



LINEAR OPTICAL PROPERTIES OF L-ALANINE ADDED CADMIUM THIOUREA ACETATE (CTA) CRYSTALS

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ABSTRACT:

Metal complex crystals of cadmium thiourea acetate (CTA) with L-Alanine additive were grown by slow evaporation solution growth technique. The linear optical properties like refractive index, reflectance, extinction coefficient and study of linear optical properties doped cadmium thiourea acetate crystal reveals various industrial applications.

KEYWORDS: Metal complex crystal, Solution growth, Optical constants, linear optical properties.

1. INTRODUCTION

Thiourea (TU) is a good ligand with high crystallographic symmetry. The crystal structure of thiourea has established the coplanarity of the C, N and S atoms in the molecule. It also has a large dipole moment and the ability to form an extensive network of hydrogen bonds. Due to these important properties of thiourea, when thiourea molecule is co-ordinated with metal ions it forms the stable coordinate complexes. Thiourea is a centrosymmetric material, but when it is coordinated with metal ions it becomes a non-centrosymmetric, which is an essential property for a crystal to exhibit non-linear optical activity. The complexes of thiourea are commonly called semiorganics, since they combine the advantageous properties of organic and inorganic materials [1].

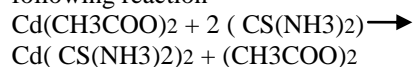
Dopants are playing the vital role in enhancing the various properties of materials. Most of the natural amino acids can individually exhibit the NLO properties. Among the amino acids L-alanine is the simplest natural amino acid with amino group and acceptor carboxyl group. In L-alanine, methyl group exists as a side chain. Hence, L-alanine is used as a dopant and it was observed that there is enhancement in the material properties [2].

As per literature survey, the effect of L-alanine, Mn(II) and glycine (Gly) on the structural, crystalline perfection, second harmonic generation

(SHG), dielectric and mechanical properties of CTA crystal was studied by V. Ganesh et al.[2] In the present investigation we have studied the linear optical properties like refractive index, reflectance, extinction coefficient, electric susceptibility & polarizability of the L-Alanine doped CTA crystal.

Synthesis and Growth

Cadmium Thiourea Acetate salt was synthesized by dissolving cadmium acetate and thiourea in the molar ratio 1:2 in deionized water according to the following reaction



The prepared salt was purified by repeated recrystallization to obtain high purity of salt. The 1 mole% of L-Alanine was added to CTA product for the growth of doped crystals. The saturated solution of CTA with L-Alanine dopant was prepared using deionized water at room temp. Constant stirring of the solution was employed to overcome the concentration gradient in the crystallizer. CTA crystals with the foresaid dopant were grown from saturated solution by slow evaporation at room temperature.

2. RESULTS AND DISCUSSION

2.1 Optical Studies:

The transmittance spectrum was recorded using Shimadzu UV-2450 spectrophotometer in the range 200-900 nm. The wide range of transmission and lower cut off wavelength makes it substantive for

second harmonic generation and UV tunable lasers [3,4]. The transmittance spectrum was used to evaluate the absorption coefficient and optical band gap using the following relation,

$$\alpha = \frac{2.303 \log \left[\frac{1}{T} \right]}{d} \quad (1)[3]$$

where T is the transmittance, α is the absorption coefficient, d is the thickness of the crystal

$$\alpha = A(h\nu - E_g)^{\frac{1}{2}}(2)[3]$$

Extinction coefficient can be obtained by the following relation,

$$k = \frac{\alpha\lambda}{4\pi} \quad (3)[4, 5]$$

Reflectance in terms of refractive index (n) is given by relations respectively,

$$R = \frac{(n-1)^2}{(n+1)^2} \quad (4)[4, 5]$$

The electrical susceptibility was calculated using the relation,

$$\chi_c = n^2 - 1 \quad (5)$$

The variation of refractive index, extinction coefficient and reflectance is shown in Fig. 1, 2 & 3. The lower values of refractive index, extinction coefficient and reflectance of L-Alanine doped CTA in entire visible region favors its suitability for antireflection coating in solar thermal devices and NLO applications [6]. The plot of polarizability and electrical susceptibility are depicted in Fig. 4 & 5. The low polarizability in entire UV region decreases the dielectric nature of material shown in Fig. 6. The lower dielectric indicates better conversion efficiency [7]. The comparative evaluation of some optical parameters is shown in Table 1. The optical studies favor the prominence of L-Alanine doped CTA for solar thermal devices, second harmonic generation, and NLO and optoelectronics applications.

