Research Paper

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# Study on Synthesis, Growth, Fundamental, optical and Dielectric Properties of Glycine doped with Potassium Iodide of a Organic Single Crystal

Physics

KEYWORDS : Slow evaporation technique, Plasma energy, Fermi energy, Electronic polarizability, Extinction coefficient, Refractive index and Dielectric constant

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## ABSTRACT

*Some organic materials exhibit exceeding by large amount of nonlinear property and they are found to be more suitable for device fabrications. Hence, in the present study Glycine doped with Potassium Iodide (GLPOI) an organic material, has been extensively studied with regard to the growth and various properties. Single crystals of Glycine doped with Potassium Iodide (GLPOI) with good degree of transparency were grown from aqueous solution by slow evaporation technique. Single crystal X-ray diffraction analysis reveals that the crystal belongs to hexagonal system. Some fundamental data such as valence electron, plasma energy, Penn gap, Fermi energy and electronic polarizability of the grown crystal were calculated. The optical absorption studies show that the crystal is transparent in the entire visible region with a cut off wavelength of 311 nm. The optical band gap energy was found to be 3.99 eV. The dependence of the extinction coefficient (K) and refractive index (n) on wavelength has also been reported. Dielectric constant measurements were carried out at different temperatures and frequencies.*

## INTRODUCTION

Organic materials attract much interest to chemists, material scientists and optical physics because of their superior performance with respect to NLO properties such as the large NLO efficient, ultrafast nonlinear response time, and high optical damage threshold [1-5]. Amino acids and their complexes belong to a family of organic materials that have been considered for photonic applications [6]. Out of 20 amino acids glycine is the simplest of all. Glycine family crystals have been subjected to extensive research by several researches for their efficient optical properties [7-10]. In the present study, a systematic investigation has been carried out and we report bulk growth, fundamental properties, optical and dielectric properties of Glycine doped with Potassium Iodide (GLPOI) single crystals.

## EXPERIMENTAL DETAILS

All reagents used in the synthesis were of analytical grade. Glycine doped with Potassium Iodide (GLPOI) was synthesized by the reaction between Glycine and Potassium Iodide by slow evaporation technique. Glycine doped with Potassium Iodide in different ratio of 5:2, 5:3, 5:4. The amount of Glycine salt was calculated and dissolved in deionized water for one and half hours to get complete dissolved solution. Then the appropriate amount of Potassium Iodide was added with a few drops of Cons.$H_2SO_4$ to the solution. The resultant solution was continuously stirred well using a temperature controlled magnetic stirrer for 6 to 7 hours to yield a homogenous mixture of solution.

The complete dissolved solution was filtered using micro filter paper and taken in a Petri dish. It was optimally closed using a perforated polythene paper and kept in undisturbed conditions. The solution was allowed to evaporate at room temperature, which results in the yield of crystalline salt of GLPOI due to super saturation followed by nucleation. The seed cryatals were harvested from the solution after 15 days and a suitable seed was selected. The selected seed was suspended in the freshly prepared mother solution. After a period of 50 days, a well developed and optically transparent defect free crystals of GLPOI were obtained from the mother solution. The dimension of the GLPOI single crystal(5:4 ratio) was found to be 30 X17 X15 $mm^3$. The photo of as grown single crystal of GLPOI with high degree of transparency was presented in fig.1.

**Fig.1 – Photograph of as - grown single crystal of GLPOI(5:4)**

## RESULTS AND DISCUSSION

### Density of GLPOI crystal

The density of GLPOI crystal was calculated using the relation[11]

$$\rho = \left( \frac{MZ}{N_A abc} \right) \quad \text{..... (1)}$$

Where M is molecular weight of GLPOI, molecular unit cell Z = 1, $N_A$ is Avagadro's number and a, b and c are the lattice parameters of GLPOI crystal. The theoretical density was found to be 1.617 g/ $cm^3$. The density of GLPOI crystal was measured experimentally by the floatation method at room temperature (33°C), and the measured density can be obtained using the expression

$$\rho = \left( \frac{M \rho_{solvent}}{m_1 - m_2} \right) \quad \text{..... (2)}$$

where $m_1$ is the mass of GLPOI crystal sample in the air, $m_2$ is the mass when the GLPOI crystal sample was immersed in solvent ( double deionized water) and $\rho_{solvent}$ is the density of the solvent used at measured temperature. The density was measured by floatation technique. From this measurement, the density of the GLPOI crystal was found to be 1.623 g / $cm^3$ which is in good agreement with the theoretically found value. Finally the mean value 1.620 g / $cm^3$ was taken as density of the GLPOI crystal.

