LINEAR AND NONLINEAR OPTICAL PROPERTIES OF L- THREONINE ACETATE

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Abstract - The optical properties of the grown crystal were studied by means of absorption measurements in the wavelength region between 200 and 1200 nm. Optical behavior has been assessed by UV-Vis analysis and found that there is minimum absorption in the entire visible region. The optical constants such as refractive index (*n*) and extinction coefficient (k) have been determined from the transmittance data. The optical band gap (E_g) the real and imaginary part of the dielectric constant of the grown crystal was determined. The relative second harmonic generation (SHG) efficiency measurement reveals that the incorporation of Acetic acid to L- Threonine leads to increase in its SHG value.

Keywords – L – Threonine, Tau'c plot, SHG,

1 INTRODUCTION

Universal contradiction exists between nonlinear optical coefficient and wavelength cutoff in organic crystals. The search for materials with relatively shorter wavelength transparency yet higher nonlinearity has been a long sought goal in many studies. In order to obtain the adjustment of the nonlinear efficiency/transparency, based on the molecular engineering and crystal engineering approach, we are trying to develop a new method to design organic nonlinear optical second-harmonic generation materials, e.g. organic inclusion complex. Optical properties have been the subject of numerous investigations by both theoreticians and experimentalists in recent years due to the potential applications in optical signal processing and computing. Detailed investigations of linear and nonlinear optical coefficients enable to fabricate materials, appropriately designed at the molecular level for specific applications such as optoelectronic devices [1-3]. Knowledge of optical constants of the materials (optical band gap and extinction coefficient) is vital to scrutinize the atomic structure, electronic band structure and electrical properties. The refractive index provides information about the chemical bonding and electronic structure of the material. An accurate measurement of the optical constant can be easily performed on semi organic crystals [4-5].

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In the present work, we report the determination of the optical constants such as refractive index, extinction coefficient, dielectric constants, energy gap and optical conductivity of the LTA using optical spectra.

2 SYNTHESIS

Analytical grade L-threonine (AR grade) and acetic acid were dissolved according to the stoichiometric ratio in double deionized water. The resulting aqueous solution was filtered and allowed to evaporate under optimized conditions to grow crystals by slow evaporation method at room temperature. The grown crystal is found to be transparent and free from defects in figure 1.

Figure 1. Photograph of LTA

3 LINEAR OPTICAL PROPERTIES OF LTA

The optical properties of a material are important, as they provide information on the electronic band structures, localized states and types of optical transitions. To determine the transmission range and hence to know the suitability of LTA single crystals for optical applications, the UV–Vis spectrum (Figure 2) was recorded in the range of 200–1200 nm. The UV-Vis spectrum gives information about the structure of molecule because the absorption of UV and visible light involves the promotion of the electrons in the σ and π orbitals from the ground state to higher energy states. The spectrum reveals that the LTA compound has a wide transparency window in the region 225–1000 nm. This data was further used for analyzing optical band gap energy (E_g) using the formula

$$(\alpha h\nu) = k\,(h\nu - E_g)^{n/2} \qquad (1)$$

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n is an integer equal to 1 for a direct band gap and 4 for an indirect band gap. The values of the direct optical band gap E_g were obtained from the intercept of $(\alpha h\nu)^2$ versus $h\nu$ curve plotted in Figure 3. Ideally the graph should be linear and the deviation from linearity at low incident photon energy can be attributed to the presence of irregularities and imperfection of the crystals. The intercept obtained by the extrapolation of the linear portion of the plot to energy axis gives the band gap energy of the crystal. The band gap is found to be 4.7 eV. The other optical constants were calculated using the theoretical formulae discussed below [6, 7]. The optical properties of the crystals are governed by the interaction between the crystal and the electric and magnetic fields of the electromagnetic waves. Extinction coefficient is the fraction of light lost due to scattering and absorption per unit distance in a participating medium. In electromagnetic terms, the extinction coefficient can be explained as the decay or damping of the amplitude of the incident electric and magnetic fields.

The extinction coefficient in terms of absorption coefficient is obtained as

$$K=\frac{\alpha\lambda}{4\Pi} \qquad (2)$$

The Reflectance is derived as a function of absorption coefficient as

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

And the linear refractive index is given by

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

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

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

Where the real and imaginary and part of dielectric constant is

$$\varepsilon_r=n^2-K^2 \qquad (6)$$

$$\varepsilon_i=2nK \qquad (7)$$

The optical conductivity as a function of frequency response of the material when irradiated with light is calculated as

