Synthesis, Crystallization, Non Linear Optical and Anti-bacterial Activity of L-Alanine Sodium Nitrate Single Crystals

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Abstract. In this present work, L-Alanine Sodium Nitrate (LASN) single crystals were grown by spontaneous nucleation solution growth method. The cell parameters and crystalline structure of the LASN crystals were analysed using powder X-ray diffraction (PXRD) technique. The numerous functional groups in the LASN crystals were confirmed by FTIR analysis. SHG efficiency of the grown LASN crystal is 1.06 times superior to the reference crystalline material KDP. The antibacterial property of LASN crystals were assessed using by agar diffusion method.

Keywords: Semi Organic Single Crystals, NLO Material, Anti-bacterial Material.

1. Introduction
L-alanine is a hydrophobic and non-polar organic compound under amino acid family composed of optically active molecule. The recent researches are focused to grow semi organic single crystals with high non-linear optical (NLO) efficiency and high optical transparency in the UV-Vis and near infra red regions which are very essential properties for the fabrication of various devices like frequency conversion, optical switching, telecommunication, optical storage devices, displays, optical-fiber amplifiers [1,2]. Bacteria’s are very adaptable organisms that live in and on animals as part of their natural foliage and they can be the reason for many infections. Bacterial infections are leading problem to public health. Recent works are focused to design and growth of new pharmaceutical drugs agents beside harmful bacteria [3]. Owing to this, the manifestation of annoying side effects of some antibiotics are also the reasons to the search for new antibacterial drug agents. Thus, in the present communication studies, the grown LASN crystals have been employed by NLO and antibacterial studies.
2. Experimental
The raw materials of L-alanine (Merck) and Sodium Nitrate (Merck) were blended in 1:2 molar ratio in a 250 ml glass beaker using 100 ml deionised water at a pH of 6. The mixed solutions were stirred for 6 hours to get clear solution. The attained homogeneous solution was filtered using Whatman No.1 filter circles in a 300 ml crystallization dish. Then, the dish was closed with a holed cover and kept in a vibration free clean crystal growth chamber and permitted for spontaneous nucleation at ambient temperature. In next 15 days of slow evaporation, the solution attains supersaturation and small crystals were developed from the solution and then they are permitted for further growth to reach good dimensional crystals with an average size of (8×4×1) mm³ and harvested in a growth period of 41 days. The photograph of the grown LASN crystals is presented in Figure 1.

3. Results And Discussion
The grown LASN crystals were finely crushed and employing to powder X-ray diffraction (PXRD) analysis using the Bruker AXS D8 Advance X-ray diffractometer with Cu Kα (λ=1.5406 Å) radiation. The obtained PXRD pattern of LASN single crystal is represented in Figure 2. The PXRD pattern affirmed that the grown LASN crystal have orthorhombic crystal structure with the non-centrosymmetric space group of P212121 which is the basic criterion for SHG applications. From the PXRD data calculated lattice parameter values are a = 5.7723 Å, b = 6.019 Å, c = 12.342 Å and α = β = γ = 90°. The sharp and strong peaks acquired in the PXRD pattern affirms good crystalline nature of the grown LASN single crystals and the obtained peaks positions well coincides with the literature work [2].

![Figure 1. The Photograph of the grown LASN Single Crystals](image1)

![Figure 2. PXRD pattern of the grown LASN single crystal.](image2)
The FTIR spectrum of the LASN single crystal have been examined within the frequency range from 400-4000 cm\(^{-1}\) by Perkin Elmer FTIR spectrophotometer and is characterised in Figure 3. The vibration peak at 2245 cm\(^{-1}\) confirms the CH\(_3\) stretching whiles the transmission peaks at 1589, 1512 cm\(^{-1}\) indicated the presence of ammonium group (NH\(_3^+\) bending). The absorption peak at 1458 cm\(^{-1}\) is attributed to the asymmetric CH\(_3^+\) bending vibrations. The absorption peak at 1412 cm\(^{-1}\) is assigned to symmetric stretching of C-COO\(^-\). The sharp peaks at 1358, 1111, 849 and 772 cm\(^{-1}\) correspond to NO\(_3^+\) stretching vibration. C-H and N-H bending vibrations are seen at 1304 cm\(^{-1}\). The observed peak at 1234 and 1150 cm\(^{-1}\) correspond to the NH\(_3^+\) rocking. The observed vibration peaks at 1011 and 918 cm\(^{-1}\) are due to the overtones of torsional oscillation of NH\(_3^+\). The COO\(^-\) in plane deformation is evident at 648 cm\(^{-1}\). The vibration peak at 540 cm\(^{-1}\) is attributed to torsional oscillation of NH\(_3^+\). The peak at 486 cm\(^{-1}\) confirms the NH\(_3^+\) in plane rocking. The nitro group presence in the obtained spectrum affirms the grown LASN single crystal [2].

