Effect of Organic Entities on the Performance of Potassium Dihydrogen Phosphate (KDP) Crystals

Sujata B. Bade[1,a)], Y.B. Rasal[1,b)], M.D. Shirsat[2,c)], and S.S. Hussaini[1,*]

[1] *Crystal Growth Laboratory, Department of Physics, Milliya Arts, Science and Management Science College, Beed-431122, Maharashtra, India*

[2] *RUSA, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad-431005, Maharashtra, India*

[a)] sujatabade02091995@gmail.com

[b)] rasyog1975@gmail.com

[c)] mdshirsat@gmail.com

Abstract

The 0.5 mol l-cystine and 2 mol oxalic acid doped in potassium dihydrogen phosphate crystals have been developed by slow evaporation solution technique at 20 °C. The powder X-ray diffraction technique was used to study the structural properties of the grown crystal. The FTIR spectral analysis method is used to identify the functional groups of grown crystals. The UV-visible was adopted to study the optical transparency of the grown crystals and their related optical parameters in the range of 200-900 nm. The optical transmittance is found to be 87 % of the grown crystal. The energy band gap (E_g) of the grown crystal observed from the graph is 3.93 eV. The Kurtz-Perry powder test is used to determine the SHG efficiency and it is observed that it is 0.5 times greater than pure KDP crystal.

Keywords:

*** Address of correspondence**
S.S. Hussaini
Crystal Growth Laboratory, Department of Physics, Milliya Arts, Science and Management Science College, Beed-431122, Maharashtra, India
Email: shuakionline@yahoo.co.in

How to cite this article
Sujata B. Bade, Y.B. Rasal, M.D. Shirsat, and S.S. Hussaini, Effect of Organic Entities on the Performance of Potassium Dihydrogen Phosphate (KDP) Crystals, J. Cond. Matt. 2023; 01 (02): 100-104

Available from:
https://doi.org/10.61343/jcm.v1i02.35

Introduction

The emerging trends in nonlinear materials NLO play a very important role in the area of optical, communication, signal processing, and optical storage devices. Potassium dihydrogen phosphate is a fundamental inorganic NLO material having good optical, dielectric, and thermal properties and plays a vital role in the field of 2nd harmonic generations and the branch of optoelectronics. The high transparency in a region of the UV-visible spectrum and the possibility of growing a big single crystal with a high growth rate are good experimental properties of KDP [1].

NLO materials are essential for various applications in optoelectronics, telecommunications, laser technology, and other fields where nonlinear optical effects are exploited. These materials exhibit nonlinear responses to intense light, which means their optical properties change with the intensity of the incident light is a well-known inorganic NLO material with good optical, dielectric, and thermal behavior, and it is widely used for second harmonic generation (SHG) and other optoelectronic applications. Doping KDP crystals with organic materials is a common practice to modify their properties for specific applications or to enhance their nonlinear optical response [2].

When an organic material is doped into the KDP crystal lattice, it can introduce new energy levels, alter the crystal structure, or create defects that can lead to enhanced NLO properties. The doping concentration and choice of the organic material are critical factors in achieving the desired optical properties. Organic materials offer advantages such as tunability, ease of synthesis, and the possibility of tailoring their optical properties by modifying their chemical structure. By combining the unique properties of organic materials with the established properties of KDP crystals, researchers can design NLO materials with improved efficiency and performance.

The molecules in pure organic crystals are often bonded by weak Vander Waals forces of hydrogen bonds, which result in poor mechanical properties. To overcome these difficulties, the large nonlinearities of p-conjugated organics and the ionic salts can be combined into a single NLO material called semi-organics. In this paper, the crystal growth of amino acids doped in KDP has been described [3-4].

Experimental

The AR-grade potassium dihydrogen phosphate (KDP) is dissolved in distilled water with constant stirring to achieve the supersaturated solution. The supersaturated KDP was added 0.5M L-cystine and 2M oxalic acid the L-cystine and oxalic acid solutions were allowed to stir at a constant speed to achieve homogeneity through the volume. The prepared solution was then filtered by Whatman filter paper & the purity of the salts was achieved good quality transparent bulk crystal was harvested within 35 days by slow evaporation method at room temperature.

