

Growth and Characterization of Barium chloride Doped with L-Alanine Single crystal

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Abstract: Single crystals of Barium Chloride doped with L-Alanine were grown by slow evaporation solution growth technique. The grown crystals were characterized by powder XRD, FTIR and UV-Visible spectroscopy. The reflection planes of the sample were confirmed by the powder X-ray diffraction study and diffraction peaks were indexed. Functional groups of the grown crystals were identified from FT-IR spectral analysis. UV-Visible spectrum studies explain the transmission ability of the grown crystals.

Keywords: Single crystal, slow evaporation, X-ray diffraction, FT-IR

1. Introduction

Several important technologies like microelectronics, optoelectronics, computers, photonics, lasers, information science, etc., need well characterized bulk single crystals. In recent years the amino acid group materials were mixed with organic¹ or inorganic salts² in order to improve their chemical stability, laser damage threshold, thermal and physical properties and linear and non-linear optical properties. Amino acids are interesting organic materials for NLO applications. They contain proton donor carboxylic acid (COOH) and the proton acceptor amino (NH₂) groups which provide the ground state charge asymmetry of the molecule required for second order non linearity [3, 4].

L-alanine is an essential amino acid with the chemical formula CH₃CH.NH₂COOH and it is an important source of energy for muscle tissue, the brain and central nervous system and also it strengthens the immune system by producing antibodies, helps in the metabolism of organic acids and sugars.

L-alanine can be considered as the fundamental building block of more complex amino acid which shows strong non linear behavior. In the present work, we report the growth of Barium chloride doped with L-alanine single crystals by slow evaporation technique. The grown crystals were characterized by powder XRD, FTIR and UV-Visible spectroscopy.

2. Experimental Procedure

The saturated solutions of Barium chloride dihydrate (99% purity) and L-alanine were prepared separately and taken in the ratio 3:1. The prepared solution was stirred continuously using magnetic stirrer for 2 hours. Then the solution was filtered and kept undisturbed in room temperature for slow evaporation. The good quality single crystals were harvested after a period of 83 days. The photograph of the grown crystal is shown in figure.1.

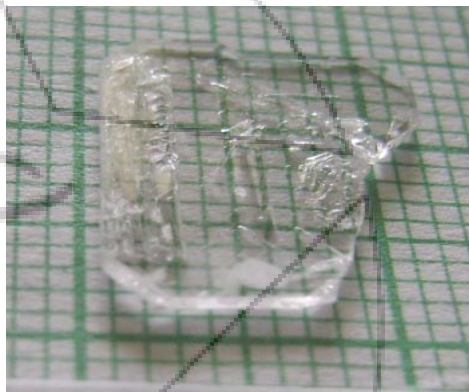


Figure 1: Photograph of the L-Alanine doped BaCl₂ crystal

3. Result and Discussion

3.1 Powder XRD Analysis

The grown crystal has been crushed to a uniform fine powder and subjected to powder X-ray diffraction technique to identify the reflection planes. The well defined peaks at specific 2θ values show high crystallinity of the grown crystal. The powder X-ray diffraction pattern of the grown crystal is shown in Fig 2. The lattice parameters are a=6.69Å, b=10.6Å, c= 7.10Å and V=503Å³