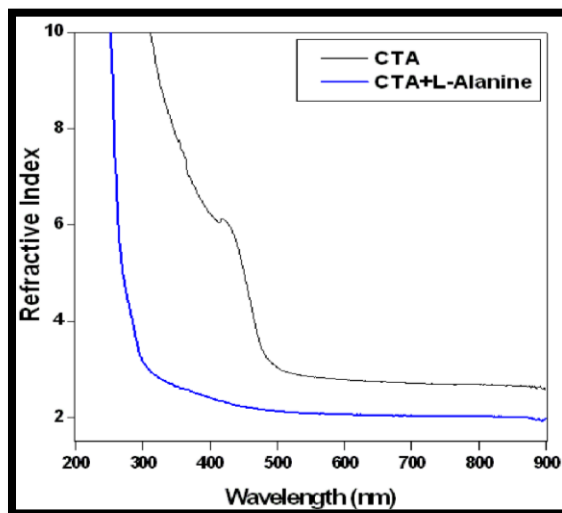


Fig.1 Refractive Index vs. Wavelength

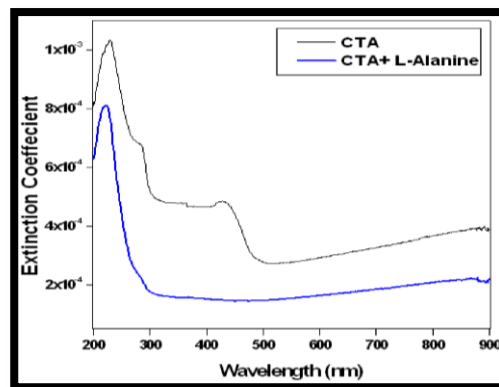


Fig.2 Extinction Coefficient vs. Wavelength

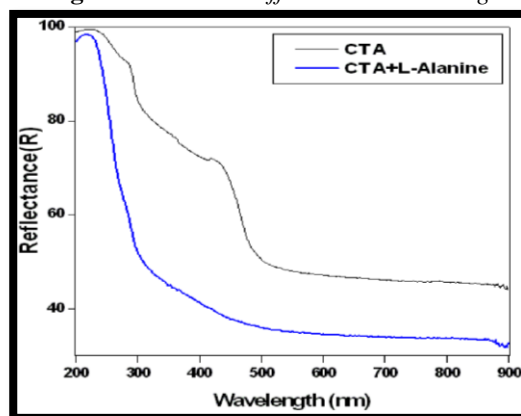


Fig.3 Reflectance vs. Wavelength

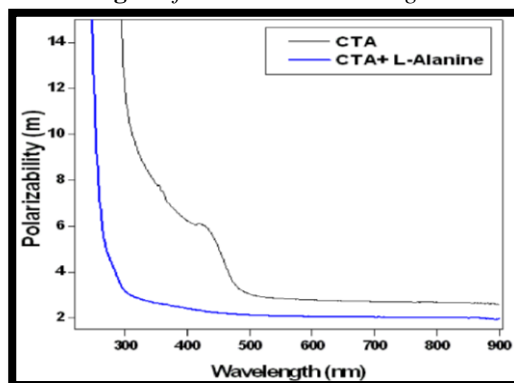


Fig.4 Polarizability vs. wavelength

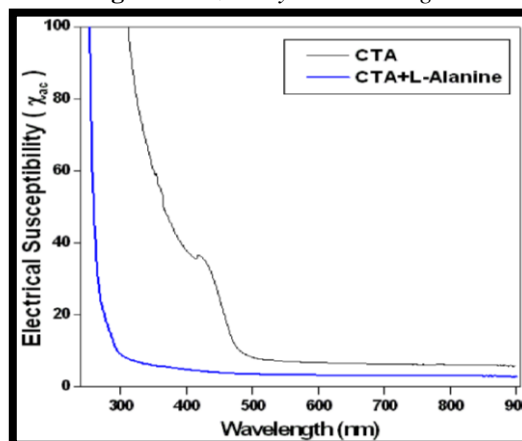


Fig.5 Electrical Susceptibility vs. Wavelength

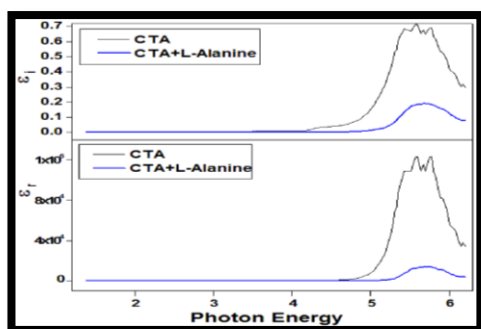


Fig.6 Real and imaginary part of dielectric Vs. Photon Energy

Parameters	CTA	CTA+Alanine
Refractive Index	3.3	2.1
ExtinctionCoefficient	2.9×10^{-4}	1.44×10^{-4}
Reflectance	51.5	36.22
ElectricalSusceptibility	10	3.7
ElectricalConductivity	77	49.8
Polaripolarizability	3.2	2.1

3. CONCLUSIONS

The high transmission, low absorbance, low reflectance and low refractive index of L-Alanine doped Cadmium Thiourea Acetate in the UV-VIS region make the material a prominent one for antireflection coating in solar thermal devices. The low extinction value (10^{-4}) and electrical conductivity (49.8 Ω/cm) shows the semiconducting nature of the material. Thus L-Alanine doped Cadmium Thiourea Acetate with many attracting linear and nonlinear optical properties is a suitable candidate for optoelectronic applications.

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REFERENCES

- [1] R.Geetha Kumari, V.Ramakrishnan, M. Lydia Carolin, J. Kumar, Andrei Sarua, Martin Kuball, "Raman spectral investigation of thiourea complexes" *Spectrochimica Acta Part A* 73,263 (2009)
