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Research Paper

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Growth and Characterization of Strontium Chloride Added Nicotinic Acid Single Crystals

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Abstract— Single crystals of strontium chloride added with Nicotinic acid were grown from aqueous solution by slow evaporation technique. The grown crystals are characterized by using single crystal XRD, FTIR spectroscopy, optical transmission, mechanical and photoluminescence spectral studies. As a result Single crystal XRD studies exposed that the crystal belongs to tetragonal system. The FTIR studies help to identify the functional groups which are present in the crystals. The optical transmission analysis shows that the crystal is transparent in the entire visible region. The cut off wavelength is 275nm. The sample is also subjected to photoluminescence analysis. Hardness was measured by the Vickers's hardness tester. The diamagnetic behavior of the grown crystal is confirmed by vibrating sample magnetometer.

Keywords— Crystal growth, single XRD, FTIR, optical studies, Mechanical strength, magnetic properties.

I. INTRODUCTION

The variety of applications of semiorganic materials in communication and optical usages result in the development of new Crystals. Due to good resistance, stability and higher transparency in the UV region shifted the researcher's attention make them to focuses towards new semi-organic crystals. The Strontium chloride ($SrCl_2$) is a salt of strontium and chloride. It forms neutral aqueous solutions. Strontium chloride is often used as a red coloring agent in pyrotechnics. Strontium Chloride is used for the medical treatment. It controls and prevents bone cancer and tooth sensitivity. It is soluble in water and the solubility in alcohol is not very great. Nicotinic acid also known as Niacin (Nicotinic acid + Vitamin) is an organic compound. It is a water-soluble vitamin, also known as vitamin B_3. Niacin is the generic term for nicotinic acid (pyridine 3-carboxylic acid) [1-4]. In recent times many NLO crystals are grown by the way of low temperature solution growth technique. The growth conditions were optimized for various concentrations and the results are compared with the parent materials. In this present research the growth of strontium chloride nicotinic acid (SCNA) single crystals have been grown by slow evaporation method. The crystals have been subjected to single crystal X-ray diffraction, UV-Vis-NIR and FTIR spectroscopic analyses. This crystal is also subjected to photoluminescence and hardness studies [5-9].

II. RELATED WORK

In the last few decades, researchers have aimed at finding high quality materials from the complex crystal family. There has been an enormous report directed towards the development of novel single crystals using the chemical compounds such as Strontium chloride and Nicotinic acid. The optical and electrical properties of Nicotinc acid doped KDP single crystals are reported by B. Deepa and P. Philominathan, in the paper titled "Enhanced NLO and antipactrial properties of nicotinic acid doped- KDP crystals: synthesis, growth and characterization". In this present work, the Strontium chloride added with Nicotinic acid (SCNA) to grow a novel single crystal. The grown crystal is subjected to study its cell parameters, optical and mechanical properties. From the observed results, their characteristics are analyzed in this work.

III. MATERIALS AND METHODS

The strontium chloride added nicotinic acid single crystals were synthesized by using Analar grade strontium chloride and nicotinic acid. They were added in the ratio 1:1, in doubly distilled water. The solution is stirred; it stirred by well using a magnetic stirrer, then the solution is filtered using filter paper and kept in a dust free environment. Slow evaporation of the solvent produced strontium chloride nicotinic acid (SCNA) single crystals takes place in the time

span of 15 – 20 days. Good transparent single crystals are harvested and are shown in Figure.1