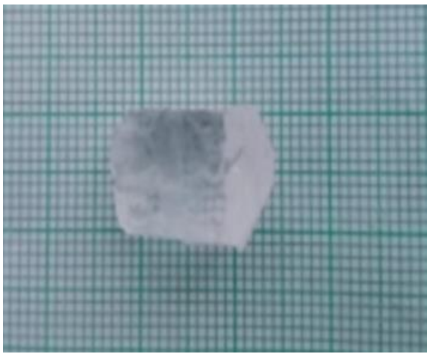

Figure 1: Dimension of resulted crystal are 8×20×8mm^3

Characterizations

X-Ray diffraction

The Single-crystal X-ray diffraction experimental technique was adopted to identify and confirm the crystallinity of the grown crystals. This technique is also used to determine the a, b, and c values. From this analysis, it was confirmed that the grown crystals belong to the tetragonal system. The lattice parameters are well matched with the reported literature [2] according to S. Sasi et al, we are getting the same pics [4]. The Oxalic acid-doped KDP crystals when subjected to X-ray diffraction show a pattern as in Fig 2. After comparing the powder XRD pattern of pure KDP and doped KDP it is found that Peak 2ϴ shifted and this suggests that the structure of KDP is slightly disturbed by dopant which tries to change the transparency [5]. The structure of the grown crystal is tetragonal.

UV-visible study

Linear optical studies are carried out by using the UV-visible spectrophotometer in the wavelength range 200 nm to 900 nm and the recorded UV-visible transmittance spectrum is shown in Fig 3. The figure shows a sharp fall in transmittance at 283 nm. For the UV-visible study, the sample was taken in the form of a solution. The spectrum shows 87% of transmittance in the visible and near-infrared regions of the spectrum. The linear optical absorption coefficient for oxalic l-cystine doped KDP crystal at different wavelengths was calculated using the relation

Where T and d denote transmittance and the thickness of the crystal. The plot of absorption coefficient versus wavelength for oxalic l-cystine-doped KDP crystal is presented in Fig 6. Using the following Tauck’s relation, the optical band gap energy (E_g) of the grown crystal is determined [2].

$$\alpha = A\left(h\nu - E_g\right)^{\frac{1}{2}}$$

Where α is the absorption coefficient, hν is photon energy and A is the band edge constant that depends on the transition probability. The plot between $(\alpha h\nu)^2$ and hν of the l-cystine oxalic doped KDP crystal is shown in Fig 6 optical band gap energy of the grown crystal is found to be 3.93 eV.

