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Effect of L-Alanine Doping On the Physicochemical Properties of Strontium Formate Dihydrate Crystals

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ABSTRACT: L-Alanine doped strontium formate dihydrate crystals were grown by slow evaporation method. The optimized growth parameters for growing the crystal were determined. The grown crystal was characterized by XRD, FTIR and UV. XRD studies showed that the lattice volume of strontium formate dihydrate crystals increase with doping concentration. Fourier transform infrared (FT-IR) studies confirm the various functional groups present in the grown crystal. The UV-Vis absorbance spectra have been recorded to find the cut-off wavelength.

KEYWORDS- L-Alanine doping, Strontium formate crystals, Physicochemical properties

1. INTRODUCTION

In recent years several studies dealing with organic, inorganic and semi organic molecules and materials called nonlinear optics (NLO) are being reported due to the increasing need for photonics applications. The nonlinear (NLO) responses induced in various molecules in solution and solids are of great interest in many fields of research [1]. Both organic and inorganic crystals were grown and characterized for NLO applications. Crystals of metal formates of I and II groups of the periodic systems exhibit marked nonlinear optical (NLO) properties comparable to that of the best nonlinear materials used for efficient frequency doubling of a Nd:YAG laser and for the phase matched SHG for ruby laser[2]. Deserno and Haussuh[3] have shown that orthorhombic Sr(CHO₂)₂ and Sr(CHO₂)₂.2H₂O crystals allow phase-matched SHG and optical mixing in the near IR to UV region and low sensitivity with respect to aperture walk off and beam divergence. With an increasing demand of materials for NLO applications there is growing interest in investigations on crystallization and properties of new materials. Strontium formate dihydrate is found to be orthorhombic with space group P212121. Strontium formate dihydrate crystals are of considerably interest, particularly for the basic studies of some of their interesting physical properties. A thorough survey of the literature shows that very little work has been done on the effect of doping on the physicochemical properties of strontium formate dihydrate crystals. Therefore in the present study we have attempted to study the effect of L-Alanine doping on the physicochemical properties of strontium formate dihydrate crystals. The results obtained in the present study are reported herein.

II. EXPERIMENTAL

The synthesis of strontium formate dihydrate was reported in our earlier work[4]. A saturated solution of strontium formate dihydrate doped with L-Alanine in the required concentration was kept in a magnetic stirrer at a temperature of 40 °C for a period of 2 hours. The dopant concentrations were 0.05 M. The solution thus obtained was filtered and transferred to the growth vessel (100 mL beaker) and kept in a constant temperature bath with an accuracy of ±0.1 °C. The temperature of the bath was maintained at 40 °C throughout the growth process. The best crystal with good morphological perfection and transparency was grown in size.

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III. CHARACTERIZATION TECHNIQUES

The powder X-ray diffraction (XRD) patterns were obtained using a powder X-ray diffractometer. [Model: Ritz-170 with Nickel filtered CuK α radiation (1.54056 \AA)]. The Infrared spectroscopy is effectively used to identify the functional groups to determine the molecular structure of the grown crystals. The FT-IR spectra of the samples were recorded using a Perkin Elmer Lambda 35 IR spectrophotometer by KBr pellet technique in the wavenumber range 400-4000 cm $^{-1}$. The optical transmission spectrum was recorded using Perkin Elmer Lambda 35 spectrophotometer in the wavelength region 200-320 nm.

IV. RESULTS AND DISCUSSION

4.1 Powder XRD

The optimum temperature for the growth of L-Alanine doped strontium formate dihydrate crystals was found to be 40 °C. Crystals of good quality and transparency appeared below the beaker in about 48 hours and grew in large crystals in about 7-8 days. The largest crystal was about 8 mm in length. It is observed that as the size of the crystal increases the transparency was reduced. The photograph of the grown crystals was displayed in fig.4.1.



Figure 4.1: Grown L-Alanine doped strontium formate dihydrate crystal

The material of the grown crystals was confirmed by x-ray diffraction studies. The grown crystals were confirmed to be L-Alanine doped strontium formate dihydrate crystals. The x-ray diffraction data compares very well with the JCPDS data (File No. 14-0824). Lattice variation and increase in lattice volume further confirm the entry of the dopant into the crystal lattice. The lattice parameters for L-Alanine doped strontium formate dihydrate crystal obtained in the present study are: $a = 7.366 \text{ \AA}$, $b = 12.126 \text{ \AA}$ and $c = 7.142 \text{ \AA}$.

