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A Study of Optical, Structural, Mechanical and NLO Properties of Sarcosine Doped ADP Single Crystal by Slow Evaporation Technique

A. T. Ravichandran[1*], S. Aron Rabi[1,2], D. Ravinder[3]
[1.] Department of Physics, National College (Autonomous), Trichy-620001, India.
[2.] Department of Physics, Loyola College of Arts & Science, Mettala, Namakkal-636202 India.
[3.] Department of Physics, Osmania University, Hyderabad, India

Abstract. **In the present work amino acid of sarcosine doped ADP crystal grown by slow evaporation solution growth method. The FTIR spectroscopy showed the vibration frequencies of functional groups in the grown crystal. The optical transmission study reveals the improved transparency of doped crystal in the entire visible region for NLO applications. The crystalline size and cell parameter were characterized by powder X-Ray diffraction and Single X-Ray diffraction analysis. The presence of dopent in the sample grown by ADP crystal with addition of sarcosine was determined by the spectral analysis. The effect of the influence of dopant on the surface morphology of sarcosine doped ADP crystal faces are analyzed by Scanning Electron Microscope (SEM). The presence of elements in the dopent grown crystal confirmed by energy dispersive X-ray analysis (EDAX). The Vickers Microhardness studies reveal the mechanical strength of the grown crystal. The SHG efficiency of pure sarcosine doped ADP crystal confirmed by Nd:YAG pulsed laser employing the Kurtz powder technique.**

KeyWords: Sarcosine, ADP, FTIR, UV, Vickers hardness test, Single and powder XRD, SHG.

1. INTRODUCTION

The nonlinear optical material enhanced of current research plying in the role of emerging trend of photonics.[1] In many optoelectronic materials for the ammonium dihydrogen phosphate (ADP) posses like piezoelectric, ferroelectric to exploit for nonlinear optical (NLO) and electro-optical properties.[2] - [5] The ADP is widely used to second, third and fourth harmonic generations for Nd:YAG, Nd:YLF lasers for electro-optical applications, Q-switches and acousto-optical applications. [6] - [9] ADP is a class of hydrogen bonded material is the both organic and inorganic dopants. In nonlinear optical properties of both donor group NH_2 and acceptor COOH group and also there is a possibility to transfer intermolecular charge in amino acids.[10] - [12] In amino acids and their compounds belong to a family of organic materials have wide applications in sarcosine of N-methylglycine (CH_3NH_2+CH_2COO) is a natural amino acid inhibiting two hydrogen atoms are located nitrogen atom is a investigating the crystal structure of sarcosine in pure and made on several crystalline complexes with organic and inorganic acid derivatives. [13-14]. The crystal grown L-gluatomic acid, L-histdine and L-Valine, L-Lysine, L-tartaric acid, TGS doped ADP crystals. Also to improve the optical transmission and NLO property of growth habit to modifications.[15] In present work is aimed at the doping of amino acid sarcosine with ADP in the growth have been slow evaporation method. The grown crystal was characterized by optical, structural, mechanical NLO properties of ADP crystals were investigated in present study.

2. EXPERIMENTAL DETAILS

2.1 Solubility and crystal growth

The saturated solution for the single crystal growth of pure and doped ADP crystal studies their solubility in double distilled water at different temperatures (30°C to 50°C). the solubility curve for pure ADP and doped sarcosine with ADP has been shown in fig 1. From figure it is clear that the solubility is decreasing with increasing the doping concentrating of metal ion with increasing the temperature.

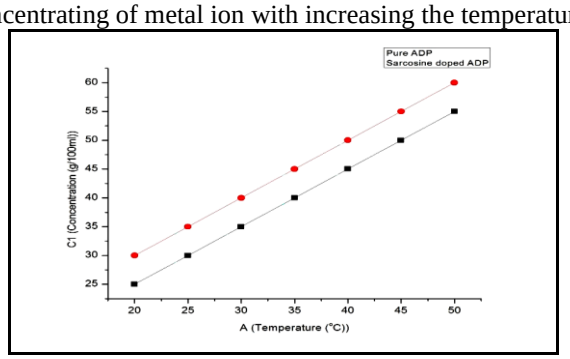

Fig.1 Solubility diagram for Pure and Sarcosine doped ADP

Pure and sarcosine doped ADP crystals grown by slow evaporation technique at room temperature. The saturated solution is prepared by dissolving the solute of ADP in 11.50g/mol per 100ml in Millipore water. The doping of sarcosine was carried out by adding 0.1 weight percentage powder form of sarcosine into 1mol percentage for 100ml solution of ADP in Millipore water. The mixture of salts was stirred for 8hrs for homogenous solution. The harvested crystal the growth period 25-35 days as shown in fig 2. The grown crystal size of 9x6x2mm^3 and were found to be colour less and transparent for the sarcosine doped ADP crystal.

