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GROWTH, SPECTRAL & MECHANICAL BEHAVIOUR OF SCZA – INORGANIC CRYSTAL

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Abstract— **The purpose of this study was to investigate the effect of trace metal like Zinc on Strontium. Trace elements can affect crystallographic properties.Therefore this study was designed to investigate how trace elements influence on crystals and ultimately its physical properties.The single crystal of the strontium chloride and Zinc acetate (SCZA) was grown by Slow evaporation technique using water as a solvent. Good quality crystals were harvested within 20 days. The grown crystals were characterized by Fourier Transform Infrared Spectroscopy (FTIR) were used to confirm the presence of the functional groups of SCZA. Optical property was established by UV-Visible spectrum and the mechanical strength of the grown crystal was estimated by the Vicker's microhardness test and itwas increased due to the effect of trace metals.**

Index terms- **Slow Evaporation, inorganic metal, FTIR, UV-Vis spectral analysis, Microhardness.**

I. INTRODUCTION

Non linear optical material plays a major role in nonlinear optical communication and in particular they have a great impact on the laser technology. NLO materials exhibit excellent mechanical and thermal properties of nonlinear optical application are combine with the favorable optoelectronics and photonic application.[1] For recent years, the effect of nonlinear mechanisms and their relation to the structural characteristics of the material has been considerably improved.[2] Trace elements are required by the body for specific functions. In crystal growth process trace elements helps to improve on crystallographic structure, hardness, resistance to crack propagation, shade lightness and carbonate content[3]. Metal complexes are synthesized, grown and characterized by trace elements which exhibits good NLO properties. Inorganic materials like strontium chloride are widely used in many devices because of their higher nonlinear optical coefficient, which favours thermal and mechanical stability and an enhance degree of chemical inertness [4]. Strontium crystals are of considerably interest, particularly for the basic studies of some of their interesting physical properties.

Hence the present work describes thesynthesis and growth of trace metals with strontium chloridecrystals (SCZA) by slow evaporation technique.The good quality singlecrystal were characterized by FTIR, UV and Microhardness analysis.

II. EXPERIMENTAL

A. SYNTHESIS AND CRYSTAL GROWTH

The starting materials were analytical grade reagents of strontium chloride and zinc acetate (99% purity)was used to synthesize SCZA crystals by slow evaporation technique. These salts were taken into equimolar ratio (1:1) and thesolution was prepared using double distilled water as the solvent using magnetic stirrerat room temperature. The prepared solution was filtered twice using a Whatman filter paper closed with sealed cover and kept in a dust free environment. After a span of 20 days, good quality single crystals of SCZA wereharvested with well optical transparency of dimension of 5×6×2 mm^3.The photograph of the as grown single crystal is shown in **Fig.1& 2** andgrowth conditions are given in **table 1.**

Table1:

Solute	Strontium chloride; zinc acetate
Solvent	De-ionized water.
Method	Slow evaporation
Growth period	20 days
Purification	Re-crystallization
Size of the crystal	5×6×2mm^3

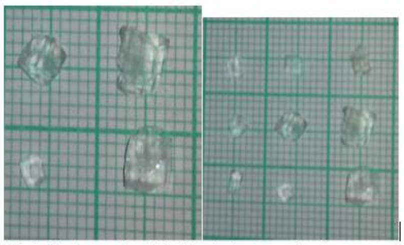

Fig:1 Photograph of the single crystal of SCZA Fig .2 photograph of group of SZCA crystals

III. CHARACTERIZATION TECHNIQUES

FTIR spectroscopy studies were used to analyze qualitatively the presence of functional groups in the synthesized pure crystal. The FTIR spectra analysis of SCZA performed in the range from 400-4000 cm^{-1}.The optical properties of the crystal examined using UV-VIS spectrometer. The micro hardnessmeasurement of SCZA crystal was carried out by Leitz Weitzler Vicker's Microhardness tester.

A. FT-IR SPECTRAL ANALYSIS

The FTIR spectrum of the SCZA crystal was recorded using a Bruker IFS 66v using KBr pellet technique in the range of 400-4000cm^{-1}.[5] The observed assignments have been tabulated in Table-2 and shown in fig 3. The presence or absence of absorption bands helps in the presence of certain functional groups in the compound.[6]. To analyze the FTIRspectrum,accurate information about structure of strontium chloride and zinc acetate is much essential.

