Journal of Advances in Applied Sciences and Technology
ISSN : 2393-8188 (print)
2393-8196 (online)
www.milliyasrcollege.org.journal.php

STUDIES ON LINEAR OPTICAL PROPERTIES OF GLYCINE DOPED DSHP CRYSTAL

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ABSTRACT

The one mole percent glycine doped di-sodium hydrogen phosphate (DSHP) crystal was grown by the slow evaporation solution growth technique. The optical transmission study reveals the wide transparency of grown crystal in the entire visible region, which is an essential requirement for NLO applications. The cutoff wavelength has been found to be 232 nm and the optical band gap is found to be 5.2eV. Theoretical calculations were carried out to determine the linear optical constants such as extinction coefficient, refractive index, reflectance, real and imaginary part of dielectric constant, optical conductivity and the electrical conductivity.

KEYWORDS: Crystal growth, DSHP, amino acid UV-visible, Optical properties.

1. INTRODUCTION

In recent years, nonlinear optical materials (NLO) have been of immense interest for their excellent applications in optical communication, second harmonic generation (SHG), photonic and optoelectronic technologies and data storage technology [1–4]. The search for new conversion materials for various device applications has led to discovery of many organic, inorganic, and semiorganic NLO materials with high susceptibilities. Disodium hydrogen orthophosphate (DSHP) is an interesting and promising inorganic NLO material of phosphate group. Crystal growth and characterization of pure DSHP crystal was reported by Gunasekaran et al and Jhon et al [5-6]. The amino acid crystals were subjected to extensive investigation by several researches for their excellent characteristics. Amino acids are interesting organic materials for NLO applications as they contain donor carboxylic (COOH) group and the proton acceptor amino (NH2) group in them, known as zwitter ions which create hydrogen bonds. Due to this dipolar nature, amino acids have physical properties which make them ideal candidates for NLO applications [7-8].In the present investigation, we have grown the 1 mole % glycine doped DSHP crystal by slow evaporation solution growth technique, characterized by UV-visible spectral analysis and its detailed optical parameters were reported for NLO applications.

2. EXPERIMENTAL

SYNTHESIS AND CRYSTAL GROWTH

The AR grade DSHP salt was dissolved in deionized water with constant stirring to achieve the supersaturated solution. The saturated solution of DSHP was added with one mole percent of glycine and allowed to stir at constant speed to achieve the homogeneity throughout the volume. The prepared solutions were then filtered and the purity of the salts was achieved by repetitive recrystallization, good quality transparent seed crystals were harvested within 6-7 days by slow evaporation method at room temperature.

Linear optical studies The grown crystals were subjected to spectral analysis for studying the linear optical properties. The transmission spectrum was recorded using Shimadzu UV-2450 Spectrophotometer in the range 200-900 nm. The optical absorption coefficient (α) was calculated using the following relation

$$\alpha = \frac{2.303\log\left[\frac{1}{T}\right]}{t} \qquad (1)$$

where T is the Transmittance and t is the thickness of the crystal. The various other optical constants were calculated using the following theoretical formulae [9].

The extinction coefficient is obtained in terms of the absorption coefficient,

$$k = \frac{\alpha\lambda}{4\pi} \qquad (2)$$

The reflectance in terms of absorption coefficient is derived,

$$R = \frac{1 \pm \sqrt{1-\exp(-\alpha t)+\exp(\alpha t)}}{1+\exp(-\alpha t)} \quad (3)$$

and the linear refractive index is given by

$$n = \frac{-(R+1) \pm \sqrt{(-3R^2+10R-3)}}{2(R-1)} \quad (4)$$

Also the complex dielectric constant is related to the refractive index and the extinction coefficient as

$$\varepsilon_c = \varepsilon_r + \varepsilon_i \quad (5)$$

where the real and imaginary dielectric constant is

$$\varepsilon_{r} = n^2 - k^2 \quad 6)$$

$$\varepsilon_i = 2nk \quad (7)$$

The optical conductivity is a measure of the frequency response of the material when irradiated with light

$$\sigma_{op} = \frac{\alpha n C}{4\pi} \quad (8)$$

where c is the velocity of light. The electrical conductivity can also be estimated by optical method using the relation