![Figure 3. FTIR Spectrum of the grown LASN single crystal.](image)

The Kurtz-perry powder technique was made to find out the second harmonic generation productivity of the grown LASN crystals [4]. The grown LASN single crystals were powdered into a uniform particle size of about 150 \(\mu\)m and then orderly filled in a micro-capillary tube of constant bore. A Q-switched Nd: YAG laser beam with 1064 nm of wavelength, input pulse energy of 1.2 mJ per pulse and pulse width of 10 ns was passed to the sample cell. The SHG behaviour was affirmed by the green (532 nm) radiation from the sample. The SHG productivity of the LASN crystals (36 mV) is 1.06 times superior to the reference crystalline material KDP (34 mV).

For the past few years numerous methods have been used to analyse the antibacterial activity of different materials [3]. Agar diffusion method was employed to find the growth inhibition of grown crystals against Advisory Committee on Dangerous Pathogens (ACDP) declared harmful pathogens which are normally used in-vitro investigation method for microorganisms. The bacterial cultures were conserved at 37°C using incubator. The required amount of culture is equipped and autoclaved at 121°C for 20 minutes for test. The prepared culture was allowed to cool under laminar airflow. Sterilized use and throw petri plates were used for this experiment. Around 20 ml of culture was aseptically transferred to every petri plates and permitted to solidify. The petri dishes were vaccinated by dunking a sterile pad into inoculums. The additional inoculum was evacuated by squeezing and rotating the swab solidly touching the side of the tube, over the level of the fluid. The swab was marked everywhere throughout the surface of the medium three times, revolving the petri plate through an angle of 60 °C after every use and the swab was passed round the edge of the agar surface.
The immunization was dried for few minutes, at room temperature, with the lid closed. Discard the drag in a plate. Add solution in the bore. The Petri plates were placed in an incubator at 37°C within 30 minutes of preparation for bacteria. After 18 hours of bacterial growth, area of inhibition was measured in mm. The antibacterial activity was measured with the width of the strong inhibition area all over the place in the dish using a measurement ruler [mm]. The grown LASN crystals were established against ACDP declared harmful pathogens such as Gram positive (Bacillus cereus, Streptococcus aures, Proteus) and Gram negative (Klebsiella, Shigella and Pseudomonas) bacterial species by agar diffusion technique. The area of inhibition of the grown LASN crystals is tabulated in Table No. 1.

| Sample          | B.Cereus | S.aures | Proteus | Shigella | Klebsiella | Pseudomonas |
|-----------------|----------|---------|---------|----------|------------|-------------|
| LASN Crystalline Powder | 14       | 14      | 16      | 16       | 17         | 18          |

Table 1. Area of inhibition for selected bacterial species [mm]

The obtained results show admirable antibacterial activity of the LASN crystals against gram negative bacterial species. Hence, the grown LASN crystals will be deliberated for drug applications.

4. Conclusion
Transparent L-Alanine Sodium Nitrate single crystals have been grown by employing Spontaneous nucleation solution growth technique. The orthorhombic crystal system and space group P212121 were affirmed by powder XRD analysis. The various functional groups of LASN crystals were identified by FTIR analysis. The SHG productivity of the grown LASN crystals is 1.06 times superior to the reference crystalline powder KDP. Thus the grown LASN single crystals with noticeable optical properties revealed its greatest reliability in manipulative apparatuses for optoelectronics, photonics and NLO devices. The excellent antibacterial property of the grown LASN crystal was confirmed by antibacterial test. Hence, the grown LASN crystals may be deliberated for drug applications.

References
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