### Single crystal X-ray diffraction

Single crystal X-ray diffraction study was carried out on the as grown GLPOI single crystal. The crystal data collection was performed by a Bruker APEX IIα CCD area detector diffractometer equipped with graphite-monochromatized MoKα radiation (λ = 0.7103 Å ). The XRD study reveals that GLPOI (5:4) belongs to hexagonal system. The unit cell parameters and crystallographic data of GLPOI crystal are given as follows: a=b=6.9785(5) Å, c=5.4579(8) Å, α=β=90°, γ=120°, and Z=1.

### Fundamental Parameters

The molocular weight (M) of the grown crystal and total number of valence electron(Z) were found to be 259.085 g / mole and 46. The density (ρ) of the grown crystal was found to be 1.620 g / $cm^3$ and dielectric constant (ε) at 1MHz and at temperature 130°C was calculated as 11.6. The valence electron plasma energy,

$$28.8\left( \frac{Z\rho}{M} \right)^{\frac{1}{2}} \quad \text{.....(3)}$$

Where Z is the total number of valence electrons, ρ is the density of the GLPOI crystal and M is the molecular weight of the GLPOI single crystal. The Plasma energy in terms of Penn gap and Fermi energy [12] is given as

$$E_p = \frac{\hbar\omega_\rho}{(\varepsilon_\infty - 1)^{1/2}} \quad \text{.....(4)}$$

and

$$E_F = 0.2948(\hbar\omega_\rho)^{4/3} \quad \text{.....(5)}$$

Polarizability, α is obtained using the relation [13]

$$\alpha = \left[\frac{(\hbar\omega_\rho)^2 S_o}{(\hbar\omega_\rho)^2 S_o + 3E_F^2}\right] \times \frac{M}{\rho} \times 0.396 \times 10^{-24} cm^{-1} \quad \text{.....(6)}$$

Where $S_0$ is a constant for a particular material, and is given by

$$S_o = 1 - \left[\frac{E_p}{4E_F}\right] + \frac{1}{3}\left[\frac{E_p}{4E_F}\right]^2 \quad \text{.....(7)}$$

The value of α so obtained agrees well with that of clausius Mossotti equation, which is given by,

$$\alpha = \frac{3M}{4\pi N_A \rho}\left(\frac{\varepsilon_\infty - 1}{\varepsilon_\infty + 2}\right) \quad \text{.....(8)}$$

where the symbols have their usual meaning. $N_A$ is Avagadro number and the calculated fundamental data of the grown crystal of GLPOI are listed in table 1.

**Table 1 : Calculated theoretical fundamental data for GLPOI single crystal**

| Parameter | Value |
|---|---|
| Plasma energy | 15.45 eV |
| Penn gap | 4.75 eV |
| Fermi gap | 11.34 eV |
| Polarizability - By Penn analysis | 4.82 x $10^{-23}$ $cm^3$ |
| Polarizability - By Clausius Mossotti equation | 4.94 x $10^{-23}$ $cm^3$ |

**Optical absorption of GLPOI**

The optical absorption spectrum of GLPOI single crystal was recorded in the wavelength region ranging from 200 – 2500 nm which shows that absorption was very less in the entire visible region and part of IR **region.** For optical fabrication, the crystal should be highly transparent over a considerable region of wavelength [14-15]. The lower cut-off wavelength($\lambda_{min}$ ) of the GLPOI crystal was found to be at 311 nm which makes it is a potential material for optical device fabrications. Using the relation $E_g$ = 1240/ $\lambda_{min}$, the band gap energy was found to be 3.99 eV.

**Optical constants ( n, K )**

The dependence of optical absorption coefficient with the photon energy helps to study the band structure and the type of transition of the electron. The absorption coefficient (α) and the optical constants ( n, K ) are determined from the transmission ( T ) and reflection ( R ) spectrum based on the following relations [16].

$$T = \frac{(1-R)^2 \exp(-\alpha t)}{(1-R^2 \exp(-2\alpha t)} \quad \text{.....(9)}$$

Where t is the thickness and α is related to extinction coefficient K by

$$K = \frac{\alpha\lambda}{4\pi} \quad \text{..... (10)}$$

The reflectance (R) in terms of the absorption coefficient can be obtained from the equation(9).

$$R = \frac{\exp(-\alpha t) \pm \sqrt{\exp(-\alpha t)T + \exp(-3\alpha t)T + \exp(-2\alpha t)T^2}}{\exp(-\alpha t) + \exp(-2\alpha t)T} \quad \text{..... (11)}$$

Refractive index(n) can be determined from the reflectance data using the following equation

$$n = -(R+1) \pm 2\frac{\sqrt{R}}{R-1} \quad \text{..... (12)}$$

Fig 2 & 3 shows that the variation of K and n with respect to λ. The refractive index (n) is found to be 2.58 at λ=800 nm.

