Volume : 2 | Issue : 11 | Nov 2013 ISSN - 2250-1991

Research Paper Physics

Growth and Electrical Properties of Thiourea Doped l-threonine NLO Single Crystal

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ABSTRACT

A organic nonlinear optical material thiourea doped l-threonine single crystal has been synthesized and grown by slow solvent evaporation technique at room temperature using water as solvent. Single-crystal X-ray diffractometer was utilized to measure unit cell parameters and to confirm lattice parameter. SHG efficiency has been tested by Kurtz powder method. Dielectric measurements were carried out at various temperatures at frequency range 10kHz to 1MHz. It shows that the electrical parameters increases with increase in temperature and the lower dielectric constant value at lower temperatures makes the grown crystal an interesting candidate for optoelectroninc applications.

Keywords : non linear optical, single crystal, dielectric studies

I. Introduction

Non linear optical materials have been extensively studied owing to their excellent nonlinearities and rapid response in electro-optic effect compared to inorganic NLO materials [1–3]. Amino acid family crystals are still gaining importance because of its high second order nonlinear optical coefficients, wide optical transparency and multifunctional substitutions [4, 5]. It is well known that all the amino acids except glycine contain chiral carbon atom, and it gets crystallized in non-centro symmetric space group. Hence, amino acids and their complexes have potential applications in second harmonic generation, optical storage, optical communication, optical switching, photonics, electro optic modulation, and optical image processing [6]. L-threonine an excellent second harmonic generation amino acid crystal is doped with organic ligand thiourea which is a good hydrogen matrix modifier. Single crystal XRD is carried out to determine the cell parameter, Kurtz Perry test proves the non linear property of the grown crystal and dielectric studies are carried out to analyse the crystal behaviour at various temperature and measure its dielectric constant, dielectric loss, behaviour of the crystal in ac and dc field.

II. Experimental Procedure

Crystal Growth

Saturated solution of thiourea doped l-threonine undisturbed at room temperature. Tiny seed crystals with good transparency were obtained due to spontaneous nucleation. Among them, defect free seed crystal was suspended in the mother solution, which was allowed to evaporate at room temperature. Large size single crystals were obtained due to collection of monomers at the seed crystal sites from the mother solution after the nucleation process was completed. Good quality crystals were obtained after 25 days. Photograph of the grown crystal is shown in Fig.1.

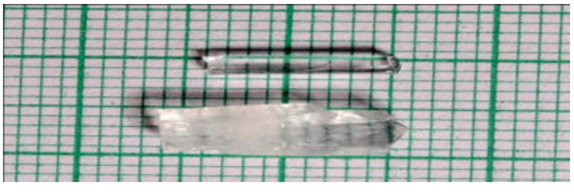

Fig.1 Photograph of as grown thiourea doped l-threonine crystal

Characterization

Single crystal XRD data of the grown crystal is found out by using ENRAF NONIUS CAD4 single crystal X-ray diffractometer with MoKl (l = 0.71073Å). The SHG efficiency of the sample was measured using Nd:YAG Q-switched mode laser (l= 1064 nm). The capacitance and dielectric loss factor (tanδ) measurements were carried out to an accuracy of +2% using an LCR meter (Agilant 4284A) with five different frequencies, viz. 100Hz, 1 kHz, 10 kHz, 100 kHz and 1 MHz at various temperatures ranging from 40 – 90oC.

Single crystal X - ray diffraction study

Single crystal X-ray diffraction (XRD) analysis of TTHU was carried out using ENRAF NONIUS CAD-4 diffractometer with Mo Kα radiation(λ= 0.7070Å). From the data it was observed that the TTHU crystallizes in non centrosymmetric orthogonal structure with lattice parameters, a=13.58Å, b=7.74 Å, c=5.14 Å, Volume=540.26 Å and space group P_{21}. The slight change in lattice parameter from that of pure L-threonine [7] may be attributed to the incorporation of thiourea in the lattice of L-threonine.

Second Harmonic Conversion Efficiency

SHG efficiency of the grown crystal was carried out by Kurtz and Perry test [8]. The source used was Q-switched, mode-locked Nd:YAG laser emitting 1.06 µm fundamental radiation. The SHG conversion efficiency of TTHU single crystal was confirmed by the intense green light emission from the sample.

