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Spectroscopic, Mechanical and Optical Properties of L-Serine Ammonium Carbonate (LSAC) Single crystal

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Abstract: *L-serine ammonium carbonate (LSAC) Single crystal have been grown by slow evaporation solution growth technique. Energy dispersive X-ray analyses (EDAX) prove the incorporation of metal ions into crystals. The presence of functional groups is identified by Fourier transform infrared (FTIR) analyses. The mechanical properties have been studied by vicker's microhardness test. UV–vis-NIR spectroscopy shows that minimum absorption in the entire visible region. The optical band gap (Eg) value of the grown crystal is obtained from the Tauc's plot of $(\alpha h\nu)^2$ vs hν which was determined by extrapolating the linear region of the curve to the hν axis where $(\alpha h\nu)^2=0$. LSAC crystals have enhanced second harmonic generation (SHG) efficiency indicating that these crystals are potential candidates for non linear optical (NLO) applications.*

Key Words: *SHG, NLO, EDAX, LSAC, UV–vis-NIR spectroscopy, FTIR*

1. INTRODUCTION

Nonlinear optical (NLO) materials, with high frequency conversion efficiency have the most required properties for optical communication and optical storage devices, and numerous device applications [1, 2]. Amino acids family crystals possess high NLO efficiency because of their noncentrosymmetric space group and chiral carbon atom [3, 4]. Amino acids are popularly referred as the building blocks of protein. Amino acid family crystals are of great interest due to their rich nonlinear optical properties. Its specific features such as Zwitterionic nature, weak Vander Waals, hydrogen bonds and wide transmittance in the visible and UV-spectral region make them an ideal candidate for NLO applications [5, 6]. In the present investigation is aimed at the growth of L-serine ammonium carbonate single crystals by slow evaporation method at room temperature. The grown crystals have been subjected to EDAX, FTIR, UV analysis, optical band gap measurements, second harmonic generation (SHG) measurement, and Vicker's hardness test.

2.SYNTHESIS

The appropriate stoichiometric amount of L-Serine and ammonium carbonate was taken with excess of doubly deionized water to synthesize LSAC. The as said molecules were dissolved in deionized water and saturated LSAC solution was prepared at room temperature and kept for slow evaporation. The grown crystal has the dimension 12mm×11mm×5mm as shown in the Fig.1.

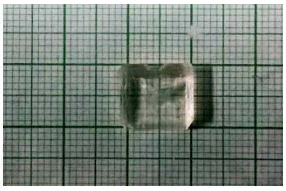

Fig.1. Photograph of as grown LSAC

3. CHARACTERISATION

3.1EDAX

Small crystal of LSAC was subjected to EDAX analysis Fig.2 and Table.1. As the presence of hydrogen ions cannot be detected by EDAX analysis due to its low atomic numbers [7]. The low percentage of incorporation of ammonia may be due to their larger ionic radii. Even though the amount of ammonia is less, it plays an important role in the enhancement of NLO property in the crystals.

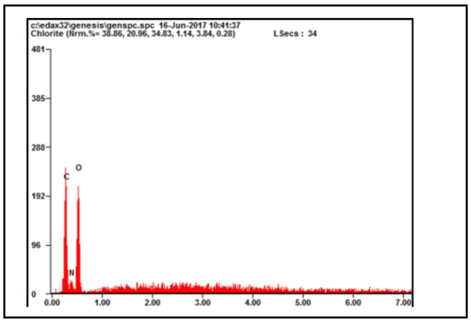

Fig.2. The EDAX spectrum of the LSAC sample recorded in electron microscope

3.2 FTIR analysis

Fourier Transform Infrared analysis was carried out for the grown LSAC crystal to find the functional groups of the crystal. A fine powdered sample of LSAC was used for the FT-IR spectral analysis and the spectrum was recorded in the range 400 cm^{-1}–4000 cm^{-1} using KBr pellet technique. The recorded spectrum is shown in Fig.3. The absorption band at 3453 cm^{-1} is assigned to OH stretching vibrations (caused by absorption of water by KBr). The absorption band at 3095 cm^{-1} is caused by NH^{3+} symmetric stretching vibrations.[7 F. Helen] The peaks at 3432 cm^{-1} and 3119 cm^{-1} having nearly good absorption in the o-H and NH^{3+}.The strong absorption peak at 1630 cm−1indicates the presence of primary amino acid group. The multiple combination and overtone bands extended the absorption of hydrogen bonded N–H stretching vibration to 2000 cm−1 [8R. M. Kumar].In the present work we have absorption peak at 1637 and 2042. The bending and rocking vibrations due to CH group have been observed at 1345 cm^{-1} and 1306 cm^{-1} respectively. C-OH bending corresponds to peak at 1220 cm^{-1}. The CN stretching vibrations produce peaks around 969 cm^{-1}. It is found that, there is a slight shift in the spectrum is due to the influence of ammonium in the crystal.[9]

