Influence of Citric Acid and Glutaric Acid on Optical Traits of KH₂PO₄ Crystal for NLO Device Applications

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ABSTRACT

In current investigation pure, citric acid (CA) and glutaric acid (GA) doped $KH_2PO_4(KDP)$ crystal has been grown by slow solvent evaporation technique. The crystallographic data such as crystal structure, space group and unit cell dimensions of grown crystals have been evaluated by single crystal X-ray diffraction technique. The significant impact of CA and GA on KDP crystal has been evaluated by UV-visible spectral analysis. The optical transmittance of pure, CA and GA doped KDP crystal has been comparatively examined within the wavelength range of 200-900 nm.

Keywords: Crystal growth, Optical studies, X-ray diffraction

1. INTORDUCTION

KH₂PO₄(KDP) is recognized nonlinear optical (NLO) crystal for high-tech industrial applications due to its versatile characteristic properties. The KDP crystal therefore finds its special place for designing NLO devices. Nowadays NLO crystals are being readily used as integral part of photonic devices which is why the KDP crystal has been under extensive investigation since its identification as NLO material. In order to explore the maximum utility and most suitable applicability of KDP crystal researchers have scrupulously evaluated the crystal growth, morphological, structural, mechanical, optical, electrical and thermal properties[1, 2]. However, decisive attempts have been made to modify the inherent qualities of KDP crystal by doping a selected organic additive which largely includes amino acids and carboxylic acids [3, 4]. They possess large H-bonding quality and abundance of pi-bond network which are prerequisite to tune the optical properties. The literature survey proved prominent impact ofamino acids and carboxylic acids on KDP crystal, thereforein current study the impact of glutaric acid and citric acid on structural and optical properties of KDP crystal has been evaluated by single crystal XRD and UV-visible spectral analysis.

2. EXPERIMENTAL PROCEDURE

The Merck make KDP salt was dissolved in double distilled water and the homogeneous solution of KDP was taken in two separate beakers. The beakers were then added by 1wt% of citric acid (CA) and glutaric acid (GA) respectively. The mixture was then stirred well for four hours in order to achieve homogeneous doping in KDP. The solutions were then filtered using the No.1 Whatmann filter paper and the filtered solution was taken in a clean rinsed beaker. The beakers were covered by the porous foil and kept in a constant water bath maintained at 35 °C. The as grown pure, citric acid doped KDP (CA:KDP) and glutaric acid doped KDP (GA:KDP) crystals are shown in Fig.1.

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Fig -1: Crystal of (a) KDP, (b) CA:KDP and (c) GA:KDP

3. RESULTS AND DISCUSSION

3.1 Single Crystal X-ray Diffraction Analysis

The structural parameters of grown crystals have been experimentally determined by single crystal X-ray diffraction (XRD) technique. The sample crystals of each were subjected to XRD analysis using the EnrafNonius CAD-4 single crystal X-ray diffractometer. The recorded structural data reveals that the Pure, CA:KDP and GA:KDP crystal have same tetragonal structure and belong to same space group while there is slight change in unit cell dimensions as observed in data given in table 1. The cell dimensions of pure KDP crystal are in good agreement with reported literature[5].

Table-1 Single	crystal XRD data
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Crystal	Unit cell values (Å)	Volume $(Å)^3$	Structure	Space group
KDP	a = b = 7.47, c = 6.98	389.49	Tetragonal	I-42d
CA:KDP	a = b = 7.44, c = 6.99	386.92	Tetragonal	I-42d
GA:KDP	a = b = 7.51, c = 6.97	393.10	Tetragonal	I-42d

3.2 UV-visible spectral analysis



The optical transmittance window of pure and doped KDP crystals has been investigated within the wavelength range of 200-900 nm using the Shimadzu UV-2450 spectrophotometer. The recorded optical transmittance of grown crystals is shown in Fig. 2. It is evident that the grown crystals show transmittance in prominent range of spectrum and it is found that the transmittance of GA:KDP (87%) > CA:KDP (84%) > KDP (79%). It is noteworthy that the transmittance of GA:KDP is significantly higher than KDP crystal. The crystal with high optical transmittance is largely desirable for NLO device applications[6]. The high optical transmittance might have favored due to reduced internal scattering from defects[7]. Thus the GA:KDP and CA:KDP crystal with superior optical transmittance can replace KDP crystal for designing distinct NLO devices.

4. CONCLUSION

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The single crystals of KDP, GA:KDP and CA:KDP have been grown successfully by slow solvent evaporation technique. The single crystal XRD analysis confirmed the tetragonal crystal structure and slight change in cell dimensions of doped KDP crystal. The UV-visible spectral analysis of grown crystal show significant optical transmittance in visible spectrum however amongst all the GA:KDP crystal express highest transmittance i.e. 87%. Thus the wide optical transmittance window of GA:KDP and CA:KDP crystal could play vital role in designing various NLO device applications.

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