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Investigation on optical, thermal and photoconductivity behavior of sodium hydrogen l-cysteine monohydrate

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ABSTRACT

In present investigation Sodium Hydrogen L-cysteine Monohydrate (SHCM) crystal has been grown by slow evaporation technique at room temperature. The optical studies were carried to examine optical transparency and determine the optical constants of the grown crystal quenching the optoelectronics applications. The optical studies ascertained high optical transparency and cut off wavelength was found to be 328 nm imperative for nonlinear applications. The optical band gap of grown crystal was found to be 5.05eV. The optical constants, extinction coefficient, nonlinear index of refraction, optical conductivity, complex dielectric, optical band gap were determined to scrutinize the electronic band structure highly demanded for optoelectronics applications. The thermogravimetric analysis (TGA) confirmed the grown crystal was stable up to 249 °C.

Keywords: Growth from solution; UV-Vis; Optical properties; Thermogravimetric analysis (TGA).

INTRODUCTION

Nonlinear optical frequency conversion materials have a significant impact on laser technology, optical communication and optical storage technology. Sodium nitrate was a potential inorganic material having wide range of applications such as electro-optic modulator, harmonic generators and parametric generators [1-2]. The literature survey confirmed the studies on improved second harmonic generation, thermal and opto-electric properties of crystals grown by mixing equimolar ratio of amino acids L-alanine, L-arginine with malic acid, oxalic acid, and nitric acid acetic acid [3-5]. The amino acids were organic materials for NLO application as they have donor carboxylic (COOH) group and the proton acceptor (NH2) amino group, known as zwitter-ions. Therefore, amino acids show high NLO activity due to chirality and donor-acceptor group [6]. L-cysteine posses a side chain with hydrogen atom which offers to charge transfer to form semi organic crystals for nonlinear optical applications [7]. Thus present study reports detailed evaluation of optical properties like optical band gap, extinction coefficient, refractive index, optical conductivity and thermal studies of Sodium Hydrogen L-cysteine Monohydrate crystal for possible application in optical limiting devices.

EXPERIMENTAL SECTION

The AR grade L-cysteine was dissolved in deionized water with continuous stirring to attain the supersaturation solution at room temperature. Sodium nitrate was introduced to supersaturated solution and stirred with constant

Azeezaa Varsha Mohammed et al

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speed for five hours to achieve the homogeneity throughout the volume. The filtered solution was kept for evaporation at room temperature. The purity was achieved by successive recrystallisation. The photograph shows good quality transparent crystals of Sodium Hydrogen L-cysteine Monohydrate cited in figure. 1. The reaction was as follows

C3H7NO2S + NaNO3 → NaHC3H5NO2S.H2O + HNO3

RESULTS AND DISCUSSION

Optical studies

The optical studies were studied using Shimadzu UV-2450 spectrophotometer within the range of 200-1400 nm. The recorded transmittance spectrum of SHCM was shown in figure 2. The grown crystal exhibits 100% transmittance in entire visible region with lower cutoff wavelength found to be 204 nm. The high transmittance and lower cutoff were imperative parameters for NLO applications [8].

The absorption coefficient was calculated using the transmittance spectrum as

$$\alpha = \frac{2.303 \log\left[\frac{1}{T}\right]}{d} \tag{2}$$

Where T is the transmittance, a is the absorption coefficient; d is the thickness of the crystal optical band gap (E_{o}) depicted in fig. 3 was calculated by

$$\alpha = A \left(hv - Eg \right)^{\frac{1}{2}} \tag{3}$$

The Band gap of the grown crystal was wide up to 5.05eV which was calculated from the Tauck's plot shown in figure 3. The wide optical band gap indicates its suitability for optical device fabrication. The relation between band gap and refractive index [9] was given as

$$E_g n^4 = 25.57$$
 (4)

The high photo response nature of the material was revealed from the above studies.

Thermo gravimetric analysis

The thermo gravimetric analysis (TGA) and the differential thermal analysis (DTA) were very important to find the thermal stability of the substance. Thermal analysis was carried out using SDT Q600V 8 build 95, simultaneous TGA/DTA analyzer in the nitrogen atmosphere at a heating rate of 20°C/min in the temperature range 20-1200°C for SHCM crystals. A powder sample of 4.396mg was used for this investigation. From Fig. 4, the compound starts to loss water at around 149.89°C and continues up to 167.28°C, in which water molecule was eliminated at around the melting point. A second dissociation with a sharp peak occurs at 249.03°C to 257.19°C with a weight loss of 22.08%, was due to the decomposition of material and rest of water molecules. Hence the compound SHCM was stable up to the temperature 249°C. The TGA curve also shows that there was a weight loss of about 22.51% in the temperature range 715.24-767.86°C due to the liberation of volatile substances probably carbon dioxide and ammonia in the compound. The DTA curve shows an endothermic peak at 149.89°C which was due to the loss of water lattice. It was followed by another peak at 249.03°C, which indicates the major decomposition of the material and this corresponds to the melting point of the substance. Then it undergoes an irreversible endothermic peak at 741.96°C which shows that the decomposition of the material. The second endothermic peak at 777.32°C may be due to the expulsion of molecules SO_2 , NH_3 and CO_2 from the chain. The thermal studies confirmed that the grown crystal was suitable for optoelectronics applications up to 249 °C.

The heat capacity at constant pressure of SHCM crystal was measured by differential scanning calorimetric (DSC) analysis in the temperature range 20- 1200°C at the heating rate of 20°C/min in the nitrogen atmosphere for the system calibration using SDT Q600V 8 build 95. Crystal weighing about 4.396 mg was placed in a sealed alumina DSC pan. The DSC curve of SHCM was shown in Fig. 5. The DSC curve observed was smooth up to 250°C and

(1)

Azeezaa Varsha Mohammed et al

shows five endothermic peaks. The peak at 156.41°C was due to the removal of weakly entrapped lattice water and the sharp peak at 248.35°C was due to the decomposition of the compound.

It was observed that the melting point of *N*-acetyl-L-cysteine was found to be 110°C. In our present work, the melting point of SHCM has been increases to 249°C. Since the melting point increases, the thermal stability of SHCM was higher than *N*-acetyl-L-cysteine [10]. This may be due to the addition of Sodium Nitrate.

Photoconductivity

The variation of both the photocurrent (I_p) and the dark current (I_d) with applied field were shown in Fig. 6. Photoconductivity study of SHCM single crystal was carried out by using Keithly 485 picoammeter. It was observed that both the photo current and the dark current of the crystal increases linearly with the applied electric field but the photo current was less than the dark current, which shows the negative photoconductivity nature of the crystal. The negative photoconductivity in the present case may be attributed to the reduction in the number of charge carriers or their lifetime, in the presence of radiation [11].



Fig 1: Photograph of SHCM



Fig 2: UV Transmittance spectrum of SHCM



Fig. 3. (ahv)² Vs Photon energy of SHCM



Fig. 6. Field dependent conductivity of SHCM

CONCLUSION

Applied field (V/cm)

The Sodium Hydrogen L-cysteine Monohydrate (SHCM) crystal was grown by slow evaporation technique. The optical studies confirmed that the grown crystal can transmit light in entire visible region. The cut off wavelength was ascertained to be 204 nm. The SHCM crystal has wide optical band gap of 5.05eV which makes it suitable for optoelectronic device fabrications. The thermal studies confirmed the suitability of grown crystal for optoelectronics device fabrication up to 249°C. The Photoconductivity study revealed that the crystal exhibits negative photoconductivity nature. All above studies revealed that the grown crystal was suitable for optoelectronics device fabrication.

Azeezaa Varsha Mohammed et al

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