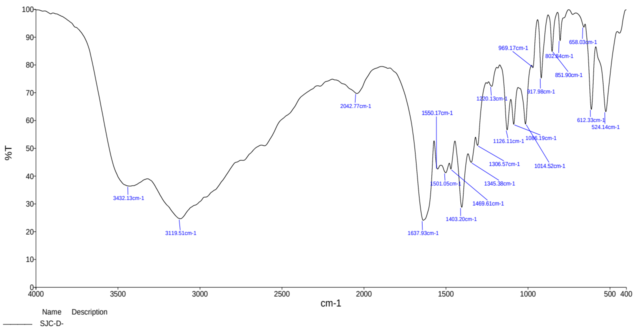

Fig.3. FT-IR spectrum of the sample.

3.3 UV–vis-NIR spectroscopy

The optical behavior of the material basically includes the interaction of light radiation over the range of the electromagnetic spectrum. The ultraviolet light absorbed by the sample gives information about the transparency window which is very essential in many optoelectronic applications. The optical transmission spectra of pure and doped crystals of good quality were recorded in the wavelength range 190–1100 nm and shown in Fig. 4. As there is no absorption, the crystals are found to be transparent in the visible and near IR region, an essential parameter required for frequency doubling process [10]. With the wide transparency window in the entire visible and near IR range, these crystals can be used for optical device fabrication. The UV cut off wavelength of the LSAC single crystal is 261nm.

The optical absorption co-efficient [α] is calculated using the following relation

$$\alpha = 2.303 \times \log (1/T) / d$$

where T is the transmittance and d is the thickness of the crystal. The energy dependence of absorption coefficient suggests the occurrence of direct band gap and hence it obeys the relation for high photon energy

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

where E_g is optical band gap and A is a constant. The variation of [hν] vs $[\alpha h\nu]^2$ is shown in Fig. 5 and E_g value is evaluated by extrapolation of the linear part to a point $[\alpha h\nu]^2 = 0$. The optical band gap is found to be 6.17 eV for LSAC single crystal . As a consequence of wide band gap, all the grown crystals have large transmittance in the visible region which enables these materials for higher harmonic generation [11].

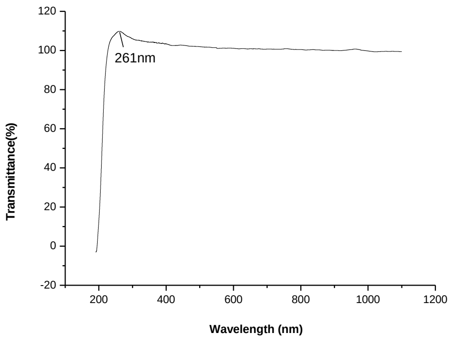

Fig.4. Optical transmittance spectrum of LSAC crystal

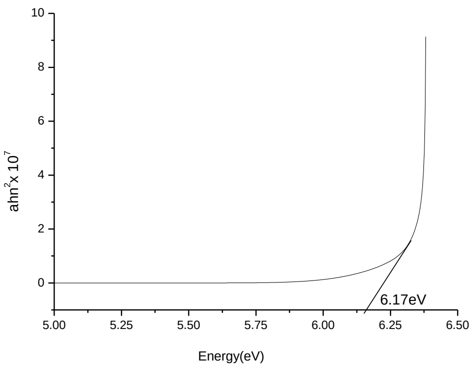

Fig.5. Energy band gap curve of LSAC crystal

3.4 Mechanical stability

Vicker's microhardness profiles as a function of the applied test loads (shown in Fig. 6and 7) clearly show that the hardness increases with increase in the applied load and suddenly decreases hence it refers to reverse indentation size effect . From the plot of log P vs log d, where P is the applied load and d is the diagonal length of the impression, the value of the work hardening coefficient (n).Following the criterion of Onitsch[12] and Hanneman[13], it can be stated that since n > 1.6, LSAC belongs to the category of soft materials.

