Linear Optical Studies of Nonlinear Optical Glycine - Phthalic Acid Single Crystal

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ABSTRACT

Good quality Glycine-Phthalic acid single crystals were grown by slow evaporation solution growth technique. Glycine and Phthalic acid materials were taken in the ratio of 1:1 for solution preparation with water as a solvent. Single crystal X-Ray diffraction of Glycine-Phthalic acid crystal was analysed to find lattice parameters, space group and crystal system. The study proves Glycine-Phthalic acid is orthorhombic crystal system and space group is Pbca. UV-Vis Transmission study was carried out on Glycine-Phthalic acid sample crystal. The lower cut-off wave length of the material is 234 nm. The optical band gap was determined as 4.979 eV. Extinction coefficient, Reflectance and refractive index of Glycine-Phthalic acid single Crystal were calculated and their variation with photon energy were analysed.

Key Words: X-Ray diffraction, Optical Band Gap, Refractive index

INTRODUCTION

Organic materials possess superior nonlinear optical efficiencies due to their large electro optic coefficient and high optical susceptibilities [1]. Crystals of such materials are used in optoelectronic applications [2-4]. In the searching of suitable crystalline material for optoelectronic applications, a novel non linear optical crystal was synthesized by the combination of Glycine and Phthalic acid with 1:1 ratio. The structure of this glycine - phthalic acid crystal has been studied and reported [5]. The FT-IR, UV-Vis absorption, TGA/DTA and Second Harmonic Generation studies of Glycine-Phthalic acid were analysed and reported [6]. The title material has SHG efficiency of 0.55 times that of KDP crystal. This report deals with linear optical studies of glycine – Phthalic acid single crystals. The sample crystals were grown by slow evaporation method. The crystals were characterized by Single crystal X-Ray Diffraction, UV-Vis transmission studies by analyzing transmittance, optical band gap determination and variation of extinction coefficient, Reflectance and refractive index with wavelength and Photon energy. As grown crystal of Glycine-Phthalic acid is shown in figure 1.

RESULTS AND DISCUSSION

Single Crystal X-Ray diffraction Analysis

Single crystal X-ray diffraction study for the grown Glycine-Phthalic acid crystal was conducted using ENRAF NONIUS CAD4 X-ray diffractometer to investigate the crystal structure. The analysis proves that the Glycine-Phthalic acid crystal belongs to orthorhombic crystal system of space group Pbca. The lattice parameters of Glycine-Phthalic acid crystal are $a = 7.975 \text{ \AA}$, $b = 23.612 \text{ \AA}$, $c = 11.414 \text{ \AA}$ and the volume $V = 2149.32 \text{ \AA}^3$, which are in very good agreement with the reported values [5].

UV-Vis Transmission Studies

The linear optical behaviour of the glycine-phthalic acid crystal was studied by recording the UV-Vis-NIR transmittance spectrum with the wavelength in the range from 200 nm to 900 nm. Figure 2 shows spectrum of optical transmission of Glycine-Phthalic acid crystals with wavelength. The UV cut-off wavelength was found at 234 nm for Glycine-Phthalic acid. In the entire visible and NIR region, the

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crystal of Glycine-Phthalic acid has very high transmission. This very high transmittance and low absorption of Glycine-Phthalic acid crystals in this region facilitates very good optical transmission of second harmonic generation frequencies and Glycine-Phthalic acid crystals are suitable for optoelectronic applications [7].

The absorption coefficient (α) in terms of transmittance (T) is given by

$$\alpha = \frac{2.3026 \log(\frac{1}{T})}{t} \quad (1)$$

Where t is the thickness of the Glycine-Phthalic acid crystal.

The equation, which relates optical band gap (E_g), absorption coefficient (α) and frequency (ν) of incident photons is given by

$$\alpha h\nu = A(h\nu - E_g)^{1/2} \quad (2)$$

Where h is the Planck's constant and A is a constant. The band gap of Glycine-Phthalic acid was determined from curve plotted between photon energy $h\nu$ and $(\alpha h\nu)^2$, which is shown figure 3. The value of the optical band gap of Glycine-Phthalic acid is 4.979 eV, which was found by extrapolating the linear portion of the curve near the onset of absorption edge to the Photon energy ($h\nu$) axis. The large band gap of the crystal authenticates the huge transmittance in the visible region and the material is appropriate for optoelectronic applications [8].

Extinction coefficient (K) was determined by the following expression,

$$K = \frac{\lambda \alpha}{4\pi} \quad (3)$$

Where λ is the wavelength and α is the absorption coefficient. The variation of the extinction coefficient of Glycine-Phthalic acid crystal with wavelength is shown in figure 4. The very low value of extinction coefficient was found in the photon energy corresponding to the visible region. This confirms the absorption of radiation by Glycine-Phthalic acid crystal is very low in the entire visible region. The very high transmittance and low absorption in the visible region indicate that the Glycine-Phthalic acid material is suitable for nonlinear optical applications [9].

The reflectance (R) in terms of absorption coefficient (α) and refractive index (n) as a function of reflectance were determined by the following relations [10].

$$R = \frac{1 \pm \sqrt{(1 - \exp(-\alpha t)) \exp(\alpha t)}}{(1 + \exp(-\alpha t))} \quad (4)$$

$$n = \frac{-(R+1) \pm \sqrt{(-3R^2 + 10R - 3)}}{2(R-1)} \quad (5)$$

Figure 5 shows the variation of reflectance with the wavelength. The graph shows low reflectance in the entire visible region. The low reflectance and low absorption of Glycine-Phthalic acid material in the visible and near infrared region reveal that the title material is appropriate to use as an antireflection coating in solar thermal devices and nonlinear optical applications [11].

Figure 6 shows the variation of refractive index with the incident photon energy. The average value of refractive index was calculated for the wavelength in the visible region is 1.79 for Glycine-Phthalic acid crystals.

CONCLUSION

Good quality Glycine-Phthalic acid single crystals were grown by slow evaporation method. The title crystals are of orthorhombic system was identified by the Single crystal X-Ray Diffraction analysis. Lattice parameters are very well matching with the reported values. UV-Vis Transmittance study shows the high transmittance and low absorption in the visible and NIR region. The variation of extinction coefficient, reflectance and refractive index were analyzed with respect to wavelength and photon energy. The results and discussions confirm the Glycine-Phthalic acid crystal is suitable for nonlinear optical optoelectronics applications.

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Figure 1: As grown crystal of Glycine-Phthalic acid.

Figure 2: Variation of transmittance with wavelength.

Figure 3: Plot to find an optical band gap.

Figure 4: Plot between extinction coefficient and photon energy.

Figure 5: Variation of reflectance with wavelength.

Figure 6: Variation of refractive index with photon energy.