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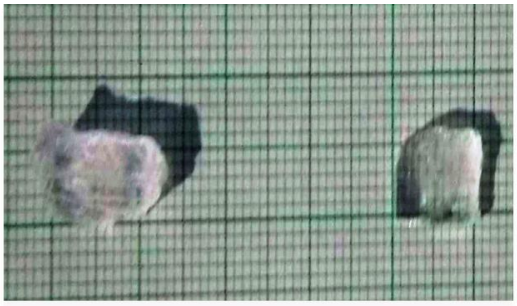

Fig.2 A photograph for Sarcosine doped ADP

3. RESULT AND DISCUSSION

3.1 Fourier-Transform Infrared Spectroscopy Studies

The FTIR Spectrum of sarcosine doped ADP was recorded in the KBr Pellet in the frequency region 400cm^{-1} – 4000cm^{-1} using Perkin Elmer spectrometer is shown in fig3. The assignments of various functional groups are given table 1. The stretching frequency at 3873cm^{-1} shows the presence of O-H stretching and 2923cm^{-1} C-H_2 symmetric stretching. In multiple fine structures at the lower energy mode indicate the strong hydrogen bonding of NH_3^+ groups. The strongest band observed at 1601cm^{-1} indicates the presence of P-O-H bending in the spectrum. The presence of strong peak ranges from 1264cm^{-1} to 1050cm^{-1} for the N-H stretching. In the lower wave number region, the bands at 803cm^{-1} and 556cm^{-1} are due to the ring asymmetric, symmetric stretching and plane deformation.

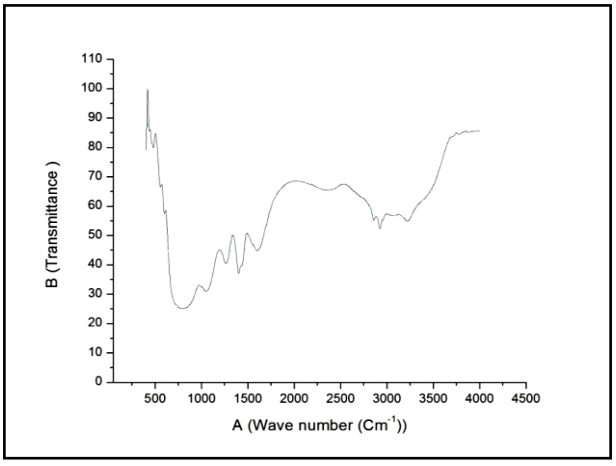

Fig. 3 FTIR Spectrum for Sarcosine doped ADP

Table 1. FTIR Spectrum for Sarcosine doped ADP

Wave Number (cm^{-1})	Assignments
3873	O-H Stretching
326	Asymmetric stretching of $NH3^+$
3079	NH stretching
2923	C-H_2 stretching
2856	C-H_3 stretching
2342	C=H stretching
1601	P-O-H bending
1264	N-H bending of dopents
1050	P=O stretching
803	P=O stretching
556	C-O bending

3.2 UV-Visible Spectral analysis

The UV-Visible spectral study of sarcosine doped ADP was carried out in the range of 200nm to 1100nm were recorded transmittance is shown in fig4. The grown crystal exhibits high transmittance above 75% for light in the visible region of electromagnetic spectrum is nonlinear application. A sharp peak is absorption 260nm of the crystal. The optical transparency of sarcosine doped ADP in the presence of grown crystal. The optical band gap semiconductor, the crystal has been absorption coefficient (α) obeying the following relation for high photon energies (hν).

