



EFFECT OF L-ALANINE ON THE GROWTH, CHARACTERIZATION AND NLO PROPERTIES OF POTASSIUM DIHYDROGEN PHOSPHATE (KDP) CRYSTAL

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Abstract:-

L- Alanine is an α -amino acid with the chemical formula $\text{CH}_3\text{CH}(\text{NH}_2)\text{COOH}$ or $\text{C}_3\text{H}_7\text{NO}_2$. The α -carbon atom of L- Alanine is bound with a methyl group ($-\text{CH}_3$), making it one of the simplest α -amino acids with respect to molecular structure and also resulting in L- Alanine being classified as an aliphatic amino acid. This methyl group of L- Alanine is non-reactive and is thus almost never directly involved in protein function. Amino acids belong to an interesting class of materials which can be used for non linear optical (NLO) applications. The L-isomer is one of the 20 amino acids encoded by the genetic code. It is classified as a non-polar amino acid. L-Alanine.L-Alanine doped potassium di hydrogen phosphate(KDP) single crystals are grown by solution growth technique .slow evaporation technique was adopted for the growth .Due to variation in the doping concentration there is a modification in the growth habit ,nonlinear optical property and mechanical hardness of the doped crystals. The KDP crystal obtained by the above technique were subjected to different characterization analysis .The lattice dimension were determined from the single crystal X-ray diffraction analysis .Fourier transform infrared (FTIR) identified the functional groups and provides information about chemical bonding or molecular structure of material & optical behavior of the crystals was identified by UV -Vis analysis.Thermogravimetric analysis (TGA) provides the information about physical phenomena such as second order phase transition including vaporization, sublimation ,absorption and desorption

Keywords:-KDP, Solution Growth, XRD, FT-IR, , UV-VIS, TGA -DTA

1.Introduction : -

Nonlinear optical (NLO) material play a major role in nonlinear optics Organic nonlinear optical (NLO) material are gives great attentions due to their potentially high non linearity's in the electro optic effect compared to inorganic NLO materials .The rapid development in the field of science and technology search for newer and efficient nonlinear optical materials. Organic materials have been of particular interest because the nonlinear optical response in this broad class of materials is microscopic in origin, offering an opportunity to use theoretical modeling coupled with synthetic flexibility to

design and produce novel materials [1, 2]. Potassium Dihydrogen phosphate (KDP) are widely used for frequency conversion and optical switching in modern optoelectronics and photonics. (KDP) crystals have created considerable interest among researcher. Its excellent qualities such as high nonlinear conversion efficiency, wide optical transmission range, with low cut of wavelength and high laser damage. The amino acid are famous organic materials, play a vital role in the field of nonlinear optical crystal growth. Thus, we will choose L- alanine as a dopant because they have a donor NH_2 and acceptor COOH group and the intermolecular charge transfer is also possible. Therefore, amino acid may be used as dopant and it was observed that, there is enhancement in the material properties such as nonlinear optical threshold [3] (NLO) and ferroelectric properties [4,5]. L-Alanine is an α -amino acid with the chemical formula $\text{CH}_3\text{CH}(\text{NH}_2)\text{COOH}$ or $\text{C}_3\text{H}_7\text{NO}_2$. The α -carbon atom of L- Alanine is bound with a methyl group ($-\text{CH}_3$), making it one of the simplest α -amino acids with respect to molecular structure and also resulting in L- Alanine being classified as an aliphatic amino acid. This methyl group of L- Alanine is non-reactive and is thus almost never directly involved in protein function. Amino acids belong to an interesting class of materials which can be used for non linear optical (NLO) applications. And because of its electro-optical properties, optical data storage system and optical switching devices and also it is widely used in X-ray monochromatic. In recent years, various growth methods and apparatus have been continuously developed to improvement in quality and growth rate. The newly develop technology have been prefer to first applied on KDP crystal. Our aim of improving the quality of KDP crystals with better optical properties, an attempt has been made in the present work to grow the KDP crystals by doping it with L- Alanine ion with different concentration by weight % and to study the effect on the nucleation parameters and structural and optical properties [6].

