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Optical and Electrical Conductivity Measurements of GLO Single Crystals for NLO Applications

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Abstract: Single crystals of semi-organic material (GLO) have been grown from aqueous solution by slow evaporation techniques. The lattice parameters for the grown crystals where determined by the single crystal X-ray diffraction analysis. The presences of functional groups was estimated qualitatively by using fourier transforms infrared spectrum source that UV cut-off wavelength for the grown is at 220 nm. The optical band gap was found to be 5.6473 eV. Finally the optical conductivity and electrical conductivity studies have been carried out on this crystal.

Key words: Glycine lithium oxalate, optical band gap, optical conductivity, nonlinear optics, India

INTRODUCTION

In the recent years, organic crystals find considerable interest among researches due to the high laser damage threshold, wide transferency range, less delinquencies, excellent NLO (Non Linear Optical) coefficient, low angular sensitivity and exceptional mechanical properties (Velsko, 1990; Gupte *et al*., 2002; Rajesh *et al*., 2004). Non linear optical materials are accomplished of producing higher values of the original frequency hence, this phenomenon can find applications in opto electronics, fiber optic communication and optical modulation. The camphene of organic materials with inorganic salts have given raise to potential materials for optical Second Harmonic Generation (SHG) as they have a tendency to combine the future of organic with the inorganic materials (Petrosyan *et al*., 2005; Razzetti *et al*., 2002). Organic crystals fall short of very important technological properties together with mechanical strength, chemical stability and performance at low and high temperature. In order to overcome the limitation of the organic materials, some new classes of semi organic NLO crystals have been developed (Pepinsky *et al*., 1957; Narayan Bhat and Dharmaprakash, 2002).

Crystal growth is a frontier area of science and technology which place a major role in the technology of photonics. Researchers report here the growth and characterization of Glycine Lithium Oxalate (GLO), single crystal, X-Ray Diffraction (single crystal XRD).

Fourier Transforms Infrared spectroscopy (FTIR), UV spectral analysis, optical band gap, optical and electrical conductivity measurements which are reported in the literature to the knowledge (Mardare and Rusu, 2001).

MATERIALS AND METHODS

Experimental procedure

Synthesis: The glycine lithium oxalate was prepared at room temperature by dissolving in water. The reaction mixture was stirred at room temperature for 3 h and then filtered using a high quality wattman filter paper. The prepared solution was allowed it does dry at room temperature and salt was recrystalised several times prior to the growth for its purity.

The single crystal of glycine lithium oxalate where grown by slow evaporation techniques. The recrystalised salt of GLO was taken as raw materials. The saturated glycine lithium oxalate solution was prepared at room temperature using deionizer water as solvent. The prepared solution was filtered with a wattman filter paper. The solution was taken in a glass vassal and closed with perforated cover and kept in a dust free atmosphere after

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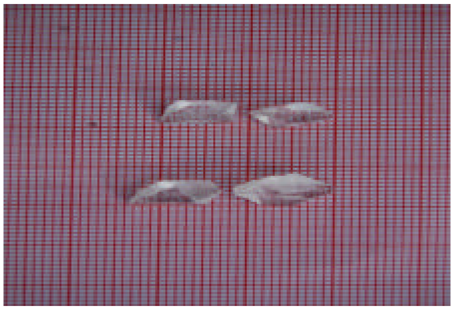

Fig. 1: Glycine lithium oxalate single crystals

3-5 days of solvent evaporation. The solution was allowed to evaporate slowly at room temperature and a crystal of size 0.30×0.25×0.20 $(mm)^3$ was harvested after 20 days. Cut and polished crystal highly transparent glycine lithium oxalate is shown in Fig. 1.

RESULTS AND DISCUSSION

Single crystal X-ray diffraction: The grown crystals were subjected to single crystal X-ray diffraction analysis using an ENRAF NONIUS CAD-4 Single crystal X-ray diffraction with CuKα radiation (λ =1.5418 Å) to determine the lattice parameters. The calculated lattice parameters are a = 6.1068 Å, b = 3.6002 Å and c = 11.8740 Å, volume V = 254.00 $Å^3$ and the crystal belong to the monoclinic system, with space group $P2_1/_C$ and Z = 2. The single crystal XRD of Glycine lithium oxalate is shown in Fig. 2.