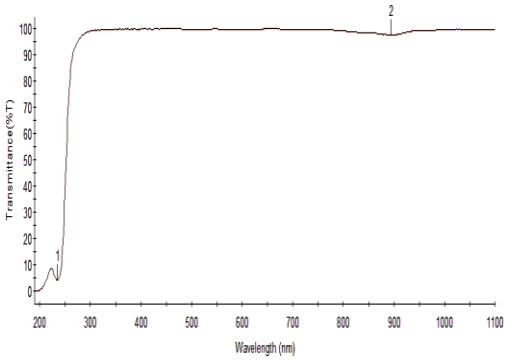

Fig.4 UV-Visible Spectral studies of sarcosine doped ADP

$$(\alpha h\nu) = A(Eg-h\nu)^{1/2}$$

Where, A is a constant, Eg is the optical band gap, h is the planck's constant and ν is the frequency of the incident photons. The plot between energy gap (hν) and $(\alpha h\nu)^{1/2}$ is shown in fig 4a.

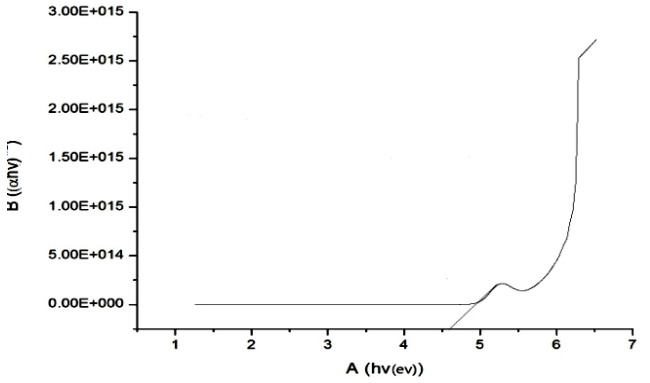

Fig.4a A graph plot for $(\alpha h\nu)^{1/2}$ band gap energy

The extraploting the slope region is found to be optical band gap energy Eg=4.7ev in the absorption coefficient with fabricating of the optoelectronics devices.

3.3 Microhardness Studies

The Microhardness study that the carried out on the grown crystal to across the mechanical property the static indentations were made at room temperature with constant time of 10s for the all indentations. The indentation marks were made on the surfaces by varying the load from 25g to 100g. The Vickers hardness number (H_v) of the Sarcosine doped ADP crystal was calculated using the relation, Hv =

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1.8544P/d^2 Kg/mm^2 Where, P is the applied in Kg, and d is the average diagonal length of the indentation in mm. A graph plotted between Hv versus applied load (P) is shown in fig5. The Hv increases as the applied load (P) for the grown crystal of beyond the 100g in the significant crack occurs to which may be due to internal stress generated with indentation the ADP crystal. The work hardening coefficient (n) for the grown crystal was softer material category in the Pure and sarcosine doped ADP single crystal.

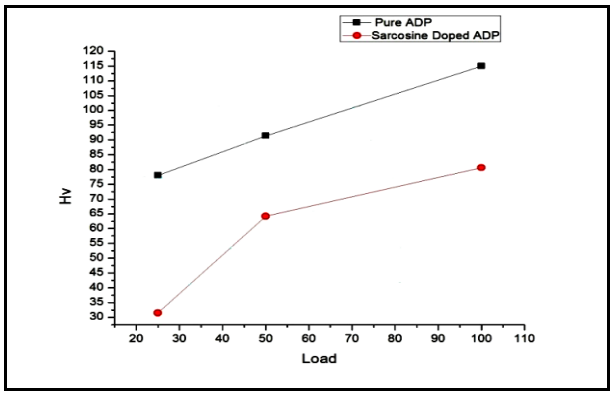

Fig.5 A graph plot for Load Vs Hv pure and sarcosine doped ADP

3.4 X-Ray Diffraction Analysis

Single Crystal X-ray Diffraction

Single crystal X-ray diffraction analysis was carried out using ENRAF NONIUS Cad4 diffractometer to identify the lattice parameters. The single crystal X- ray diffraction studies confirm the tetragonal structure with the space group of I-42d. The lattice parameters of sarcosine doped ADP are a=b=7.268A°, C=8.95A°, with volume V=368.35$A°^3$. The crystal parameters and cell volume were found to be reported value as shown in table2.