Dielectric study

Figs. 2 and 3 show the variation of dielectric constant and the dielectric loss of TTHU crystal as a function of frequency at different temperatures on a- direction (40 - 90 °C). Single crystals of (TTHU) have been cut in the appropriate orientation and subjected to dielectric measurements. A thin coating of carbons was applied on both the surfaces of the samples for firm contact. The capacitance and dissipation factor of the specimen were measured as a function of frequency in the range from 100 Hz to 1 MHz using Agilent 4284A LCR METER. Fig. 2 shows the dielectric constant as a function of frequency for TTHU single crystals along a- direction. The dielectric constant of the material is mainly due to the contribution of space charge polarization at low frequencies (below 10 kHz). The magnitude of dielectric constant is a measure of the electrostatic binding strength between ions. The ε_r and tanδ values are found to decrease whereas the σ_{ac} value is found

 ISSN - 2250-1991

to increase with the increase in frequency along a- direction at all temperatures. This is a normal dielectric behaviour. This can be understood on the basis that the mechanism of polarization is similar to the conduction process. The electronic exchange of the number of ions in the crystal gives local displacement of electrons in the direction of the applied field, which in turn gives rise to polarization. It could be noticed that the crystal has a low εr value, hence such dielectric material is gaining more importance in the microelectronics industry. The variation of dielectric loss with frequency at different temperatures is shown in Fig. 3. It is well observed that the dielectric loss decreases with increasing frequency. The low value of dielectric loss indicates that the grown crystals are of moderately good quality [9].

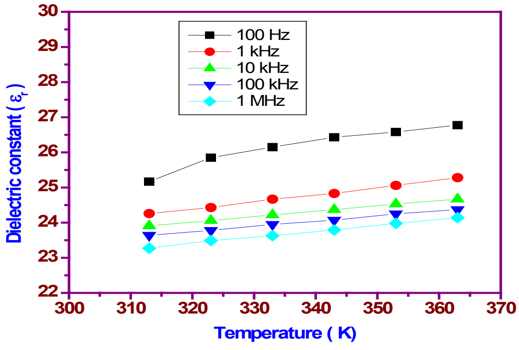

Fig. 2 Temperature dependence of dielectric constant

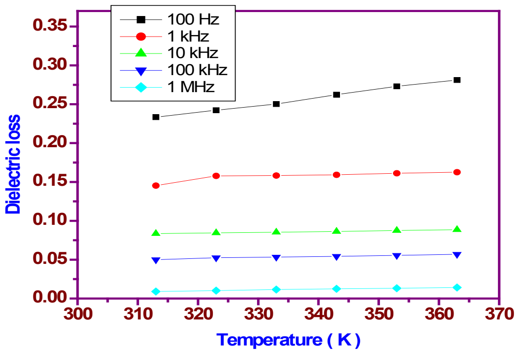

Fig. 3 Temperature dependence of dielectric loss

AC and DC Conductivities

Figs. 4 and 5 show the σ_{ac} and σ_{dc} values obtained for TTHU single crystal. Both the electrical conductivities (σ_{ac} and σ_{dc}) increase, in the TTHU crystal studied, smoothly through the temperature range considered in the present study; the ε_r and tanδ values are found to decrease whereas the σ_{ac} value is found to increase with the increase in frequency along a- direction and at all temperatures. There is no sharp increase that would be characteristic of a superprotonic phase transition.

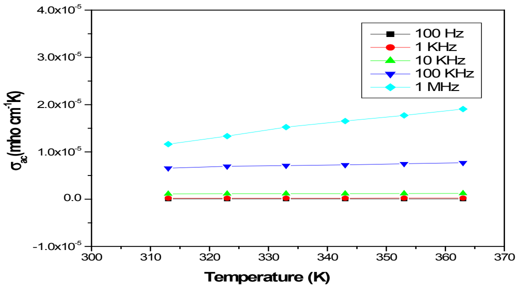

Fig. 4 AC electrical conductivities along a direction

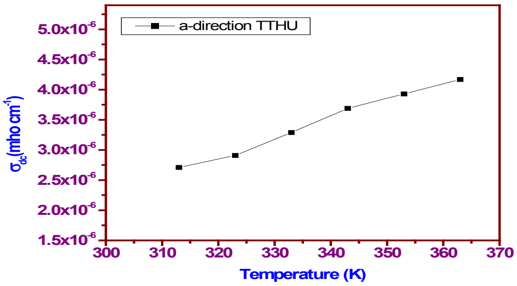

Fig. 5 The DC electrical conductivities along a- direction

III. CONCLUSION

Single crystals of TTHU of appreciable size were grown by the slow evaporation technique. Single crystal XRD confirms the grown crystal. Kurtz and Perry test confirms the NLO property of the grown crystal. The dielectric studies prove the low values of dielectric constant and dielectric loss in the sample at high frequency. The variation of dielectric constant observed with temperature could be understood as essentially due to the temperature variation of ionic polarizability.

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