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ChemTech

International Journal of ChemTech Research
CODEN (USA): IJCRGG ISSN : 0974-4290
Vol.6, No.3, pp 1578-1581, May-June 2014

ICMCT-2014 [10th – 12th March 2014]
International Conference on Materials and Characterization Techniques

Spectral, Second Harmonic, Third Harmonic and Thermal analysis of Phosphorous acid admixtured L-Alanine Crystals (PALA)

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Abstract: Tranparent and colourless single crystals of phosphorous acid admixtured L-alanine (PALA) were grown by solution method for the first time at room temperature. In this work, L-alanine and phosphorous acid were used to synthesize PALA salt. XRD analysis confirms orthorhombic structure of the grown crystal. Suitability of PALA crystal for NLO application was determined by optical transmission and SHG efficiency analysis. Thermal stability of PALA crystal was determined by TG-DTA analysis. Third-order nonlinear (THG) studies of PALA crystal have been investigated by Z-scan method. The values of nonlinear refractive index (n_2), the nonlinear absorption coefficient (β) and third-order nonlinear susceptibility ($\chi^{(3)}$) were estimated for the sample.
Keywords: Amino acid complex; single crystal; XRD; SHG; TG/DTA; Z-scan.

1. Introduction

Organic nonlinear optical (NLO) materials have high nonlinearities and rapid response in electro-optic effect compared to inorganic NLO materials. There has been considerable interest in the study of organic NLO crystals with good nonlinear properties because of their wide applications in the area of optical communication, optical information processing and optical data storage technology [1]. Among organic crystals for NLO applications, amino acid like L-alanine is an efficient NLO crystal. Here for the first time we report the growth of a promising nonlinear organic crystal of phosphorous acid admixtured L-alanine crystals (PALA) by slow evaporation growth technique and the grown crystals were subjected to various studies like XRD, UV-visible spectral studies, SHG, third harmonic generation measurement and thermal studies.

2. Synthesis, Solubility and Crystal Growth

PALA salt was synthesized at 50^{o} C from L-alanine and phosphorous acid (H_3PO_3) taken in the molar ratio 2:1. Solubility of synthesized sample was found by gravimetrical method [2]. Fig.1 shows that PALA crystal has positive temperature coefficient of solubility.

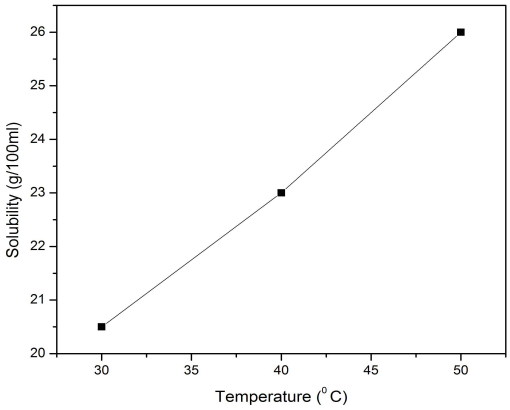

Figure 1: Solubility curve of PALA sample

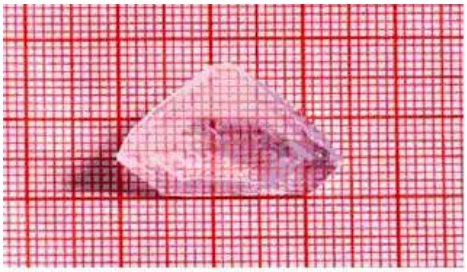

Figure 2: As grown crystal of PALA crystal

Based on the solubility data, the saturated solution was prepared and stirred well for about 3 hours using a magnetic stirrer and then it was allowed for growth by slow evaporation. A transparent and colourless crystal was harvested after 25 days and it is shown in figure 2.

3. Results and Discussions

3.1. Unit cell parameters

The obtained lattice parameters from a single crystal X-ray diffractometer are a=5.775 Å, b=6.011Å, c=12.415 Å, α=β=γ=90° and V = 430.95 $Å^3$. The structure of the sample is orthorhombic crystal system. The obtained structure of grown crystal is almost coincided with those of L-alanine crystal. Slight changes in lattice parameters may be due to incorporation of admixture element.