FTIR analysis: In order to analysis the presences of functional groups qualitatively in the grown crystal, the FTIR spectrum was recorded between 400 and 4000 cm^{-1} using Ferkin Elmer spectrophotometer and the resultant spectrum is shown in Fig. 3. The broad band at 3178 cm^{-1} is due to O-H stretching. The peak at 1407 indicates the presences of C-O-H bending a sharp band absorbed at 694 and 895 cm^{-1} has been assigned to the symmetric stretching vibrations.

The peaks at 1325, 1314, 1030, 606 and 505 cm^{-1} corresponds to asymmetric stretching, symmetric as well as asymmetric deformation, symmetric and asymmetric bending, respectively. The peaks 2889 and 2614 cm^{-1} corresponding to CH_2 symmetric stretching. The sharpness with high intensity at the peaks indicates that the grown crystals are almost free from the structural defects (Sidorov *et al*., 2007).

UV-vis-NIR spectral analysis: The UV-vis-NIR spectrum for the grown crystal was carried out between 190 and 1100 nm using Lambda 35 spectrophotometer and is shown in Fig. 4. It is observed from the spectrum but there is very low absorption in the entire visible region and shows maximum absorption at UV region. It is one of the most desirable properties of the crystals for the fabrication of optoelectronics devices. The UV cut off wave length was found to be at 220 nm.

