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# Nucleation, Growth and Characterization of L-Tyrosine Sodium Nitrate Single Crystal

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**Abstract:** L-tyrosine sodium nitrate (LTSN) single crystal was grown by slow evaporation solution growth technique. Nucleation kinetics of the material was studied to optimize the growth conditions. The crystal system and lattice parameters were analysed using single crystal XRD analysis. The transparent nature of the grown crystal was determined using optical studies. The different compositions of the grown material were studied using EDAX analysis. The dielectric behaviour and solid state parameters such as Penn gap ($E_P$), Fermi Energy ($E_F$) and polarizability ($\alpha_p$) were estimated using dielectric studies.

**Keywords:** Slow evaporation, Single Crystal XRD, Microstructure, Polarizability.

## 1. Introduction and Experimental:

Amino acids are interesting organic nonlinear optical materials for NLO applications. When the amino acids are coordinated with strong acids or metallic ions, they form a compound with improved NLO activity and mechanical, thermal stability [1,2]. In the present work, a new amino acid complex, L-tyrosine sodium Nitrate (LTSN) has been grown and characterized using various studies. The classical nucleation theory was used to optimize the growth conditions with a view to improve the quality and size of the crystal. The material (LTSN) was synthesized by taking L-tyrosine and sodium nitrate with stoichiometric ratio of 2:1.The starting materials were dissolved in double distilled water according to stoichiometric ratio. The solution was continuously stirred with a magnetic stirrer for about 24 hours to attain homogeneous solution and allowed to undergo slow evaporation. The photograph of the as-grown LTSN crystal is shown in the Fig.1. When a crystal nucleus of LTSN is formed in the mother solution due to supersaturation, the change in Gibbs free energy ($\Delta G$) is written as-

**Fig.1. Photograph of as-grown LTSN crystals**

$$\Delta G = 4\pi r^2 \sigma_0 + \frac{4}{3}\pi r^3 \Delta G_v \qquad \text{------(1)}$$

where $\sigma_0$ is the interfacial or surface energy per unit area and ΔGv is the volume free energy change per unit volume and it is a negative quantity. At the critical stage, the condition d(ΔG)/dr = 0 is applied to obtain the radius of the critical nucleus ($r^*$) and critical Gibbs free energy change ($\Delta G^*$) and nucleation rate J. The expressions for nucleation parameters are thus obtained as

$$r^* = \frac{-2\sigma_0}{\Delta G_v} \qquad \text{------(2)}$$

$$\Delta G^* = \frac{16\pi \sigma_0^3}{3\Delta G_v^2} \qquad \text{------(3)}$$

$$J = A \exp\left(\frac{-\Delta G^*}{KT}\right) \qquad \text{------(4)}$$

where A is the pre-exponential factor and it is found to be $10^{26}$ [3].

The nucleation parameters have been calculated for the LTNS crystal at different supersaturations at room temperature. The critical radius ($r^*$) and critical free energy change ($\Delta G^*$) vary between 336nm and 313nm and $2.78 \times 10^{-16}$ mJ and $2.46 \times 10^{-16}$ mJ respectively for the supersaturation range 1.100 – 1.108. The supersaturation for which nucleation rate J=1 is called critical supersaturation ($S_c$). The predicted critical supersaturation was found to be 1.105 at room temperature. The theoretical prediction was tested when the crystal was grown at room temperature and its supersaturation was measured from the start till the completion of the growth process. It was found to be between 1.11-1.25.

## 2. Results and discussion:

Single crystal XRD was studied using Four Circle Enraf NoniusCAD4/MACH3 single crystal diffractrometer coupled with a computer program. Single crystal XRD analysis reveals that LTSN crystal belongs to orthorhombic system with space group $P2_12_12_1$. The calculated unit cell parameters are found to be a= 5.866 Å, b=6.95 Å, c=21.24 Å; α=β=γ=90°and volume V=860 $Å^3$ [4]. Fig.2 shows the EDAX spectra of LTNS crystal. The EDAX spectral analysis confirms the presence of sodium, carbon, nitrogen and oxygen in the grown crystal.