- [2] V. Ganesh a, T. Bhaskar Rao c, K. Kishan Rao c, G. Bhagavannarayana d, Mohd. Shkir, "Effect of L-alanine, Mn(II) and glycine dopants on the structural, crystalline perfection, second harmonic generation (SHG), dielectric and mechanical properties of BTCA single crystals" *Mater. Chem. Phys.* 137, 276 (2012)
- [3] P. Vivek, P. Murugakoothan, "Growth and anisotropic studies on potential nonlinear optical crystal imidazole-imidazolium picrate monohydrate (IIP) in different orientations for NLO device fabrications" *Opt. Laser. Technol.* 49, 288 (2013)

[4] P. Vasudevan, S. Sankar, D. Jayaraman, "Synthesis, Optical and Electrical Studies of Nonlinear Optical Crystal: L-Arginine Semi-oxalate" *Bull. Korean Chem. Soc.* 34, 128 (2013)

[5] Ferdousi Akhtar, Jiban Podder, "A Study on Structural, Optical, Electrical and Etching Characteristics of Pure and L-Alanine Doped Potassium Dihydrogen Phosphate Crystals" *J. Cryst. Procs. Technol.* 1, 55 (2011)

[6] T. C. Sabari Girisun, S. Dhanuskodi, "Linear and nonlinear optical properties of tris thiourea zinc sulphate single crystals" *Cryst. Res. Technol.* 44, 1297 (2009)

[7] S. Shahil Kirupavathy, S. Stella Mary, P. Srinivasan, N. Vijayan, G. Bhagavannarayana, R. Gopalakrishnan, "Investigations on the growth and characterization studies of cadmium thiourea acetate (CTA) single crystals" *J Cryst. Growth* 306, 102 (2007)