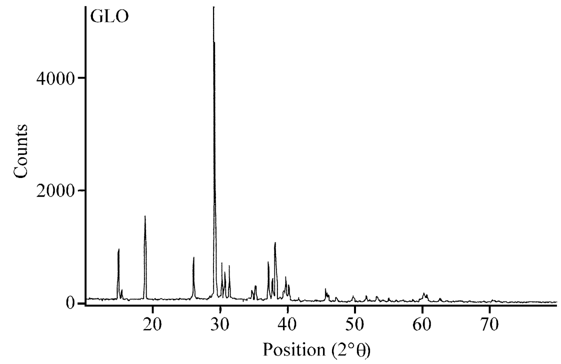

Fig. 2: XRD analysis of GLO crystal

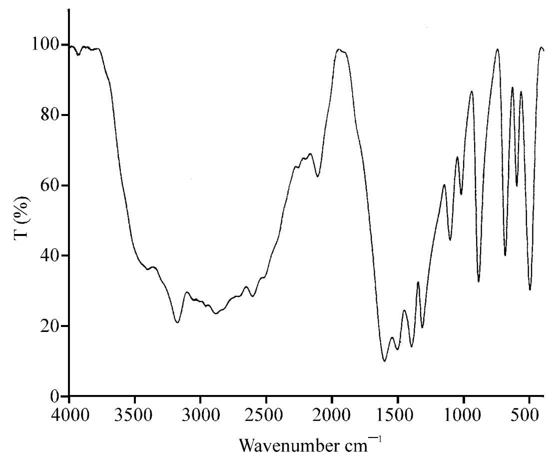

Fig. 3: FTIR spectrum of GLO crystal

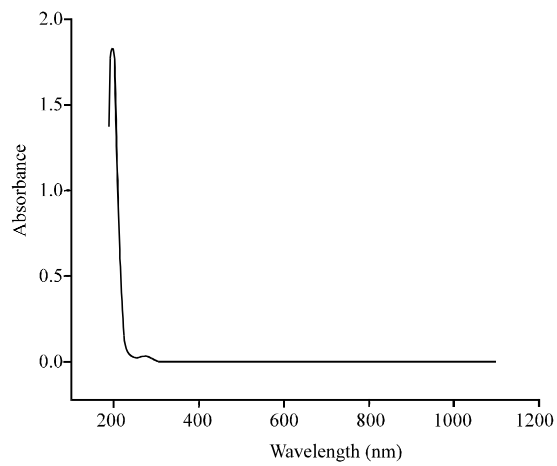

Fig. 4: UV-absorption analysis of GLO crystal

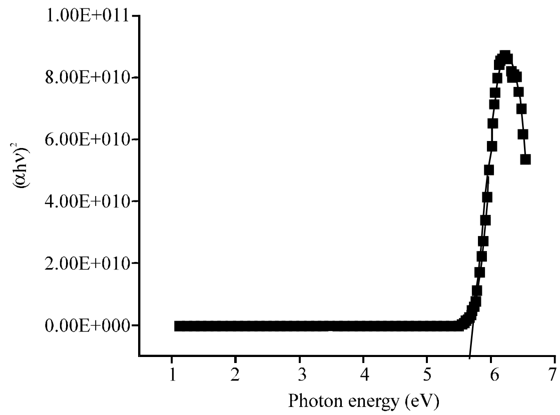

Fig. 5: Photon energy versus $(\alpha h\upsilon)^2$ in GLO crystal

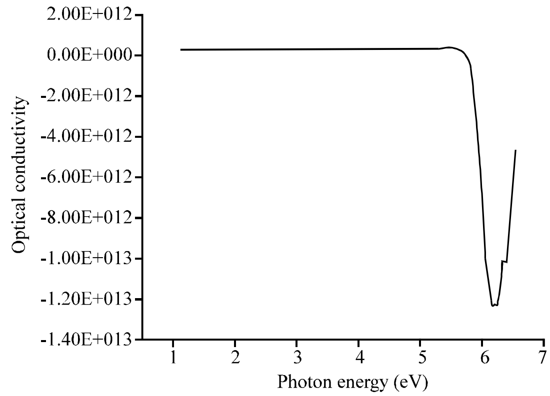

Fig. 6: Photon energy versus optical conductivity in GLO crystal

Optical band gap measurement: The absorption plot, the threshold at which absorption data shown in abrupt rise is indicative of the band gap of the material that is calculated using the equation:

$$E_g = \frac{hc}{\lambda}$$

Where:

h = The blank's constant
c = The velocity of light
λ = The absorption wavelength range the optical band gap of GLO crystal is found to be 5.6473 eV

The wide optical band gap absorbed in GLO as suggest that the crystal has a large transmittance in the visible region. The photon energy versus $(\alpha h\upsilon)^2$ graph is shown in Fig. 5. From the graph the optical band gap value is found to be 5.64001 eV. The optical band gap values both from theory and the graph are more or less the same (Shankar *et al*., 2010; Shankar and Joseph, 2010).

Density measurement: One of the important techniques to study the crystal purity is the measurement of density. The density of the crystal determined by the floatation method while the calculated volume assuming two formula units in a cell is obtained from the crystallographic data. Using the equation:

$$\rho = \frac{MZ}{NV}$$

Where:

N = The molecular weight
Z = The number of molecules per unit cell
N = The Avogadro number
V = The volume of unit cell

Conductivity measurements

Optical conductivity: The variation of optical conductivity against photon energy is shown in Fig. 6. The optical conductivity remains at zero up to an energy of 5.5 eV where the optical conductivity drops down to the lowest value. Beyond that the optical conductivity shoots up towards less negative value which could be explored in Fig. 6. As incident photon energy is given by E = hυ where it depends only on frequency. The optical conductivity from the Shankar relation:

$$\sigma_{op} = \frac{Knc}{\lambda}$$

Where:

K = The optical extinction coefficient
n = The refractive index
c = The velocity of light
λ = The wavelength of light

Electrical conductivity measurement: The electrical conductivity measurement using the Shankar relation:

$$\sigma_{ec} = \frac{2Kcn}{\alpha}$$

Where:

K = The optical extinction coefficient
n = The refractive index
c = The velocity of light
α = The optical absorption coefficient

The Fig. 7 shows that the electrical conductivity verses photon energy. The photon energy increases up to 1.25 eV the electrical conductivity suddenly shoots up. Beyond that the electrical conductivity slowly decreases and finally reached at zero value. The electrical conductivity is inversely proportional to the optical absorption coefficient.