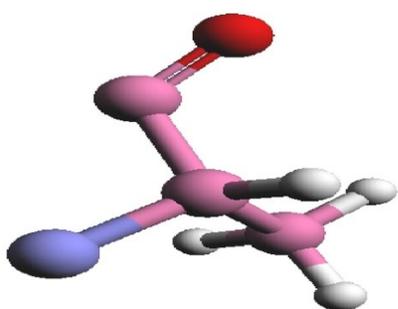
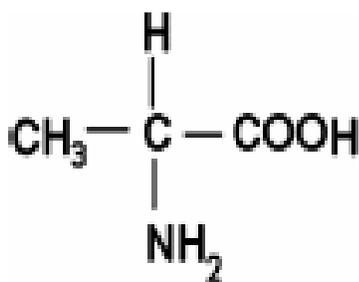


Fig-1(Molecular structure of L- alanine)



(2-Aminopropanoic acid)

In the present study the L-Alanine was added in KDP. Therefore pure and 0.2 mole %L- Alanine doped KDP were grown by slow evaporation technique and subjected to X-ray diffraction, FTIR spectroscopy, TGA and DTA

analysis and UV analysis. In the present investigation, the L- Alanine doped KDP crystals have been grown and characterized by FT-IR, powder XRD, TGA-DTA, and UV-Vis transmission spectroscopy, to identify the improvement in various properties of the grown crystals due to doping.

2. EXPERIMENTAL

2.1 Synthesis and growth:

Slow evaporation technique was employed to grow crystals. The doping of L- Alanine into KDP (GR grade) was carried out by adding 0.2 weight percentage powder form of L-Alanine into 1 molar 100 ml solution of KDP in double distilled water. The mixtures were thoroughly stirred for 8 hours for homogenization. The solution filtered by whatman filter paper pore size 11. The purity of the crystals was improved by successive recrystallization. Grown crystals were found to be color-less and transparent. Figure 1 shows a photograph of 0.2 wt. % L- Alanine doped KDP crystal.



Fig. 2: 0.2 wt % L-alanine doped KDP crystal

3. Characterization:-

The KDP crystal, which was developed by Slow Evaporation method, was studied by using X-ray diffraction analysis (XRD), Fourier transformation infrared spectroscopy (FTIR), Thermo gravimetric analysis/Differential thermal

analysis (TGA/DTA), Ultraviolet-visible (UV-visible) analysis and Dielectric measurements. The details of the various studies were mentioned below under various heads.

3.1 Powder crystal XRD analysis

The powder XRD study conducted to verify the single phase nature of the samples. Fig. 3 shows the powder XRD patterns of 0.2 wt. % L-alanine doped KDP crystals. These are our expected results. KDP crystal belongs to the tetragonal symmetry having dimensions $a=6.8996 \text{ \AA}$, $b=7.5443 \text{ \AA}$, $c=7.4688 \text{ \AA}$. The sample was scanned in the range $10-90^\circ$ at a scan rate 2° per min. The variation in the intensities of various diffraction patterns on changing the concentration of doping was observed. The expected results are given as follows.