$$\sigma_e = \frac{2\lambda\sigma_{op}}{\alpha} \quad (9)$$

3. RESULTS AND DISCUSSION

Linear optical properties

The optical transparency of the grown crystal has been assessed using the Shimadzu UV-2450 spectrophotometer in the range of 200–900 nm. The recorded transmittance spectrum shown in Fig. 1 revealed that grown crystal is optical transparent up to 90% in entire visible spectrum. The lower cut-off (232 nm) of grown crystal is contributed due to electronic transition n to π offered by nitrogen and hydrogen bonds in organic compound glycine [10]. The high transmittance and lower cut-off wavelength are essential optical parameters for applications in SHG transmission devices [11].

The energy dependence of the absorption coefficient suggests the occurrence of direct band gap and hence it obeys the relation for high photon energy,

$$\alpha h\upsilon = A(h\nu - E_g)^{\frac{1}{2}} \quad (10)$$

where E is the optical band gap and A is a constant.

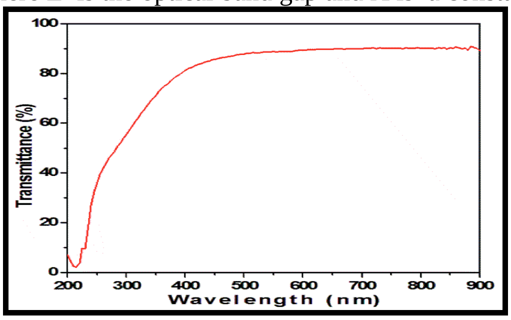

Fig.1 *UV-Vis. Spectrum of DSHP crystal.*

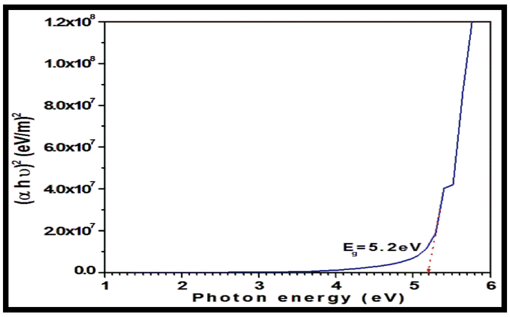

Fig.2 *Tauc's plot of DSHP crystal.*

The variation of $(\alpha h\upsilon)^2$ versus hυ in the fundamental absorption region is plotted in Fig. 2 and E_g is evaluated by the extrapolation of the linear part. The band gap is found to be 5.2 eV. As a consequence of enhanced wide band gap and high transmittance in the visible region makes it potential candidate for optoelectronic applications [12].

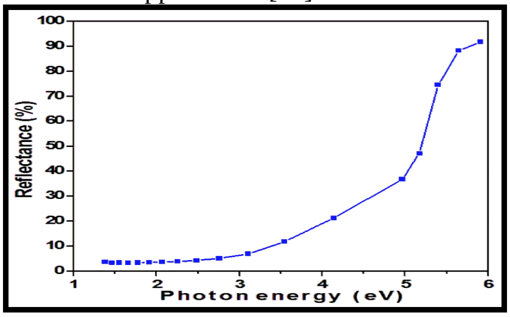

Fig. 3 *Plot of reflectance vs. hυ.*

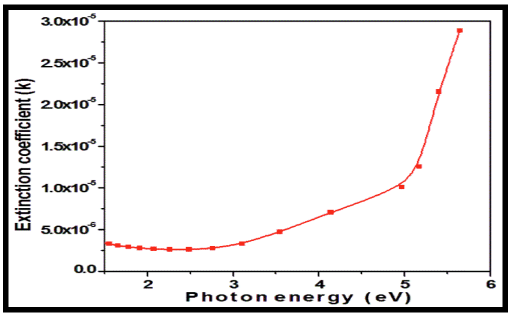

Fig.4 *Plot of extinction coefficient vs. hυ.*

From the recorded transmission spectra, the linear optical constants of 1 mole% glycine added DSHP as a function of photon energy is plotted (Figs. 3-8). For understanding the interaction of light with matter, it is very essential to study the refractive index and the extinction coefficient. The refractive index of the material at 900 nm is 1.45. Also the extinction coefficient shows exponential decay as the photon energy decreases. Refractive index being the measure of percentage of intensity of light reflected, the reflectance shows an increasing value along the photon energy.

