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Advances in Applied Science Research, 2015, 6(1):11-14

Advances in Applied Science Research
Pelagia Research Library

ISSN: 0976-8610
CODEN (USA): AASRFC

Effect of low and high concentration of glycine of properties of KDP crystals

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ABSTRACT

Crystals of potassium dihydrogen phosphate (KDP) doped with Glysine has been grown by solvent evaporation technique at 32^0 C. The crystalline nature of the crystal is verified by powder X-ray diffraction studies. The presence of functional groups has been identified by both Fourier transform infrared spectrum. The optical nature of grown crystal is analyzed using UV- Visible spectrum. The effect of different concentration of dopant on the dielectric constant is studied shows that the dielectric constant goes on decreasing on increasing the frequency.

Key words: FTIR spectra, X-ray diffraction, SHG efficiency, Transparency, nonlinearity and molecular alignment etc.

INTRODUCTION

The simplest amino acid is glycine, which has just a hydrogen atom as its side. In solution of neutral P^H the glycine is predominantly dipolar ion or Zwitterions, in Glycine the PK of carboxylic (COOH) group is 2.3 and of the amino group is 9.6 [9].

KDP is among the most widely used NLO material. It is characterized by good UV transmission, high damage threshold but still their nonlinear coefficients are relatively low. In addition they are also excellent electro-optic crystals used as a pocket cells, Q- switches etc. [1-2]. Many methods have been tried to improve the NLO properties of KDP crystal [3-4]. The addition of dopants and their influence on the growth process and properties of crystals have been tried in recent years [5-6]. The amino acids are the famous organic materials, play a vital role in the field of nonlinear optical crystal growth. Many members of natural amino acids are individually exhibiting the nonlinear optical properties because they have a donor group NH_2 and acceptor COOH group and the intermolecular charge transfer is possible. Especially natural amino acids such as Arginine, Lysine and γ glycine are evidently showing NLO activity because additional COOH group in first and NH_2 group in second. Therefore amino acids may be used as a dopant.

In present work the Glycine (NH_2CH_2COOH) was added as 2M%, 4M% and 6M% in KDP. It was observed that the SHG efficiency enhanced by that of pure KDP crystal. It was found to be 1.36 times more than pure KDP. Therefore pure and 2M%, 4M% and 6M% Glycine doped KDP crystals were grown by slow evaporation technique and subjected to X- ray diffraction, FTIR spectroscopy, UV- visible spectral analysis and dielectric studies.

MATERIALS AND METHODS

Synthesis and Growth:
Single crystals of pure and 2, 4, and 6M% Glycine doped KDP crystals were grown by slow evaporation of the saturated solution at 32^0C. Analytical grade (AR) samples of potassium dihydrogen phosphate and glycine along doubled distilled water were used for the growth of single crystals. A solution of KDP and Glycine was prepared using doubled distilled water as solvent. The P^H of the solution was 4. The solution was stirred using magnetic

stirrer at room tempeture for about one hour and filtered using Whitman filter paper, filtered solutions were kept in constant temperature bath set at 32^0 C. After a period of 14 days, transparent, colourless crystals were harvested.

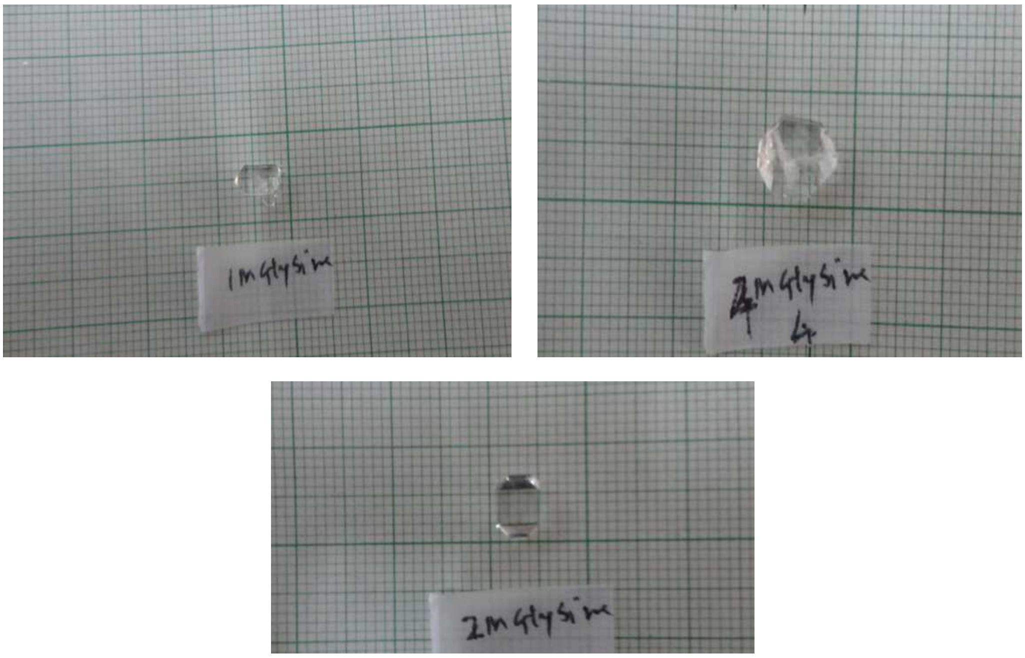

Figure 1

1.1.2 Characterization

The grown glycine doped KDP crystals were subjected to various characterization viz. NLO tests, powder X-ray diffraction, FTIR analysis, UV-visible spectral studies and dielectric studies.