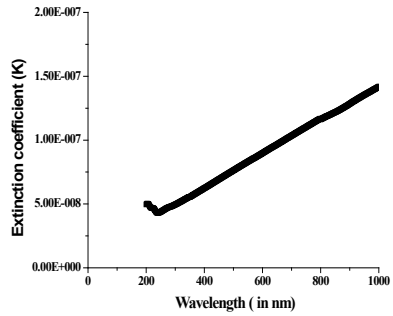


**Fig. 2 Extinction coefficient Vs wavelength**

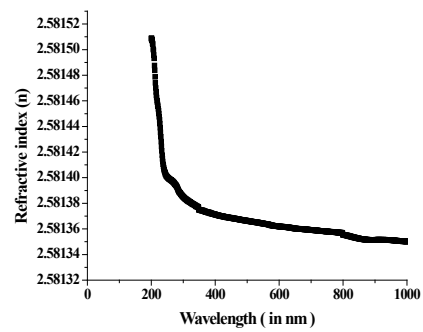


**Fig. 3 Refractive index Vs wavelength**

**Dielectric Studies**

The dielectic constant of GLPOI crystals was studied at different temperatures using HIOKI 3532 LCR HITESTER in the frequency region 1000 Hz to 1MHz. Fig. 4 shows that plot of dielectric constant ($\varepsilon_r$) Vs log frequency for the temperature of 40°C, 80°C and 120°C. The dielectric constant has high values in the lower frequency region and the decreases with the applied frequency. The very high value of $\varepsilon_r$ at low frequencies may be due to the presence of all the four polarizations namely, space charge, orientation, electronic and ionic polarization and its low value at higher frequencies may be due to the loss of significance of these polarizations gradually. Fig.5 shows the temperature dependence of dielectric constant of the GLPOI crystals at frequency 1KHz and 1MHz. From the plot, it is observed that the dielectric constant increases with increase in temperature, attributed to space charge polarization near the grain boundary interfaces, which depends on the purity and perfection of the crystal. Space charge polarization is generally active at lower frequencies for high temperatures and indicates the perfection of the crystals [20].

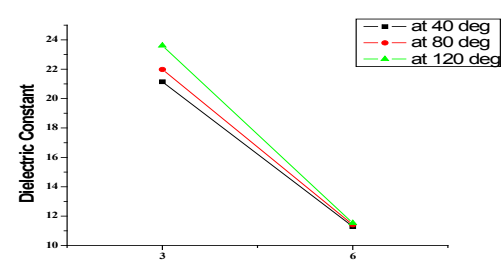


**Fig. 4 Dielectric constant Vs log f**

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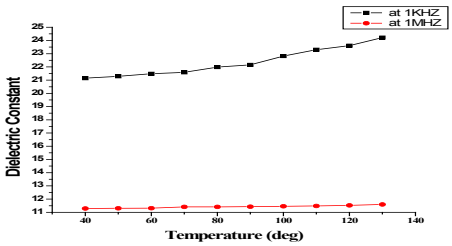


**Fig. 5 Dielectric constant Vs Temperature**

**CONCLUSION**

Good quality and optically transparent single crystals of GLPOI were grown by slow evaporation technique at room temperature. Single crystal XRD analysis confirmed that the crystals belongs to hexagonal system. Fundamental parameters like Plasma energy, Penn gap, Fermi energy and electronic polarizability of the crystal have been calculated. Optical absorption study reveals high transparency of the crystal with a lower cut off wavelength of 311 nm and the band gap energy of the crystal was found to be 3.99eV. The optical investigations show a high value of both extinction coefficient (K) and refractive index (n) indicating high transparency of the crystal which confirms its suitability for optical switch device fabrications. The frequency dependence of the dielectric constant decreases with increasing frequency at different temperatures.

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