Table2. Lattice Parameter for Pure ADP and Sarcosine doped ADP

Compound	Crystal system	Space group	Unit cell parameters
ADP	Tetragonal	I-42d	a=b=7.055Å, c=6.275 Å. α=β=γ=90°
Sarcosine Doped ADP	Tetragonal	I-42d	a=b=7.268A°, C=8.95A° α=β=γ=90°

Powder Crystal X-ray Diffraction

Powder X-ray diffraction pattern of the grown crystal was analysis using XPERT PRO powder X-ray diffractometer employing CUKα radiation (λ=1.5405 A°). The pattern of sarcosine doped ADP crystal is shown in fig6.

$$D = \frac{K\lambda}{\beta \cos\theta}$$

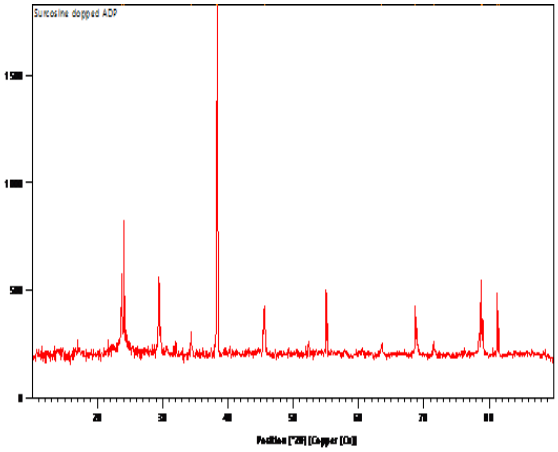

Fig.6 Powder XRD for Sarcosine doped ADP

The observed sharp peaks is spectrum indicated of grown crystal to tetragonal crystal structure. The crystalline size was calculated following scherrer's formula. The crystalline size was calculated as 76.85nm in the sarcosine doped ADP grown crystal.

3.5 Scanning Electron Microscope (SEM)

Scanning electron microscope is the surface with a high energy beam of electron in a raster scan pattern is called electron microscope. The shape and size of the particles making up the object can be studied as shown in fig7. (a,b,c,d) of the grown sarcosine doped ADP crystal. The grown crystal of surface layer growth observed to the addition of the dopent was sarcosine with ADP. The vertical and cross sectional layer growth is observed and hence sarcosine doped ADP as a growth modifier in the optoelectronic applications.

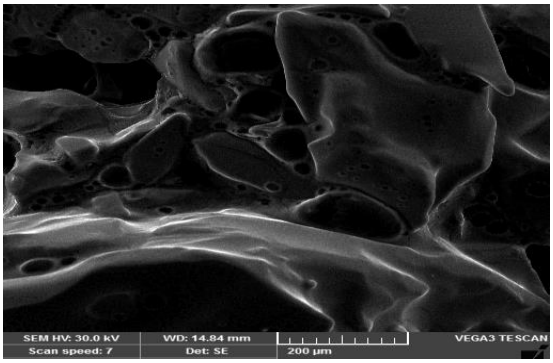

Fig.7a SEM image for sarcosine doped ADP

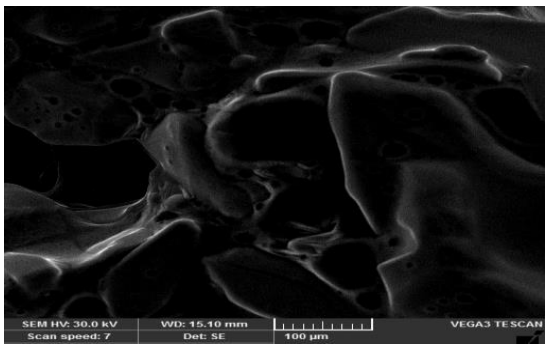

Fig.7b Magnified SEM image sarcosine doped ADP

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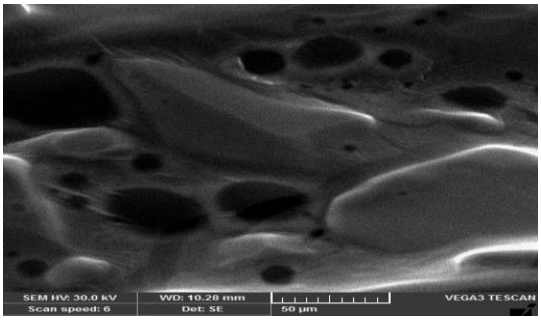