3.2. Linear optical study

To determine the optical transmittance range and hence to know the suitability of PALA single crystal for optical applications, the UV-visible spectrum was recorded for the crystal. The crystal is found to show a good transmittance (~85%; Fig. 3) in the visible region and it is noted that the UV transparency cut-off occurs at 238 nm. The good transparency and lower cut-off wavelength of this material enable it to be a good candidate for optoelectronic applications [3]. The band gap value of PALA sample is found to be 5.21 eV.

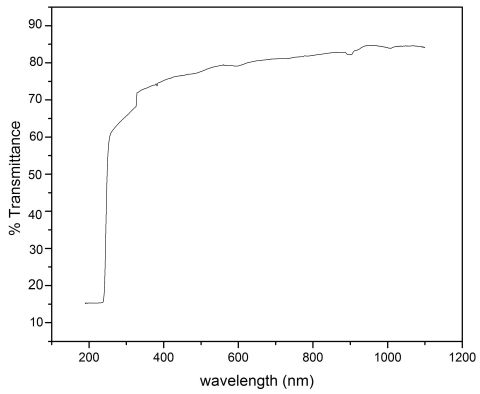

Figure 3: Optical transmission spectrum of PALA crystal

3.3. Second harmonic generation analysis (SHG)

The powder technique of Kurtz and Perry was used to study the NLO behavior of the grown crystalline specimen [4]. Nd:YAG laser of wavelength 1064 nm coupled with the energy meter, pulse width of 8 ns and pulse energy of up to 300 mJ was used for the SHG measurement. The SHG efficiency of PALA crystal is found to be 0.82 times that of KDP material. So it is a promising material for NLO applications and comparable with L-alanine.

3.4. Third harmonic generation analysis

Third-order nonlinear optical studies were performed using Z-scan technique for the grown PALA crystal in order to estimate the intensity dependence of nonlinear absorption and nonlinear refraction process. Z-scan technique is based on the conversion of amplitude distortion from phase distortion during the propagation of beam in sample. The theory part and experimental part for Z-scan technique was reported already [5]. The nonlinear absorption coefficient (β), nonlinear refractive index (n_2) and third-order susceptibility of the grown crystal have been measured in open and closed aperture modes and the obtained third-order nonlinear parameters are n_2 = 1.12x10-^{10} cm^2/W, β = 1.69 x10^{-5} cm/W and third-order nonlinear susceptibility ($\chi^{(3)}$) = 7.15 x10^{-4} esu.

3.5. Thermal analysis

The TGA/DTA of PALA crystal is shown in Fig. 4. The initial mass of the material was taken to be 5.868 mg and the final mass left out after the experiment was only 0.5002 mg of initial mass. The PALA sample was stable up to 210 ^{o}C. There is a major weight loss of sample between 210 ^{o}C to 325^{o}C which was assigned to decomposition of PALA crystal.

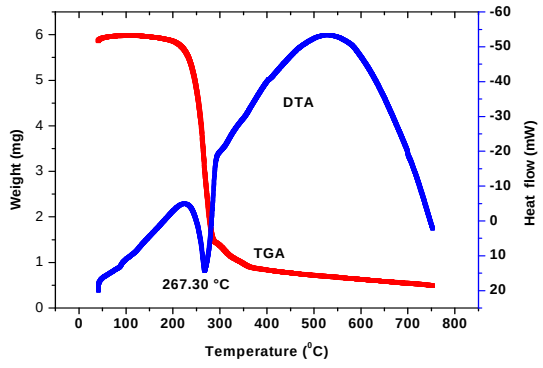

Figure.4: TGA/DTA curve of PALA crystal

From the observation it was concluded that the crystal decomposes only at 267.30°C. The sharp exothermic peak shows the good degree of crystallinity of the sample [6].

3.6. Conclusion

The good quality of transparent single crystals of PALA is grown by slow evaporation solution method. XRD analysis confirms its orthorhombic structure. The improved NLO efficiency, good degree of crystallinity, the good transparency and lower cut-off wavelength of this material enable it to be a good candidate for optoelectronic applications. The third-order NLO parameters for the sample have been evaluated by Z-scan technique.

Acknowledgement

The authors are grateful to Department of Science and Technology (DST), Government of India for the financial support to carry out this work. The authors thank the management of Aditanar college of Arts and science, Tiruchendur for providing the excellent research facilities.

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