The spectra of SCZA crystal can be interpreted as follows:

The FTIR spectra observed for the mixed crystals show a shift in the frequency bands in the low frequency region. The peak observed at 467 cm^{-1} is attributed to OCO rocking, which is observed in zinc acetate at 477cm^{-1}. OCO rocking vibration (486 cm-1) of zinc acetate appears shoulder at 620cm^{-1} in SCZA crystal. Sharp peaks at 673 and 952 cm^{-1} are assigned to

O-C-O symmetric bending and C-C stretching vibrations respectively. The same peaks are observed at 695 and 954 cm^{-1} in pure zinc acetate. The peak appears at 736 cm^{-1} may be due to the presence of metal oxygen inclusion in the material.[7]The presence of peaknear 3100-3400cm^{-1} is observed at OH stretching vibration of the water molecule of zinc acetate dihydrate.

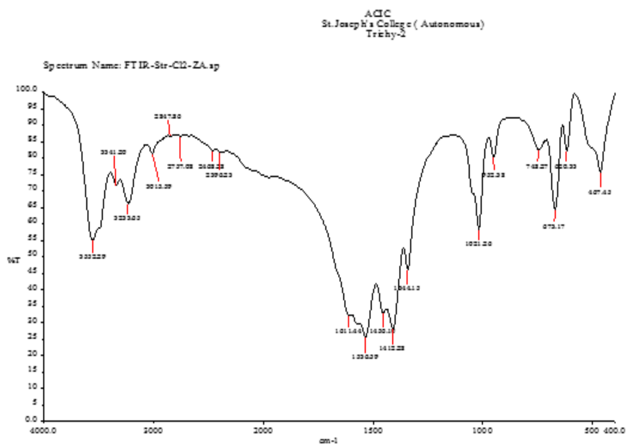

Fig.3 FTIR spectrum of SCZA

TABLE2: FTIR Spectrum of SCZA crystal

$SrCl_2$ (cm^{-1})	Zinc Acetate (cm^{-1})[1]	SCZA (cm^{-1}) (Present Work)	Frequency assignment
486	477	467	In plane OCO rocking
592	-	-	Influention of metal bonding vibration
-	622	620	Out of plane OCO rocking
-	695	673	OCO symmetric bending
721	-	748	Due to metal oxygen bonding vibration
-	954	952	C-C stretching
-	1020	1021	In plane CH_3 rocking
1360	1350	1344	CH_3 symmetric bending
1464	1415	1412	CH_3 asymmetric bending
-	1558	1536	CH_3 asymmetric stretching
1609	-	1611	Metal bonding of vibration
2854	-	2847	Influence of metal bonding vibration
2955	2960	3015	CH asymmetric stretching
3320	3100	3233	OH stretching vibration of H_2O
3444	3400	3552	OH stretching vibration of H_2O

B. UV – VISIBLE SPECTRUM

The single crystals are mainly used for optical applications in theabsorption region plays an important role of the grown crystal. The ultra violet light absorbed by the sample gives information about the transparency window which is very essential in many optoelectronic applications. The optical transmission spectrum of the grown crystal was recorded by using Perkin Elmer Lambda 35 spectrophotometer in the wavelength region 190-1100nm. The UV-Vis NIR observed in the present study is shown in fig4. Efficient non linear optical crystal have an optical transparency lower cut-off wavelength between 200-400nm. The lower cut-off lies in the range 384nm.Variation in the transmittance may be due to the presence of zinc acetate.[7]. Very low absorbance in the entire visible region would be attributed to the delocalization of electronic cloud through charge transfer. The absorption in the visible and NIR regions along with low cut off wavelengths confirm the suitability of the grown crystals for NLO applications.

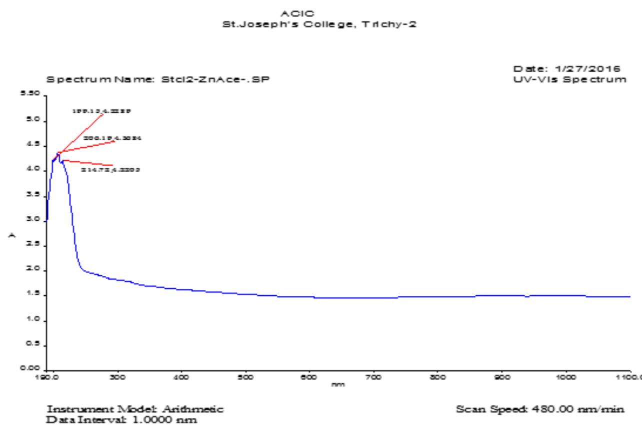

Fig.4 UV spectrum analysis

C. MICROHARDNESS MEASUREMENT

Microhardness testing provides useful information concerning the mechanical stability of solids. Microhardness measurement of PPM crystal was carried outusing Leitz-Wetzlar Vicker's microhardness tester fitted with a diamond pyramidal indenter attached to an optical microscope fordifferent loads varying from 25 to 100 g. The indentation hardnesswas measured as the ratio of applied load to the surface area of theindentationAmong the different tests of hardness measurements, the most simple and reliable methods is Vicker's micro hardness test method in which a pyramid indenter is used for indentation .The mechanical behavior of SCZA crystal was investigated by applying load of 25, 50 and 100 g and keeping the time of indentation constant at 10 seconds, using Shimadzu HMT-2T microhardness analyzer.[8,9]The Vickers microhardness number was determined by using the relation,