Fig.7c SEM image for sarcosine doped ADP

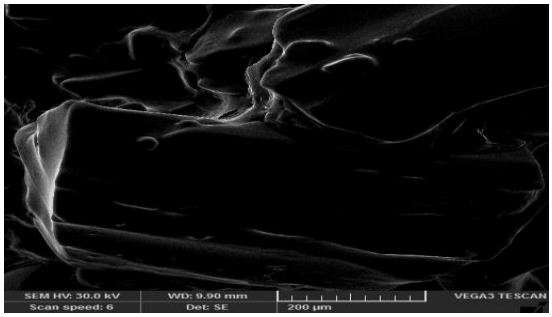

Fig.7d Magnified SEM image sarcosine doped ADP

3.6 Energy Dispersive X-ray Spectroscopy (EDAX)

EDAX spectrum of sarcosine doped ADP crystal is shown in fig8. The peaks shows the presence of carbon, oxygen, nitrogen, phosphorus in the crystal. The table 3 shows the elements and atoms percentage of the C, O, N, P. It was observed that the atomic percentage of the good agreement with stoichiometrically expected atomic weight to 39.69, 38.47, 19.12, 2.72 in the sarcosine doped ADP crystal.

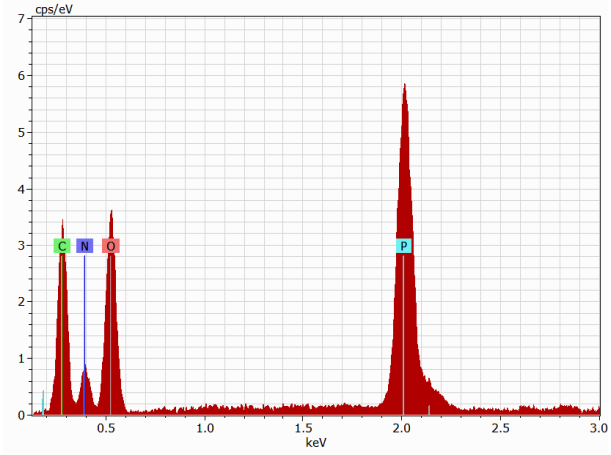

Fig.8 EDAX Spectrum for Sarcosine doped ADP

Table.3 Elemental Composition for sarcosine doped ADP

Element	Wt%	At%
C	31.89	39.69
O	43.82	38.47
N	18.48	19.12
P	5.81	2.72

3.7 Second harmonic generation (SHG)

The sarcosine doped ADP crystals was made in to fine powders of the size of 10µm. The micro particles were exposed to 1067nm laser beam from a pulsed Nd:YAG laser to the second harmonic generation efficiency. The input pulse of 1.9MJ/pulse an signal amplitude on the oscilloscope indicates the efficiency of the sample. The Pure ADP crystal an output 76mv grown crystal increase in the SHG efficiency. The sarcosine doped ADP crystal an output of 83mv. The SHG efficiencies of the doped crystals are 1.3 times greater than the standard ADP crystals were grown.

4. CONCLUSION

Good quality of Sarcosine doped ADP single crystal was grown by slow evaporation method at room temperature. The single crystal was analysis of lattice parameter and Space group to be calculated. The powder X-Ray Diffraction was indexed of tetragonal system and calculated to be crystalline Size. The FTIR was confirmed to be analysis of functional group of the grown crystal. The UV-visible to be analysis of the transmittance is found to be maximum in the visible near infrared region in sarcosine doped ADP crystal at the lower cutoff wavelength range in 260nm. The Vicker's microhardness was calculated in order to understand the mechanical stability of the grown crystals. Hardness measurement also shows that the soft material than Sarcosine doped ADP crystals. The SEM studies suggested vertical and cross sectional layer growth. EDAX studies reveals that grown crystals are Sarcosine doped ADP indeed. The SHG was observed using a Q-switched Nd:YAG laser and its efficiency were found to be better than KDP.

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