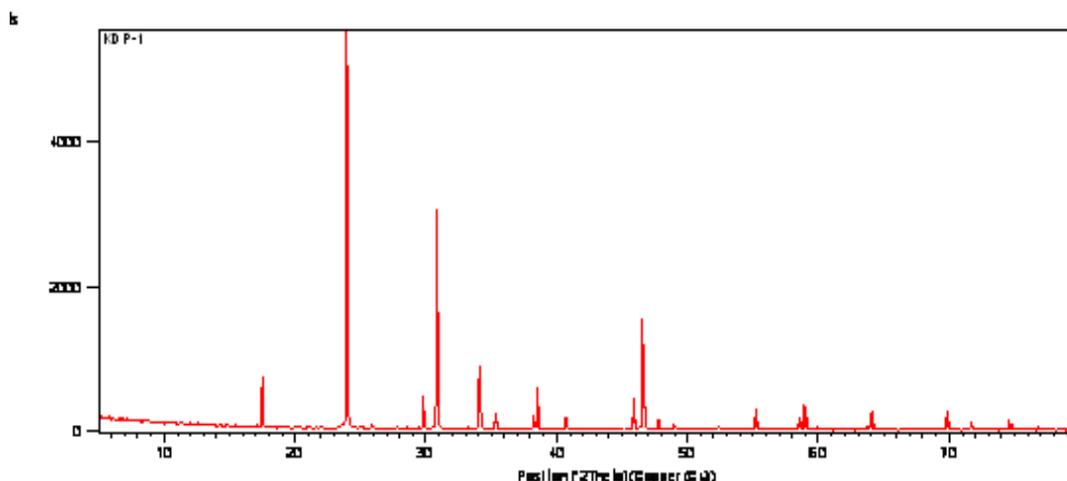


Fig. 3: Powder XRD pattern of 0.2 mole % L-Alanine doped KDP

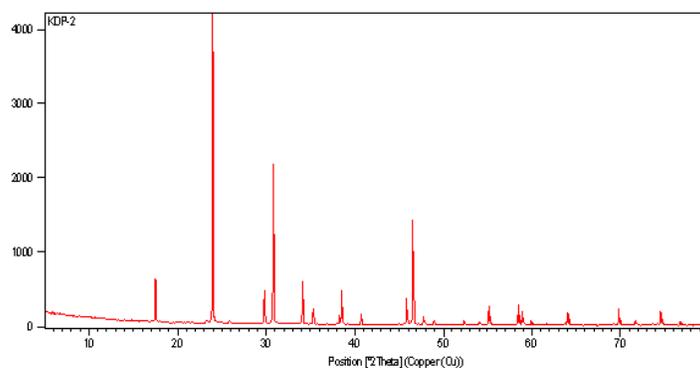


Fig.4-Powder XRD pattern of KDP pure crystal

3.2 UV-Visible Spectral Study:

The UV-Vis transmission spectra were recorded in the region 200-1400 nm. The transparent single crystalline samples were used and mounted in a standard manner so that equal area of samples was exposed to the radiation. It gives the information about structure of molecule. This analysis shows that transparency of crystal in entire visible region. It is an important requirement for NLO material having nonlinear optical applications [07]. The optical transmission range and the transparency cut-off limits are important for NLO materials. The UV-Vis optical transmission spectra of pure and L-Alanine doped KDP crystals are shown in Fig. 5. It is inferred from the spectra that both pure and doped KDP have large transmission window in the entire visible region. The UV transparency cut-off limits decrease slightly on doping L-Alanine in KDP crystals from 350 nm to 390 nm. Altogether, the percentage optical transmission increases on increasing the doping of ALANINE in KDP crystals. On the sacrifice of slight the UV-transparency cut-off limit, the L-Alanine doping increases the transparency of grown crystals. Similar results have been obtained in the case of doping of L-threonine [08] and L-lysine in KDP. A complex is formed of ALANINE with iron, similar potassium complex might have progressively increased the optical transparency of KDP on increasing the doping of L- ALANINE. Recently, a change in the UV-Vis absorbance in amino acid has been studied in the femto-second laser radiation.