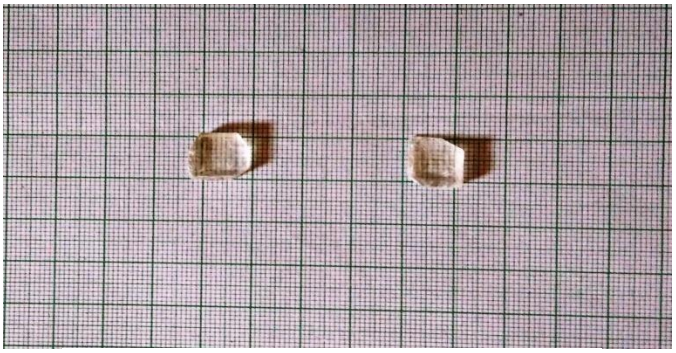

Figure- 1. Strontium chloride nicotinic acid (SCNA) crystal

IV. RESULTS AND DISCUSSION

4.1. Single crystal X-ray diffraction

The grown (SCNA) crystals were subjected to single crystal X-ray diffraction analysis using ENRAF NONIUS CAD4 X-ray diffractometer to determine the cell parameters which exposes that the strontium chloride nicotinic acid crystallize in monoclinic system. The lattice parameters were found to be a=6.318 (Å), b= 10.549 (Å), c = 6.037(Å), $\alpha=\gamma=90^0$, $\beta=112.97^0$ V=387.1 Å

4.2. Fourier Transform infrared (FTIR) analysis

FTIR spectrum of the grown (SCNA) crystal is shown in Fig (2). It was recorded on Perkin Elmer FT-IR Spectrophotometer within the wave number range in the 4000-400 cm^{-1}. The broad OH stretching absorption appears nearly at 3391 cm^{-1}. The peaks at 1598 and 1481 cm^{-1} are due to the C-C bond C=C stretching. The C=N strong stretching appear at 1193 cm^{-1}[10-11]. The C-H out of plane bending vibrations is observed at 1032 cm^{-1}. A band occurring around 574 cm^{-1} corresponds to C-C-O deformation [10-11].

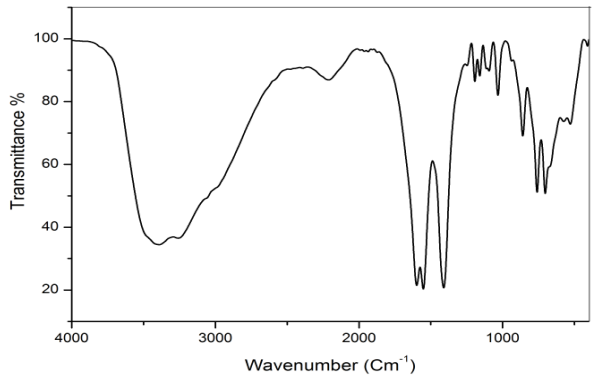

Figure-2. FTIR Spectrum of SCNA crystal

Table 1. Functional group assignment of SCNA crystal

Wave number in cm^{-1}	Assignments
3391, 3258	OH stretching of COOH absorption
2210	-C≡C- stretching
1598	N-H bending
1552, 1488	C=C stretching
1193	C=O stretching
1159,1094	C-N stretching
1032	C-H out-of-plane bending
859	=C-H bending
759, 703	C-Cl stretching
574	O-C-O deformation
528	COO^- In-plane-bending

4.3. UV-Vis- NIR spectral studies

The UV-Vis-NIR spectral studies are mainly used to assess the optical applications of the grown crystals. The Fig. 3 shows the transmittance spectrum of grown crystal. From the spectrum, SCNA crystal exposes lower cut-off wavelength around 275nm. The spectrum also indicates the applicable transmission of the crystal elongate from 300 to 1100nm which makes the crystals valuable for the applications requiring blue/green light. The high transmittance in the entire visible region enables it to be a good one for optoelectronic applications [12]. From Tau's plot, the calculated band gap energy is 4.5eV and is shown in Fig (4).