4.2 FT-IR analysis

The FT-IR spectrum obtained in the present study for grown crystal is similar to the IR spectrum of strontium formate dihydrate crystals reported earlier [5-6]. In L-Alanine doped strontium formate dihydrate crystal, the absorption peaks at 3301 due to water. The bands observed at around 3130.64 cm $^{-1}$ are due to stretching and bending vibrations of the -CH group. The band observed at around 2169.29cm $^{-1}$ is attributed to stretching vibration of the -CO group. The symmetric and asymmetric vibration modes of formate ions(-COO) are observed at around 1595.50 cm $^{-1}$ and 1363.73cm $^{-1}$.The bands observed at around 784.97cm $^{-1}$ due to stretching and bending vibrations of the -CH group. The FT-IR spectrum obtained for the doped crystal resembles that of the pure crystal. In addition to the peaks described

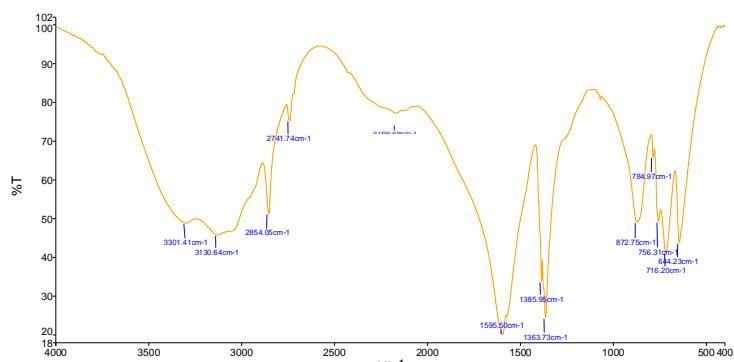
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above, few absorption peaks are observed between $500 - 660 \text{ cm}^{-1}$ indicate an appreciable shift of peak positions to lower and higher values suggesting incorporation of dopants in the crystal lattice. These peaks are attributed to metal-oxygen bonds. It is noted from figure 4.2, the vibrational modes are unaffected in the doped crystals; indicating that there is no interaction between the formate ion and the dopant added.



. Figure 4.2. FTIR spectra of the grown L-Alanine doped strontium formate dehydrate

4.3 UV–Visible spectral analysis

The single crystals are mainly used for optical applications. Thus the study of optical transmission range of grown crystal is important. The optical absorbance spectrum was recorded using Perkin Elmer Lambda 35 spectrophotometer in the wavelength region 200-320 nm. The absorbance spectra show the grown crystals have lower cutoff wavelengths at around 218 nm for L-Alanine doped strontium formate dihydrate crystal. The grown doped crystal has good transmission in UV as well as in visible regions, it is shown in Fig.4.3. The wide range of transparency in UV, visible and IR regions enables good transmission of the second harmonic frequency of Nd:YAG laser. The forbidden band gap for the grown crystal was 5.699 ev. This work was calculated using the relation $E=hc/\lambda$, where 'h' is the Planck's constant, 'c' is the velocity of light and ' λ ' is the cut-off wavelength. Thus grown crystal has good absorbance in UV as well as in visible region. This is an added advantage in the field of optoelectronic applications.

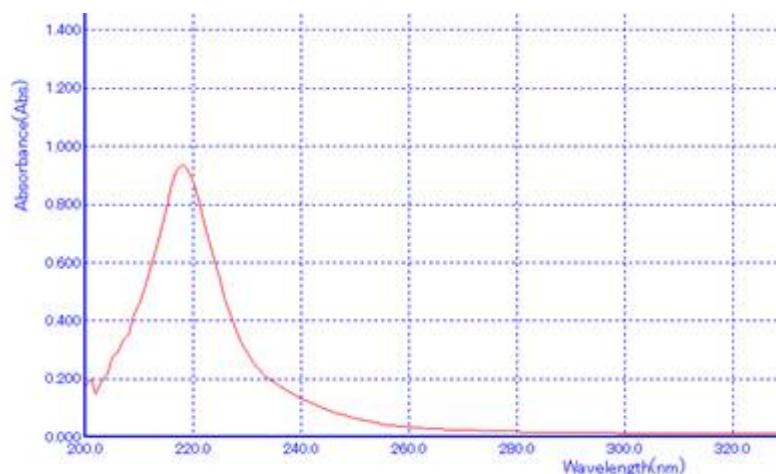


Figure 4.3: Absorbance spectrum of L-Alanine doped strontium formate dihydrate crystal

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V. CONCLUSION

L-Alanine doped strontium formate dihydrate crystals were successfully grown by slow evaporation method. The grown crystals were characterized by XRD, UV and FTIR analysis. Lattice variation and increase in lattice volume further confirm the entry of the dopant into the crystal lattice. The presence of various functional groups was confirmed by FT-IR analysis. From FTIR spectra it was observed that the vibrational modes are unaffected in the doped crystals, indicating that there was no interaction between the formate ion and the dopant added. UV-Visible study shows that the grown crystal has wide range of transparency in UV and entire visible region and cutoff wave length is around 218 nm.

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