RESULTS AND DISCUSSION

2.1 SHG test

The Kurtz's powder SHG test was carried to study the enhancement in nonlinearity of KDP due to addition of Glycine. It was found that the SHG efficiency of KDP increased with addition of glycine in different mole percent but maximum enhancement was observed with addition of 1M% Glycine. It was 1.36 times more than the pure KDP. This increase is due the fact that the Glycine has Zwitterions and it may be connected with KDP by short O-H-O hydrogen bonds. In Glycine there is more dipole moment due to presence of NH_3 amino group [9]. Hence the reaction with KDP optically active amino group may replaces some potassium ions and increases its non Centro symmetry which results increase of nonlinearities of the grown crystals. Hence this glycine doped KDP crystals with large SHG efficiency may be useful for laser fusion experiment and frequency conversion applications.

2.2 X-ray diffraction analysis

The single crystal XRD data of Glycine doped KDP crystal has been collected using ENRAF NONIUS CAD4X-ray diffract meter and calculated cell parameters values are a= $7.4490A^0$, b= $6.9666A^0$, c= $7.4486A^0$ and V= $386.5366A^{03}$. It indicates that the dopant does not change the original crystals structure of KDP.

2.3 FTIR anal

FTIR spectra indicates that 3820.98 free O-H stretching hydrogen bonded of KDP, $2856cm^{-1}$ P-OH asymmetric stretching, $2374cm^{-1}$ P-OH bending of KDP,898 P-OH stretching and $545cm^{-1}$ is due HO-P-OH bending, and 1076 to $1544cm^{-1}$ corresponds to P=O and O-H Vibrations.

It was found that the 1M% and 6M% glycine doped KDP showed extra peaks at 3801, 3367.71, 3292.49.3151.69,$2924.09cm^{-1}$and extra peaks for 6M% are 3820,3446,3367,3292,3151,2922.2856,$2922cm^{-1}$ confirmed the presence of Glycine in the doped crystals. Good refractive index changes in 1M% and 6M% Glycine doped crystals are expected to have enhanced SHG efficiency.