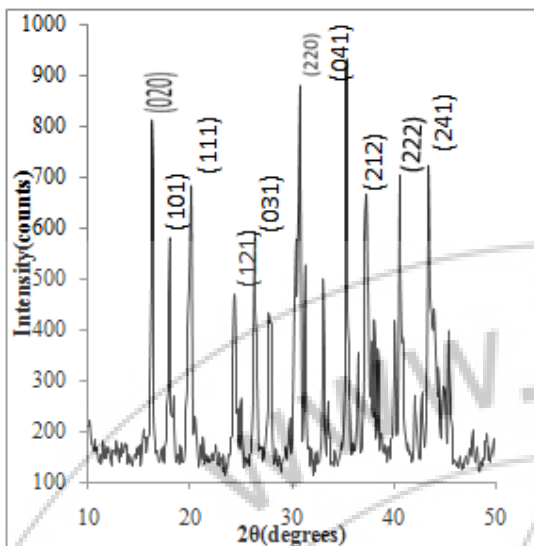


Figure 2: Powder XRD Fig.2.Powder XRD pattern of the grown crystal

3.2 FTIR Spectrum Analysis

The FTIR spectrum of the grown crystals was recorded in the range 400–4000 cm^{-1} from KBr pellets on a Perkin Elmer FTIR spectrometer. The recorded FTIR spectrum is shown in Fig.3. The band 569 cm^{-1} represents the C-Cl stretching. The peak at 1463.97 cm^{-1} in the spectra is assigned to -NO_2 stretching. The region at 2318.44 cm^{-1} represents the NH stretching. The peak at 3317.56 cm^{-1} in the spectra is assigned to O-H stretching. All the functional group assignments are summarized in table 1.

Table 1: FTIR assignments for the grown crystal

Wavelength(cm^{-1})	Band assignments
569	C-Cl stretching
1463.97	-NO_2 stretching
2318.44	NH stretching
317.56	O-H stretching

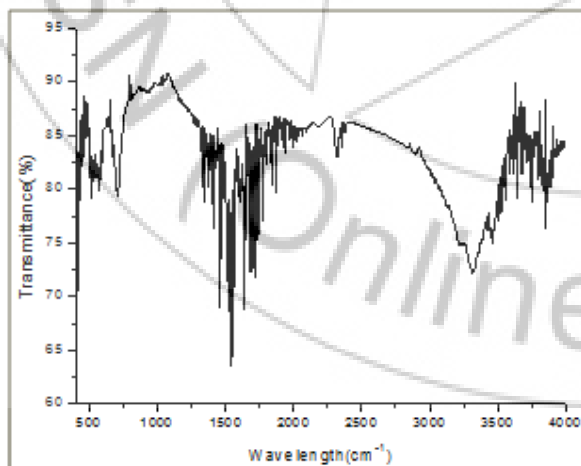


Figure 3: FTIR spectrum of the grown crystal

3.3 UV-Visible Spectrum Analysis

The optical transmission spectrum of the grown crystals were recorded in the range 200–800 nm using LAMBDA 35 Model UV spectrometer and the transmittance spectrum is shown in Fig.4. It is observed that the grown crystal has lower cut off wavelength at 230 nm and good transmission in the entire visible region. The absorption spectrum of the grown crystal is shown in Fig.5.

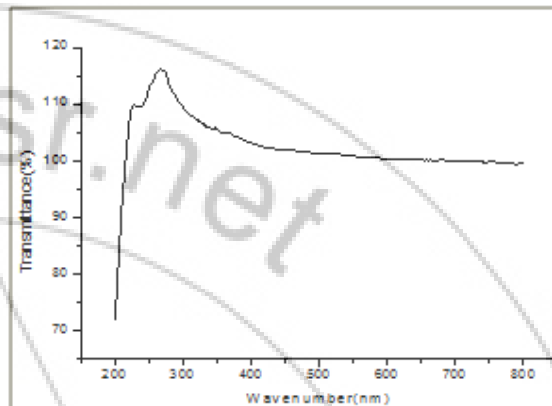


Figure 4: UV-Visible transmittance spectrum of the grown crystal

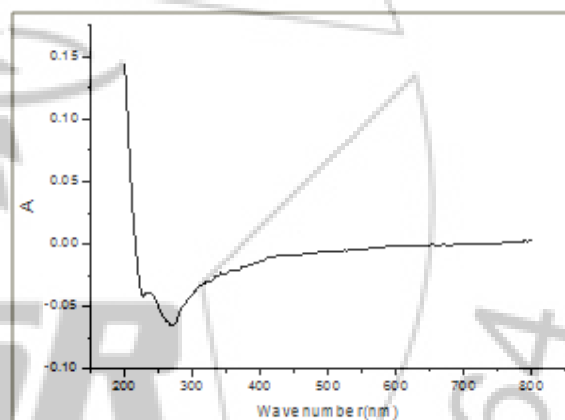


Figure 5: UV-Visible absorption spectrum of the grown crystal

4. Conclusion

Barium Chloride doped with L-alanine crystals were successfully grown by slow evaporation solution growth technique. The lattice parameters were calculated from the powder X-ray diffraction analysis. The FTIR spectrum reveals the functional groups of the grown crystal. The crystal is transparent in the UV-Visible region and the cut-off wavelength is 230 nm.

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