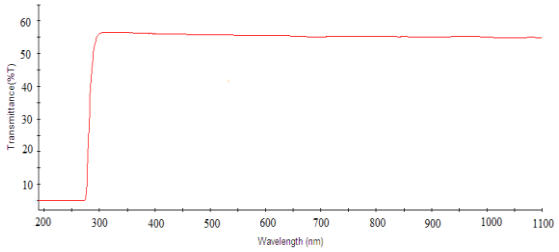

Figure-3. Optical Transmittance of SCNA crystal

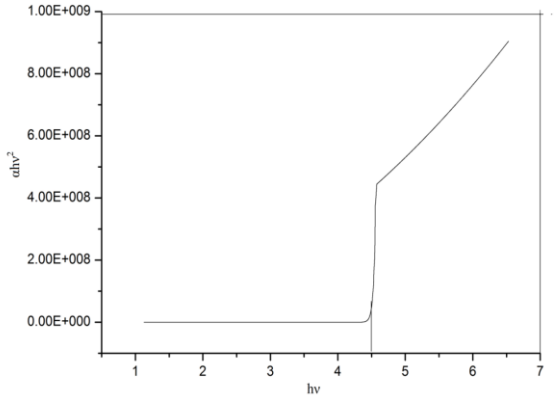

Figure - 4. Tauc's plot of SCNA crystal

4.4. Photoluminescence studies

Photoluminescence comprises both fluorescence and phosphorescence processes and originates from an absorption/emission process between different electronic energy levels in the material.

The PL spectrum recorded using crystal indicates LS45. The sharp peak in the spectrum shows the purity and crystalline nature of the grown crystal. The peak at 453 nm indicates the sample suited for optoelectronic applications [13]. Also it indicates that the crystal may possess the frequency doubling capacity. The other peaks at 490 and 681nm indicate the proper coordination of strontium chloride with nicotinic acid.

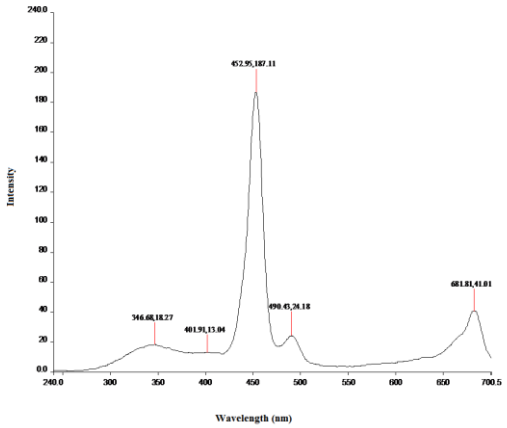

Figure - 5. Photoluminescence spectrum of SCNA crystal

4.5. Hardness studies

The mechanical property of the grown crystal was analyzed using LEITZ tester fitted with a Vicker's diamond rhombus indenter. The well powdered form of the crystal was placed on the rostrum of Vickers microhardness tester and the loads of different magnitudes were applied in fixed intervals of time. The depression time was kept as 5s for all the loads. The Vicker's hardness number of the grown crystal was calculated from the relation

$$Hv = (1.854xP)/d^2 \text{ kg/mm}^2$$

Where Hv is the Vicker's hardness number in kg/mm^2, P is the applied load in kg, d is the average diagonal length of the indentation mark in mm.

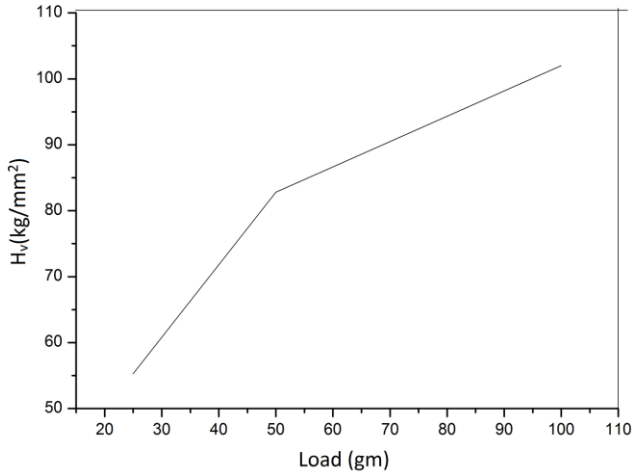

Figure - 6. Load P and Vs Hardness number of SCNA crystal

A graph was plotted between hardness number (Hv) and applied load P as shown in Fig .6. From the graph it was found that hardness value increases with increase in load [14]. In order to find the work hardening coefficient, a graph was plotted between log p and log d. A linear graph is obtained and is shown in Fig .7. From this observation it can be found as the mechanical quality of the material. The slope of the line gives the work hardning co-efficient. From the slope value, it is concluded that the material belongs to hard category.