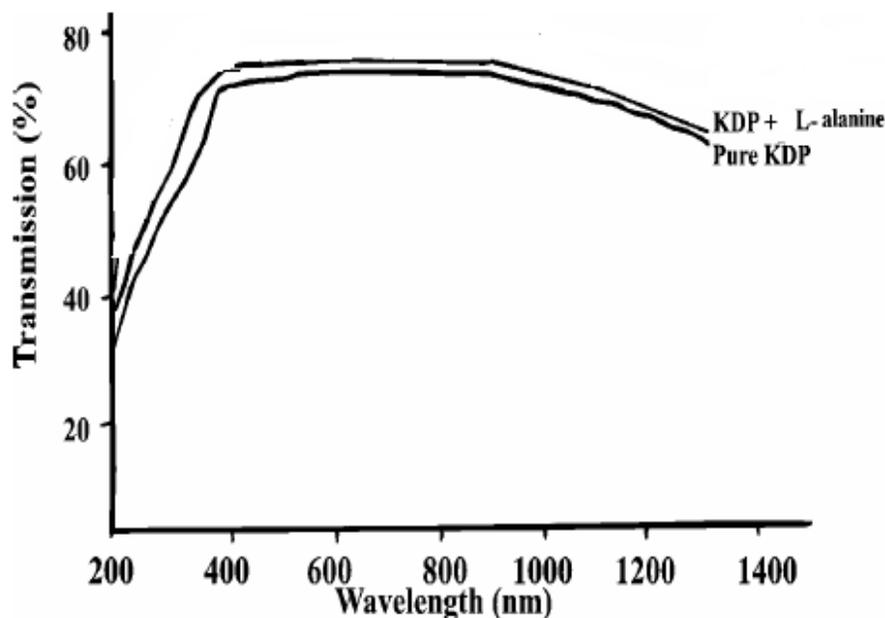


Fig. 5 UV-Vis of pure and L-alanine doped KDP crystals.

3.2 Fourier Transform Infrared spectroscopy-

To obtained result testifies that all the IR spectra are practically identical and agree with the available literature data [09]. The assignments confirm the presence of various functional groups present in the material. FT-IR spectra of powdered samples was studied in the range from 400-4000 cm^{-1} . The FTIR Spectrum of 0.2 wt %L- Alanine doped KDP crystal as shown in **Fig. 2**. The broad band at the frequency 2171.70 cm^{-1} and 2723.30 cm^{-1} may represent O-H stretching of COOH group of amino acid .A broad absorption in FTIR spectra at 1747.39 cm^{-1} . The prominent bands between 2675 and 2171.70 cm^{-1} indicates combination of asymmetrical bending vibration and torsion oscillation of the NH_3^+ group. C-H stretching of CH_2 observed at 1487.01 cm^{-1} and C-O bending attribute the absorption at 1747.39 cm^{-1} Instance absorption observed at 534.25 cm^{-1} . It was easily concluded that, L-Alanine doping was successfully achieved due to N-H, C=O, C-H, remained absent in pure KDP crystals..