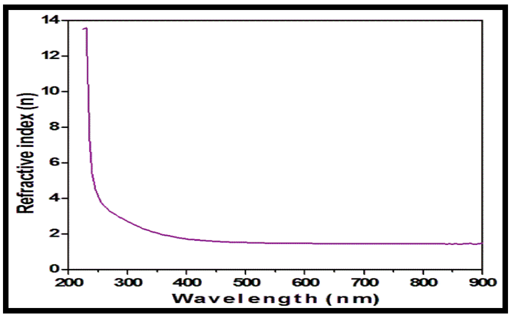

***Fig. 5** Plot of refractive index vs. wavelength*

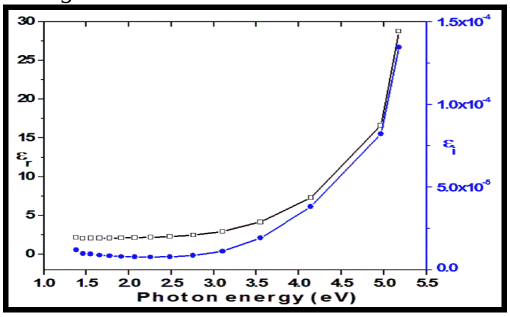

***Fig. 6** Plot of real and imaginary part of dielectric constant*

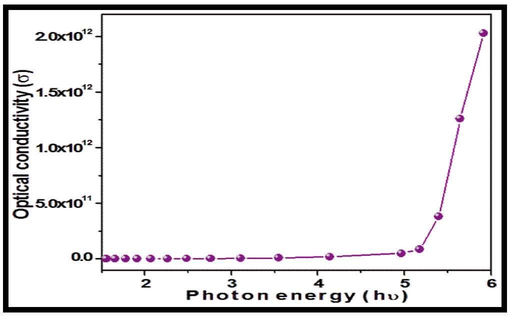

***Fig. 7** Plot of optical conductivity vs. hυ.*

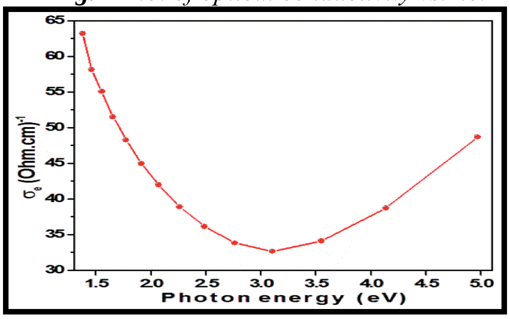

***Fig. 8** Plot of electrical conductivity vs. hυ.*

From figures 3 and 4, it is clear that the reflectance and the extinction coefficient depend upon the absorption coefficient. The internal energy of the device depends on this absorption coefficient. The high transmission, low reflectance and low refractive index of DSHP in the UV-vis. region makes the material a prominent one for antireflection coating in solar thermal devices and nonlinear optical applications [13]. The low extinction value and electrical conductivity show the semiconducting nature of the material. The high magnitude of optical conductivity confirms the presence of very high photo response nature of the material [13]. This makes the material more prominent for device applications in information processing and computing.

4. Conclusions

The amino acid one mole percent glycine doped DSHP crystal has been grown by slow evaporation solution growth technique. The high transmittance (90%) and lower cut-off wavelength (232 nm) are essential optical parameters for applications in SHG transmission devices. The wide band gap was found to be 5.2eV makes it potential candidate for optoelectronic applications. The high transmission, low reflectance and low refractive index in the UV-vis region makes the material a prominent one for antireflection coating in solar thermal devices. The low extinction and electrical conductivity value shows the semiconducting nature of the material. The high magnitude of optical conductivity confirms the presence of very high photo response nature of the material.

Acknowledgment

The authors are thankful to the Department of Science and Technology (DST/SR/S2/LOP-22/2010), and University Grants Commission (UGC/41-591/2012/SR), New Delhi, for financial assistance.

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