$$\sigma_{op}=\frac{\alpha nc}{4\Pi} \qquad (8)$$

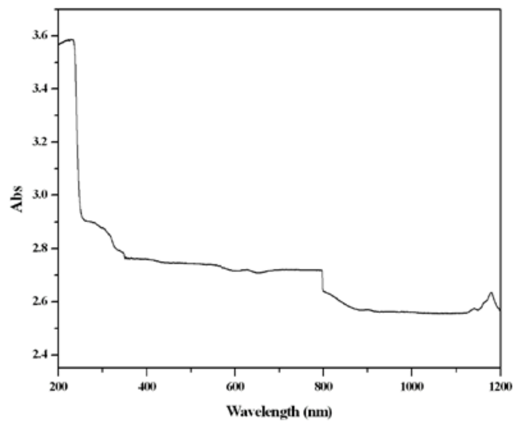

Figure 2. Optical absorption spectrum of LTA

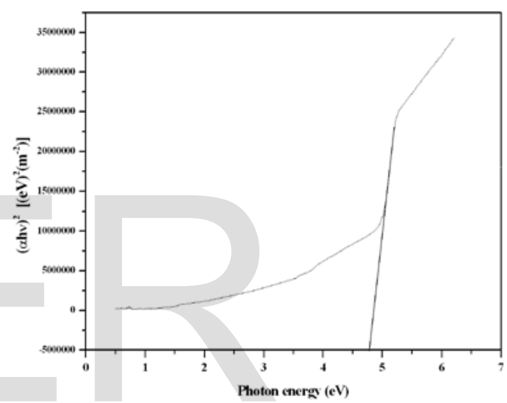

Figure 3. Energy band gap of LTA

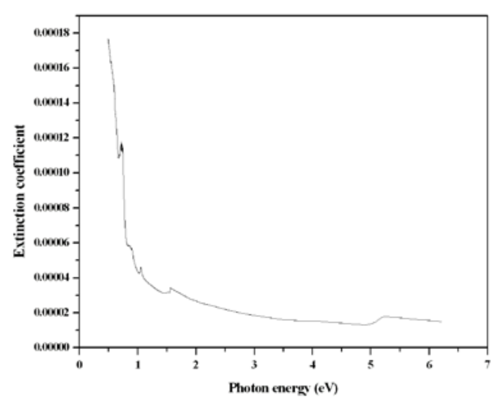

Figure 4. Extinction coefficient Vs Incident Photon Energy

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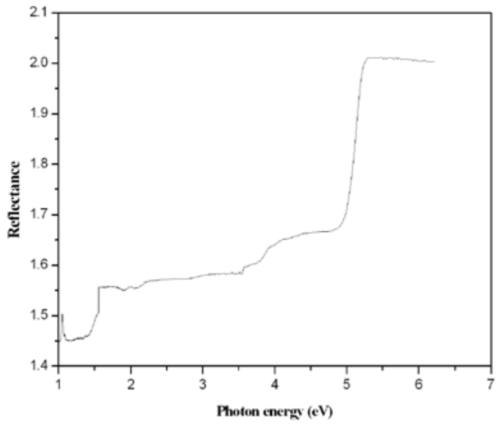

Figure 5. Reflectance Vs Incident photon energy

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

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

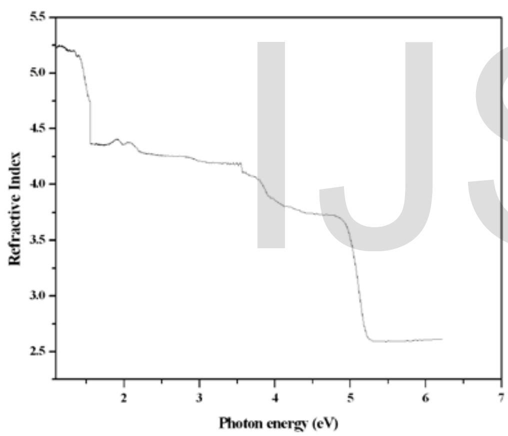

Figure 6. Refractive index Vs Incident photon energy

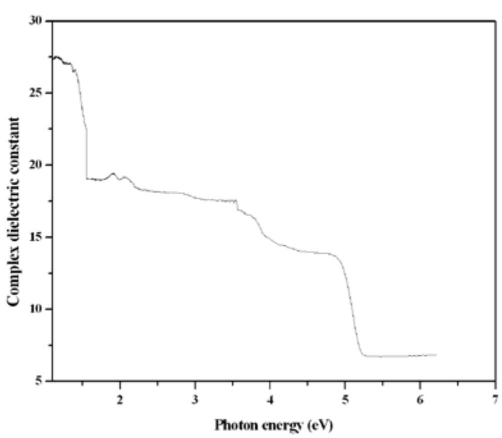

Figure 7. Complex dielectric constant Vs Incident photon energy

Figure 4 and Figure 5 shows the plot of extinction coefficient and reflectance against incident photon energy. It's found that extinction coefficient remains constant for incident photon energy of 1.1 eV to 6.5 eV and reflectance increases linearly with photon energy Figure 6 depicts the variation of refractive index with incident photon energy. Initially the refractive index decreases with increasing photon energy then becomes constant. Variation of complex dielectric constant of the material with incident photon energy is analyzed from Figure 7.

4 NLO studies

An input pulse of 6.2 mJ was used to illuminate the freshly powdered sample of particle size (above 150 μm). The NLO property of the grown LTA single crystal was analyzed by Kurtz technique [8]. This study confirmed the green emission of a crystal carried out by SHG test. A relevant comparison was made on KDP with LTA. The reference material was also powdered and used for further studies. The experimental samples reported an input pulse of 6.2 mJ, the second harmonic signal (532 nm) of 89.02 mW for KDP and 268.50 mW for LTA. It is thus elucidated that the SHG efficiency of LTA is 3.0 times higher than that of KDP.

5 CONCLUSION

A good quality single crystal of LTA was grown successfully by slow evaporation technique. Its Energy band gap is calculated from Tauc's plot as 4.7eV.The optical absorption spectrum is used to study various linear optical parameters as a function of incident photon energy. The lower dielectric constant and the higher optical response suggest the better conversion efficiency of the material. It is found that LTA is a suitable material for NLO applications

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