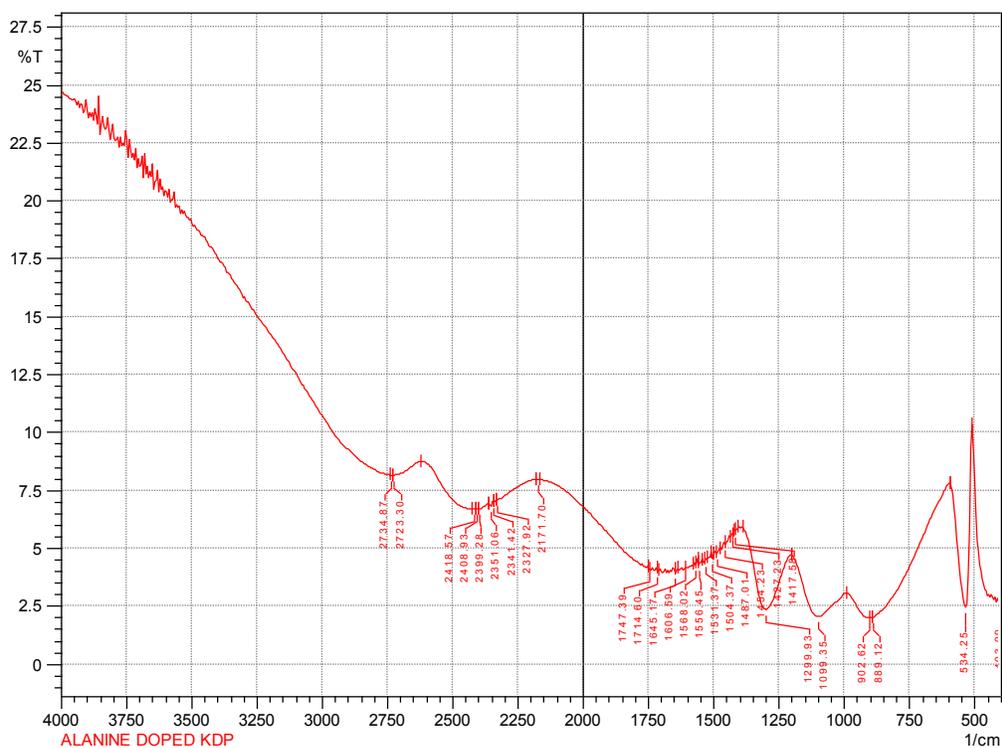


Fig 6- FTIR OF L-ALANINE DOPED KDP

3.3 TGA-DTA Analysis-

In the present investigation, the effect of L-Alanine doping on thermal stability of KDP crystals is studied by employing the thermogravimetry analysis (TGA). **Fig. 7** indicates thermo grams for pure KDP and 0.2 wt % L-Alanine doped KDP, respectively. It has been observed that initially increasing the level of L-Alanine doping the dehydration process starts early and the crystal becomes anhydrous faster than the pure KDP. The grown crystal was subjected to thermo gravimetric analysis (TGA) at heating rate 25 °C/min to 800 °C. In given fig. the thermo gram indicates that short weight loss is at temperature near 215.49 °C. It may be due to physically absorbed water. The fig of (TGA) shown below. Thermo gravimetric analysis (TGA) carried out simultaneously is very much useful in interpreting the melting point and thermal stability of a sample[10].

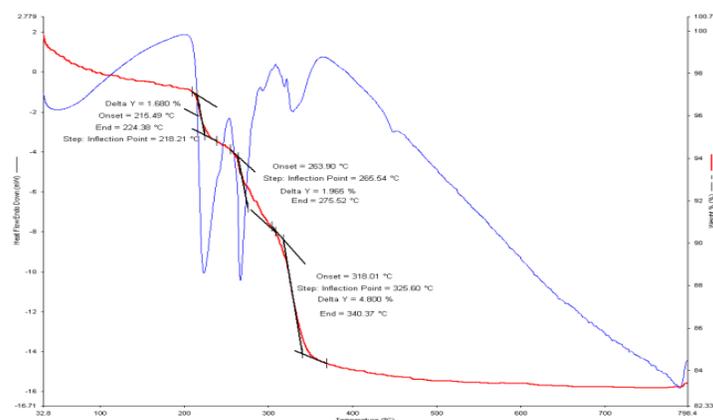


Fig. 7 Thermo grams of 0.2 wt % L-Alanine doped KDP,

4. Conclusions-

Pure and L-Alanine doped KDP crystals were grown by slow solvent evaporation technique. The FT-IR spectra confirmed the presence of amino acid L-Alanine in KDP crystals. Thermo grams of pure and L-Alanine doped KDP crystals suggested that as the doping increased the crystals became thermally less stable and it indicate that this crystal can be exploited for NLO applications up to the temperature of 218.21 °C. The study of cell parameters calculated by powder X-ray diffraction analysis confirmed that the crystal structure of KDP does not change by doping of L-Alanine. The higher values of activation energy and standard entropy of activation suggested more stable condition for pure KDP than L-alanine doped KDP crystals. For obtaining higher SHG efficiency and percentage optical transmission in KDP crystals by doping L-Alanine slight sacrifice in the UV cut-off limits and the thermal stability of crystals was given. The effect of L-Alanine as dopant has considerably enhanced the optical transparency, NLO property and mechanical properties compared to pure KDP. It is observed that doping of KDP with L-Alanine has made KDP much more efficient with improved its qualities and facilitate its application in the field of nonlinear optics.

5. References-

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