Hv = 1.8554 P/d2 Kg mm-2 ------------ **(1)**

where, P is the applied load in (Kg) and d is the average diagonal length in (mm).It is observed that hardnessnumber increases with increasing load (Fi). This phenomenon isknown as reverse indentation size effect (RISE).Using Meyer's law,the Meyer's index (n) is calculated to analyze the nature of the material. The size of indentation and load are related through Meyer's law [10-12]

$P=A1d^n$ ------------ **(2)**

Where,A1 is the material constant and n is the meyer index or work hardening co-efficient. The work hardening coefficients (n) were determined from the slopes of log d vs log pin shown in fig 6. They are found to be <2**.** The increases in Hv for increasing P observed in present study in theoretical prediction exhibiting the normal size indentation effect,

$P=W+A1d^n$ **--------------(3)**

The hardness dependent parameters;

Yield strength ($\sigma y = (0.1)n\text{-}2\ Hv/3$) and elastic stiffness ($C_{11}= Hv7/4$)were also calculated.

Table 3 Hardness dependent parameters

SCZA crystal load	Hv(kg/mm-2)	n	σy	d^2	C_{11}
25	25.53	0.3	426.43	1859.55	44.6775
50	38.0	0.3	634.72	2469.34	66.5
100	48.42	0.3	808.77	3771.18	84.735

The increase in Hv for increasing load (P) observedin the present study is in good agreement with the theoretical prediction and the grown crystals belong to soft materials.

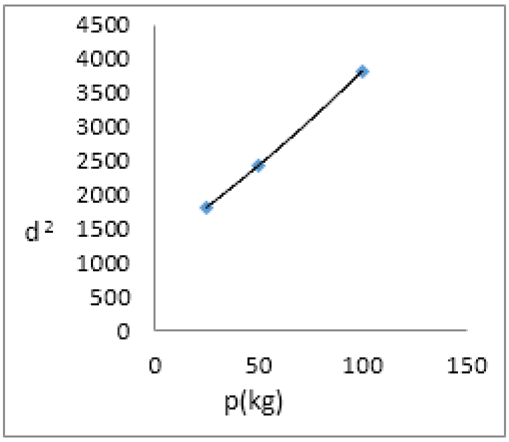

Fig.5 d^2 vs P

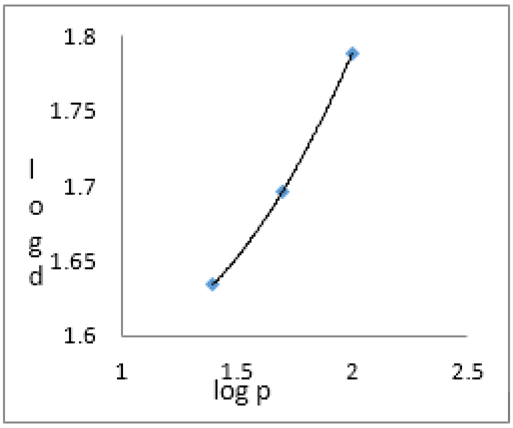

Fig.6 log d vs log p

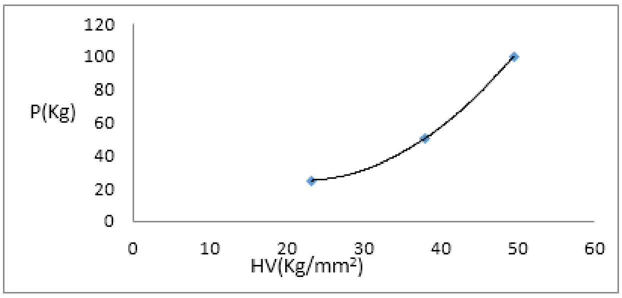

Fig.7 P vs HV

IV. CONCLUSION

The good quality of single crystal of SCZA have been grown by slow evaporation technique at room temperature. The well-defined and defect free crystal were harvested in span of 7 days by slow evaporation method. From the FTIRspectroscopy analysis, the various functional groups present in the grown crystals were identified. Fromthe UV-visible spectroscopy analysis, the grown crystals are transparent in the visible region and the cutoffwavelength is 226nm. The crystal possesses good mechanical stability due to the inclusion of strontium chloride which is confirmed by theVickers microhardness analysis. By Meyer's law, the value of Meyer's index n estimated which indicatesthat the crystal belongs to hard material category of the grown crystals.

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