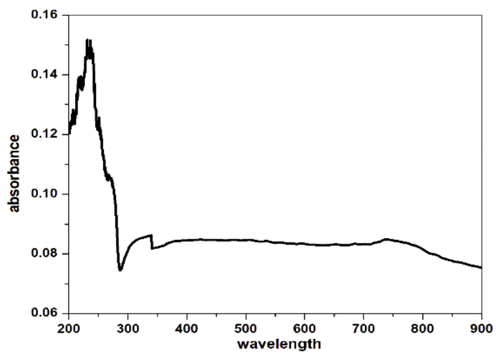

Figure 2: wavelength vs. absorbance

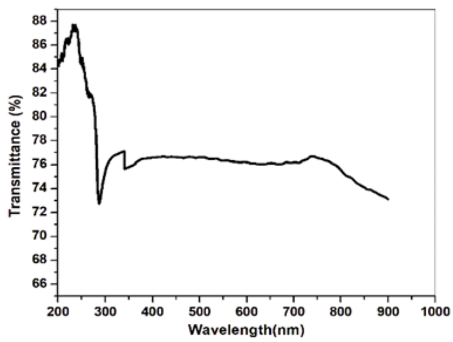

Figure 3: wavelength vs. transmittance

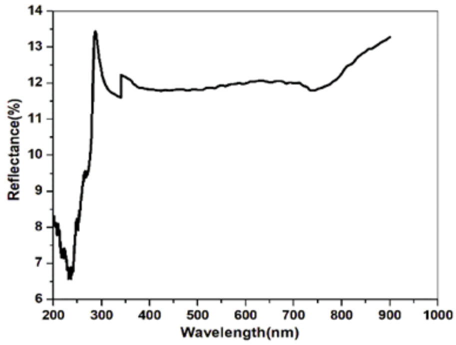

Figure 4: wavelength vs. reflectance

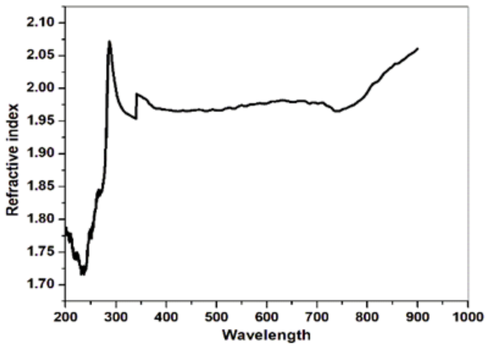

Figure 5: wavelength vs. refractive index

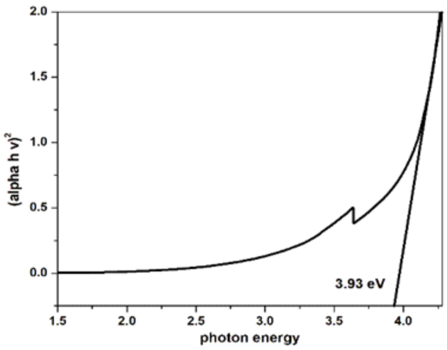

Figure 6: photon energy vs. band gap energy

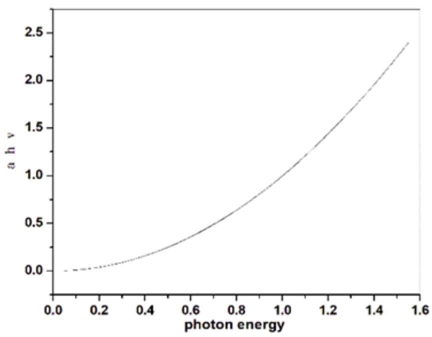

Figure 7: photon energy vs. αhν

The transmittance spectrum utilized to determine the refractive index and reflectance of the grown crystal has been calculated by using the reported formulae [3]. The related plots were shown in Fig 4 and 5 simultaneously. It is observed from the graph that refractive index and reflectance in the entire visible region are suitable for calibrating optical components such as filters, resonators, and reflectors [4]. The photo-refractive materials also have different applications in storing and processing holographic data. The various optical parameters shown in the grown crystal could serve better for fabricating electro-optic modulation and photonic devices [5].

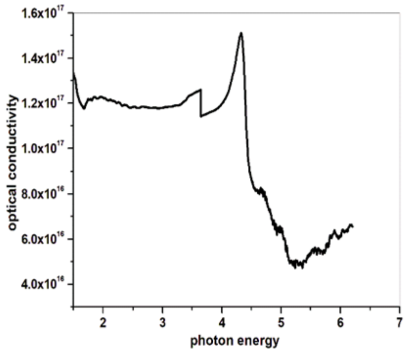

Figure 8: photon energy vs. Optical conductivity

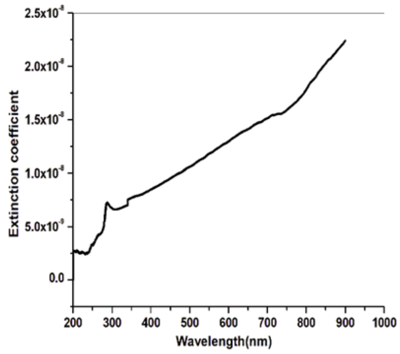

Figure 9: Wavelength vs. extinction coefficient

Fourier Transform Infrared Spectroscopy

FTIR is a powerful analytical technique used to study the molecular structure and vibrations of materials, including NLO (Nonlinear Optical) crystals. FTIR is a nondestructive analytical technique, that allows researchers to analyze NLO crystals without altering or damaging the sample. This is particularly important for the characterization of precious or delicate crystals. Using Bruker spectrometer of KBR pellet technique for wave number region 500-4500 cm-1. The Fourier transform infrared spectrum of l-cystine oxalic doped KDP crystal is reflected in Fig 10. the peak at 554 belongs to C=O bending, 718 shows Ring bend out of phase, 1097 shows C-O-C out of phase, 1248 shows C-O stretching

1324 shows NH2 stretching, 1620 shows NH2 deformation, 2347 shows P-H stretching, 3411 shows NH2 in phase, 3747 shows OH stretching, 1637 shows O-P-OH symmetric stretching [3,5].