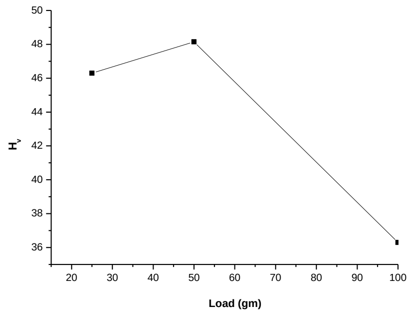

Fig.6- Hardness Graph H_v vs load

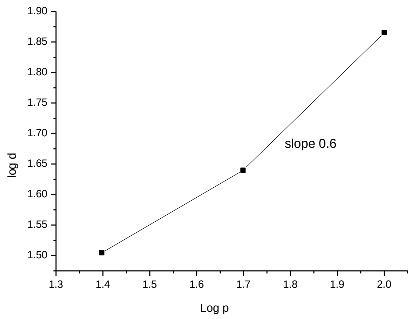

Fig.7.Hardness Graph log d vs log p

3.5 Second harmonic generation

The second harmonic efficiency of LSAC crystal has been measured by Kurtz-Perry powder technique [14]. The SHG signal was confirmed by the emission of green light (λ = 532 nm) from the sample. The output signal of 305 mV for LSAC crystal was obtained for an input of 30 mJ/pulse compared with the SHG output signal of standard KDP crystal of 295 mV for the same input energy. The SHG efficiency of the grown LSAC crystal is 0.81 times that of KDP crystal.

4. CONCLUSION

Single crystal of LSAC was grown by slow evaporation technique. Linear optical studies show the transparency of the crystal in the entire visible region. SHG studies confirm the nonlinearity of the grown crystal by the emission of green light and the SHG efficiency of the grown LSAC crystal is found to be 0.84 times that of KDP crystal. FT-IR spectrum of the crystal elucidates the presence of various functional groups in the crystal. The Vickers micro hardness study of the crystal was carried out and the crystal is found to be of hard material category.

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REFERENCES

[1] H. O. Marey, L. F. Warrn, M. S. Webb, C. A. Ebbers, G. C. Kennedy, and G. C. Catella, Applied Optics, vol. 31, no. 24, pp. 5051–5060, 1992.

[2] X. Q. Wang, D. Xu, D. R. Yuan, et al., Materials Research Bulletin, vol. 34, no. 12-13, pp. 2003–2011, 1999.

[3] M. Kitazawa, R. Higuchi, and M. Takahashi, Applied Physics Letters, vol. 64, no. 19, p. 2477, 1994.

[4] L. Misoguti, A. T. Varela, F. D. Nunes et al., Optical Materials, vol. 6, no. 3, pp. 147–152, 1996.

[5] Sweta Moitra, TanusreeKar, J. Cryst. Growth 310 (2008) 4539.

[6] Tianliang Chen, Zhihua Sun, Cheng Song, Yan Ge, Junhua Luo, Wenxiong Lin and Maochun Hong, Cryst. Growth Des. 12 (2012) 2673.

[7] F. Helen, G. Kanchana, Optik - International Journal for Light and Electron Optics Volume 125, Issue 9, May 2014, Pages 2051-2056

[8] R. M. Kumar, D. R. Babu, D. Jayaraman, R. Jayavel, and K. Kitamura, Journal of Crystal Growth, vol. 275, no. 1-2, pp. e1935–e1939, 2005.

[9] V. Vasudevan, R. Ramesh Babu, G. Bhagavanarayana, K. Ramamurthi, Effect of metal and amino acid dopants on the growth and properties of l-lysine

monohydrochloride dehydrate single crystal, Mater. Chem. Phys. 124 (2010) 681–688.

[10] C.N.R. Rao, Ultraviolet and Visible Spectroscopy of Organic Compounds, Pren-tice Hall Pvt. Ltd., New Delhi, 1984, pp. 60–66.

[11] V. Krishnakumar, S. Manohar, R. Nagalakshmi, Semiorganic nonlinear optical l-lysine sulphate growth and characterization, Spectrochim. Acta A 75 (2010) 1394–1397.

[12] E. M. Onitsch, Mikroskopia, Vol. 2, 1947, p. 131.

[13] M. Hanneman, Metallurgia Manchu, Vol. 23, 1941, p. 135.

[14] S. K. Kurtz and T. T. Perry, Journal of Applied Physics, vol. 39, no. 8, p. 3798, 1968.