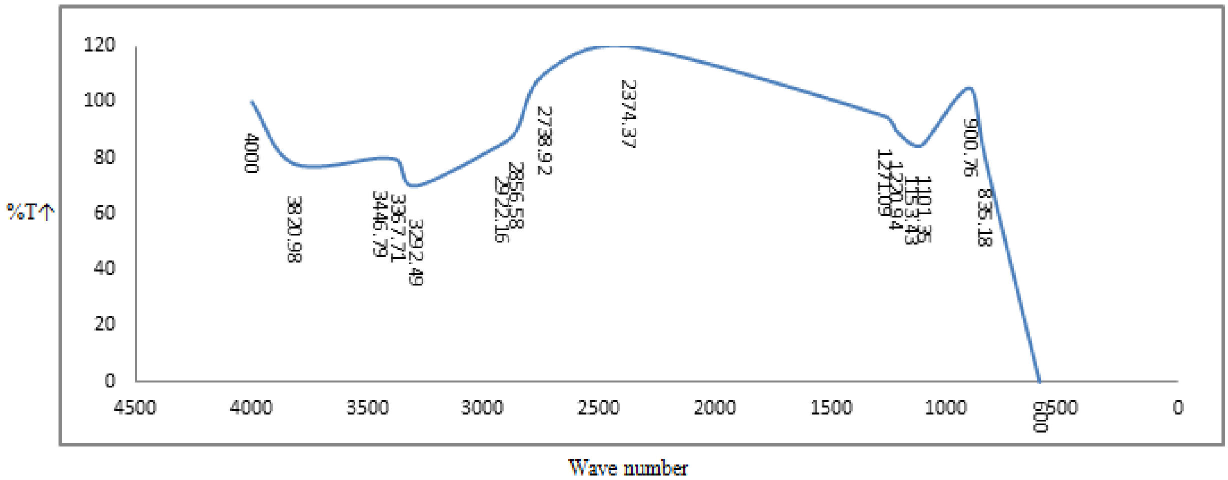

Figure 2 FTIR Spectrum of K6M%G

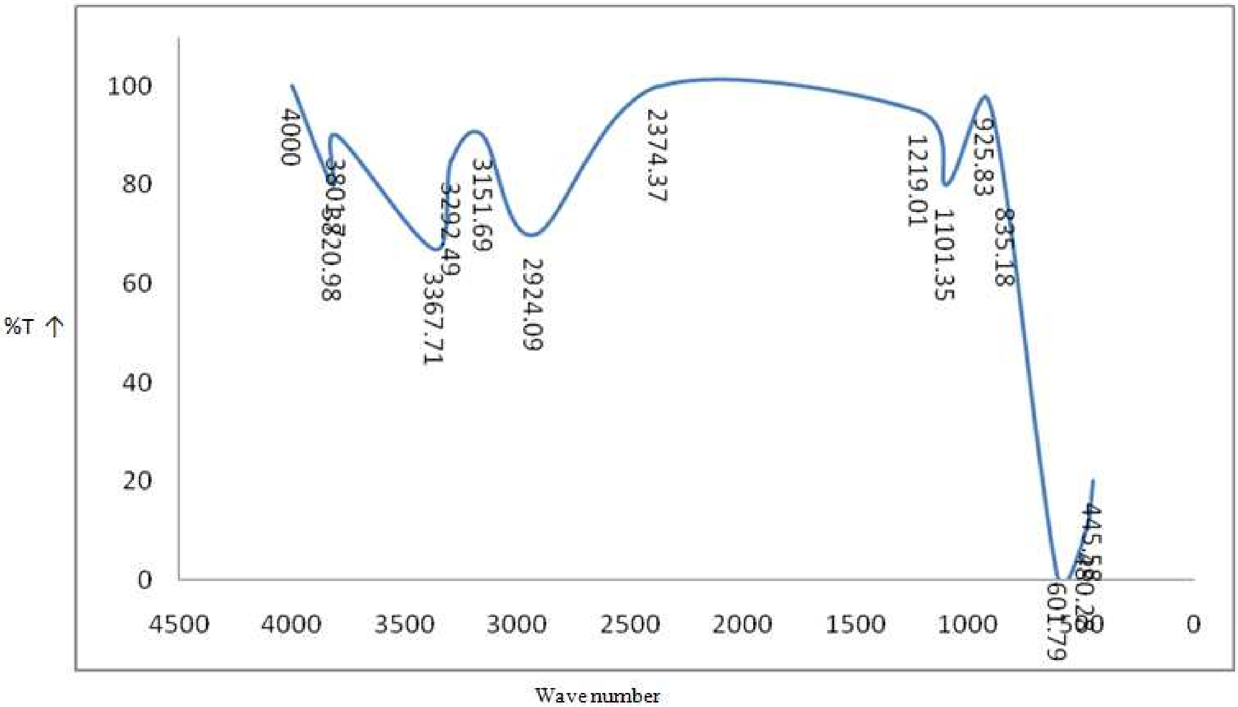

Figure 3. FTIR spectrum of K1M%Glycine

2.4UV-Visible spectral study

The UV-visible study analysis shows that the crystal is transparent in the entire visible region. There is strong absorption near the wavelength of 300nm, it may be assigned to electronic excitation in the Glycine doped KDP crystal. The lower cut off wavelength in glycine doped KDP is slightly shifted to the higher wavelength side from KDP which may be due to the incorporation of glycine.

2.5Dielectric study

The capacitance was measured using convectional parallel plate capacitor method with frequency range (100Hz to 10 KHz) using Falcon LCR-010B LCR meter. The dielectric properties are correlated with the electro- optic properties of the crystals. The magnitude of dielectric constant depends on the degree of polarization charge displacement of the crystals. The dielectric constant of materials is due to the contribution of electronic, ionic and dipolar and space charge polarization which depend on the frequency [10]. At lower frequency all the polarizations are active. The space charge polarization is generally active at low frequency and at high temperature [11]. In KDP and ADP crystals many reports are available about its behaviour and in our present work the measured dielectric constant values are in good agreement with the reported results [12]. For K1M%G and 6M%G the values of dielectric constant at 100Hz,1KHz and 10KHz are 91.8, 52.8, and 14.8 and 13.44, ----, 9.6. The value of dielectric constant decreases with increase in frequency and 6M%G have lower value of dielectric constant may suggest the purity of the crystal and high damage threshold of the crystal.

CONCLUSION

Amino acids, Glycine doped KDP single crystal has been grown by slow evaporation technique with extended SHG efficiency than pure KDP. The study of cell parameters calculated by single X-ray diffraction analysis confirmed that the crystal structure of KDP does not changed by doping of Glycine. The FTIR analysis confirmed the presence of all functional groups. The absence of absorption and excellent transmission in entire visible region makes this crystal a good candidate for optoelectronic application. The dielectric constant study reveals the purity of crystal.

Acknowledgement
The authors sincerely thanks to Dr. PK Das, IPC lab, IISC, Bangalore, Dr. Raghuwanshi, Dr. Wadatkar, Vidyabharti Mahavidyalaya, Amravati, Dr. Charde, Government Pharmacy college, Amravati, Diya lab, Navi Mumbai and Dr. G G Muley, department of Physics, Sant Gadge Baba Amravati University, Amravati.

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