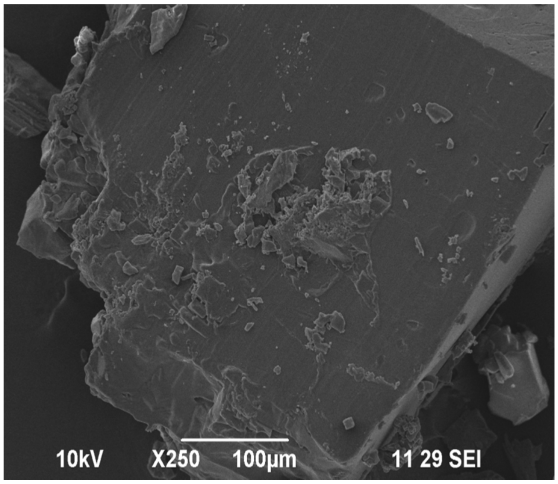

Fig.4.SEM photograpth of GTU Crystal

5.CONCLUSION

Single crystals of GTU were grown by slow solvent evaporation technique. In powder X-ray diffraction pattern, appearance of sharp and strong peaks confirms the good crystallinity of the grown crystals also the prominent of peaks has been indexed. UV-Vis-NIR study reveals the suitability of the crystal for NLO applications and the lower cut off wavelength is found to be 271 nm. There is no absorption of wavelength in the entire visible region. The emission of green signal confirms the second harmonic generation efficiency of the crystal. Thus, the moderate SHG efficiency lower cut off wavelength of the crystal indicate the suitability of this crystal for photonic device fabrication.

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