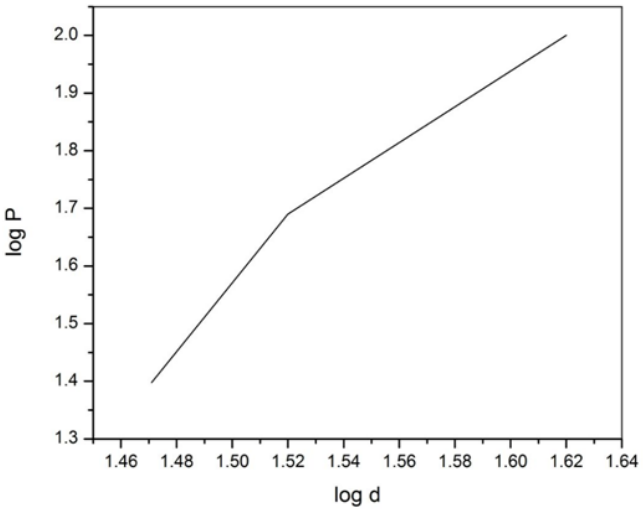

Figure - 7. Log p vs Log d

4.6. VSM

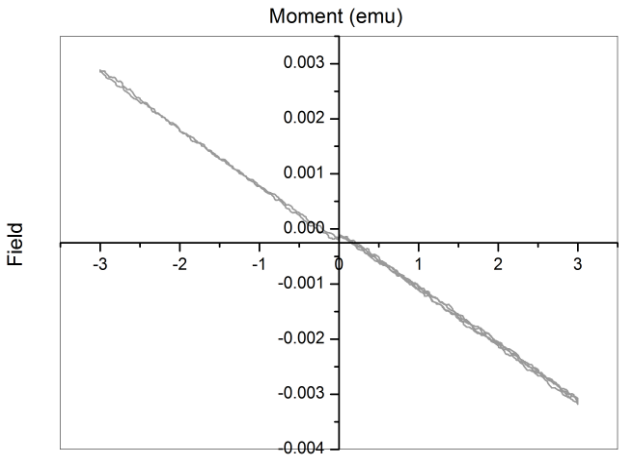

Figure – 8. Hysteresis loop of the grown SCNA crystal.

Vibrating sample magnetometer systems are used to measure the magnetic properties of materials as a function of magnetic field. They are ideally suited for research and development, production testing, quality and process control. In the present case, the magnetic study was carried out using a vibrating sample magnetometer CR155 quantum design. A plot of typical magnetic moment Vs magnetic field, hysteresis path traced at room temperature for the grown crystal as shown in Fig.7. It is observed from the graph that the sample SCNA is exhibiting the diamagnetic behavior [15].

V. CONCLUSION AND FUTURE SCOPE

The single crystal of strontium chloride nicotinic acid NLO material has been grown by slow evaporation technique. The single crystal XRD analysis confirms the structure of the crystal as monoclinic system. Functional groups and modes of vibration were identified from FT-IR spectrum. The lower cut off wavelength is determined using UV- VIS- NIR spectrum of the grown SCNA crystal is studied. The photoluminescence spectrum is recorded for the grown SCNA crystal. From these studies, this crystal is well suited for optoelectronic applications. Mechanical properties are clarified by Vickers hardness test. The VSM graph confirms the diamagnetic nature of the grown crystal.

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