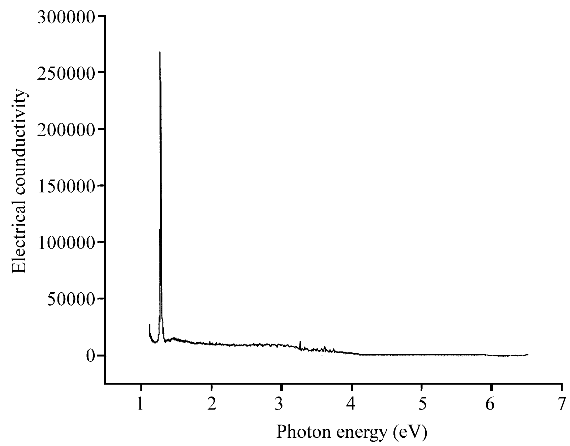

Fig. 7: Photon energy versus electrical conductivity in GLO crystal

CONCLUSION

Good, optical high quality single crystals of GLO of dimension is 0.30×0.25×0.20 $(mm)^3$ have been grown successfully by continuous slow solvent evaporation techniques. Single crystal X-ray diffraction studies confirm that the grown crystal belongs to monoclinic structure with the space group $P2_1/c$. The optical absorption studies infer that the crystal possess very low absorption in the entire visible and IR region. The presence of functional groups as confirmed by FTIR analysis. The crystal purity was confirmed by density measurement. Due to the presence of wide transference range, high damage threshold values and high second harmonic efficiency its crystals may be used for NLO applications. The present study on GLO single crystal reveals excellent optical properties along with good crystalline perfection and hence GLO may be a good candidate for the fabrication of optical devices. Finally optical and electrical conductivity for suggest that the GLO crystals are suitable fabrication of opto electronics, electro optic and photonic devices.

REFERENCES

Gupte, S.S., R.D. Pradhan, O.A. Marcano, N. Melikechi and C.F. Desai, 2002. Laser damage studies in zinc (tris) thiourea sulfate: Nonlinear optical crystal. J. Applied Phy., 91: 3125-3128.

Mardare, D. and G.I. Rusu, 2001. On the structure and optical dielectric constants of TiO_2 sputtered thin films. J. Opto. Electron. Adv. Mater., 3: 95-100.

Narayan Bhat, M. and S.M. Dharmaprakash, 2002. New nonlinear optical material: Glycine sodium nitrate. J. Cryst. Growth, 235: 511-516.

Pepinsky, R., Y. Okaya, D.P. Eastman and T. Mitsui, 1957. Ferroelectricity in glycine silver nitrate. Phys. Rev., 107: 1538-1539.

Petrosyan, H.A., H.A. Karapetyan, M.Y. Antipin and A.M. Petrosyan, 2005. Nonlinear optical crystals of L-histidine salts. J. Cryst. Growth, 275: e1919-e1925.

Rajesh, N.P., V. Kannan, M. Ashok, K. Sivaji, P. Santhana Raghavan and P. Ramasamy, 2004. A new nonlinear optical semi-organic material: Cadmium thiourea acetate. J. Cryst. Growth, 262: 561-566.

Razzetti, C., M. Ardoino, L. Zanotti, M. Zha and C. Paorici, 2002. Solution growth and characterisation of L-alanine single crystals. Cryst. Res. Technol., 37: 456-465.

Shankar, G. and P.S. Joseph, 2010. High energy optical resistivity study on nonlinear optical pyrrolidinomethylpthalamide crystal. Res. J. Applied Sci., 5: 212-214.

Shankar, G., P.S. Joseph, M. Yosuva Suvakin and A. Sebastiyan, 2010. Investigation of optical band gap in pyrrolidinomethylphthalimide crystal. Phys. B: Phys. Condens. Matter, 405: 4231-4234.

Sidorov, N.V., M.N. Palatnikov, V.T. Gabrielyan, P.G. Chufyrev and V.T. Kalinnikov, 2007. Raman spectra and structural perfection of nominally pure lithium niobate crystals. Inorg. Mater., 43: 60-67.

Velsko, S., 1990. Laser program annual report, Lawrence, Livermore. National Laboratory, CA., USA.