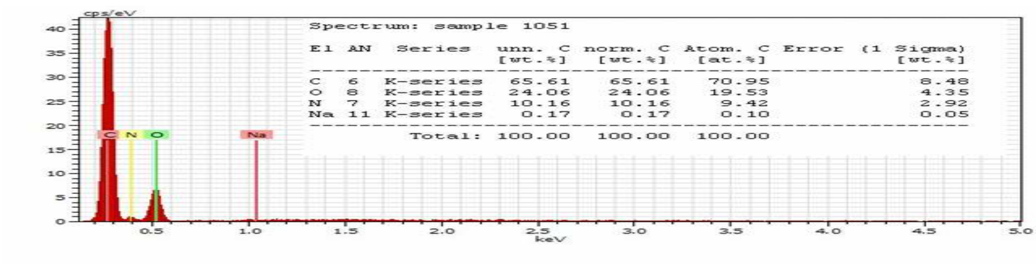


**Fig.2.EDAX spectra of LTSN crystal**

The UV-vis-NIR transmission spectrum (Fig.3) has been recorded using Lamda-35 UV-vis-NIR spectrophotometer in the wavelength range of 190-1100nm. From the spectrum the cut-off wavelength of LTSN is found to be around 219nm. The spectrum clearly indicates the transparency of the material in the region 300-1100nm.

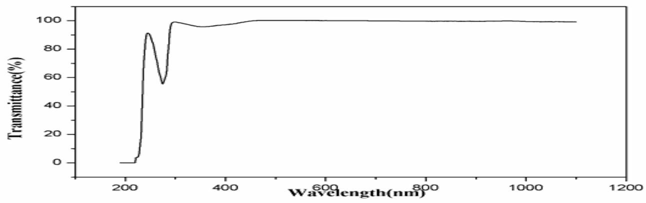


**Fig.3. UV-vis-NIR spectrum of LTSN crystal**

Fig.4 shows the FTIR spectrum of LTSN crystal recorded in the region 400-4000 $cm^{-1.}$ The presence of O-H symmetric vibration is indicated due to the peak at 3778.07 $cm^{-1}$. The peaks corresponding to the region 2500-3000$cm^{-1}$confirms the carboxylic acid group ($COO^-$). The stretching vibrations of $NH_3^+$ result in two bands one near 3205 $cm^{-1}$ and another near 3125 $cm^{-1}$ respectively. The strong peak at 1589 $cm^{-1}$ is assigned to $NH_3$ asymmetric bending vibrations. The peaks in the range 1039 – 1100 $cm^{-1}$ are due to addition of nitrate in the grown material. Hence, the presence of $COO^-$ and $NH_3^+$ indicates the characteristics of amino acid group material. The predicted functional groups are found to be in good agreement with the available report [4].

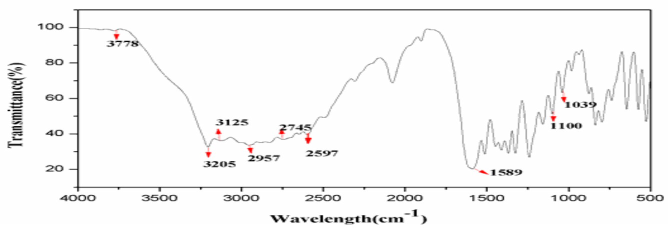


Fig.4. FTIR spectrum of LTNS crystals

Dielectric properties of the crystal are important to establish the dielectric behaviour and elucidate the solid state parameters of the grown crystal. The dielectric constant and dielectric loss were calculated for the frequency range from 5Hz to 5MHz. for the grown LTSN at different temperatures. The dielectric constant is found to decreases rapidly at the beginning with the applied frequency. The higher values of dielectric constant at low frequencies may be due to the presence of all the four polarizations namely space charge, orientation, electronic and ionic polarization and its lower values at higher frequencies may be due to the loss of significant polarizations gradually.

The NLO activity can be theoretically interpreted from the evaluation of solid state parameters. The value of dielectric constant at 1MHz is found to be $\varepsilon_{\infty}$ =280 from dielectric measurement. The valance electron plasma energy ($\hbar\omega_p$) is expressed as $\hbar\omega_p = 28.8(\frac{Z.\rho}{m})^{1/2}$ where Z is the total number valance electron,$\hbar = \frac{h}{2\pi}$ and $\omega_p$ is plasma angular frequency. Using the plasma energy, the Penn gap (Ep) and fermienergy ($E_F$) were calculated. These values are used for calculating the polarizabilty $\alpha_p$

$$\alpha_p = [\frac{(\hbar\omega_p)^2 S_0}{(\hbar\omega_p)^2 S_0 + 3Ep^2}] \times \frac{m}{\rho} \times 0.396 \times 10^{-24}$$

where $S_0$ is a parameter [2]. By comparing the polarizability ($2.723\times 10^{-23}cm^3$) of LTSN crystal with that ($2.14\times 10^{-23} cm^{3}$) of KDP crystal, it is concluded that the NLO activity of LTSN will be more than that of KDP. The nonlinear optical property was confirmed using Kurtz perry powder technique with Nd:YAG laser source of wavelength 1064nm. The grown crystal LTSN is found to be a promising NLO material for optoelectronic and photonic applications.

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