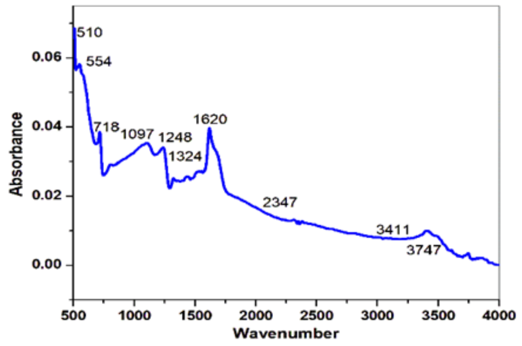

Figure 10: wavenumber vs. absorbance

Thermal studies TGA/DTA

TGA is a thermos analytical technique used to measure the weight changes of a sample as a function of temperature (or time) under a controlled atmosphere. Understanding the thermal behavior of NLO crystals is crucial to ensuring their performance and reliability in practical applications cystine oxalic doped in KDP crystal studied for TG/DT analysis. The pulse of temperature value was kept for each test is 10 °C per minute. TG/DTA study was performed simultaneously in the temperature range 50 °C to 900 °C. TG/DTA analysis in Fig 11 shows that l-cystine oxalic doped KDP crystal. The TG curve shows that the compound is used up to 260 °C for any applications. The Endothermic peak at 260 °C indicates the breaking-up point of the sample. The endothermic peak at 346 °C indicates further decomposition of the compounds present in the crystal. This indicates the vaporization of H_2O in the crystal lattice of l-cystine oxalic doped KDP.

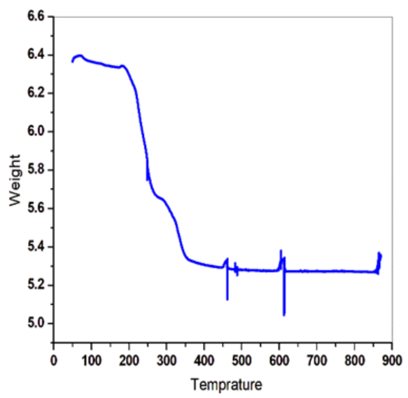

Figure 11: temperature vs. weight

Second harmonic generation

Second-harmonic generation (SHG) is a non-linear optical experimental technique in which two photons with the same frequency interact with two photons with the same frequency with a nonlinear material are combined and generate a new photon with twice the energy of the initial photons that conserves the coherence of the excitation [17]. SHG technique was adopted to measure the nonlinear efficiency of oxalic l-cystine doped KDP crystal by the Kurtz- Perry powder method [6]. In this experiment laser source used is Nd: YAG (Yttrium-Aluminum-Garnet) laser which emits 10640 Å laser light accelerated on the powdered sample. The output ray beam was collected, filtered, and detected by a photomultiplier tube for further wavelength detection and output energy measurement. It is concluded that green emission at the output confirms the wavelength of the incident beam was disintegrated and confirms the nonlinearity of the subjected sample. The results confirm SHG efficiency of the subjected crystal is 0.5 times higher than that of the parent. It is to be mentioned that oxalic l-cystine-doped KDP crystal shows the second harmonic emission. Hence oxalic l-cystine doped KDP crystal can be used for any frequency conversion applications. The laser radiation produced by harmonic generations could be applicable in optical communication, optical computing, optoelectronics optical storage and processing, and other laser applications [5].

Conclusions

In present studies, l-cystine and oxalic acid doped in KDP crystal have been grown by slow evaporation solution technique at 20 °C. The tetragonal structure of pure and doped KDP was determined by PXRD analysis. The compound groups detected in the FT-IR spectrum of l-cystine and oxalic acid affirmed the presence of dopants and KDP in grown crystals. The UV-visible analysis confirmed that l-cystine and oxalic-doped KDP crystal (87%) crystal possess superior optical transmittance than the referred paper. The SHG efficiency is 0.5 than that of Pure KDP. All the above studies infer that l-cystine and oxalic doped KDP crystals are used for designing laser frequency conversion and electro-optical modulator devices.

References

1. Y. B. Rasal, M. Anis, M. D. Shirsat & S. S. Hussaini, Mater. Res. Inno. 21, 45-49 (2016).
2. P. Kumaresan, S. Moorthy Babu, P.M. Anbarasan, J. Crys. Grow. 310, 1999-2004 (2008).
3. Y. B. Rasal, R. N. Shaikh, M. D. Shirsat, S. Kalainathan & S. S. Hussaini, Mater. Res. Express 4, 036202 (2017).

4. S. Sasi, R. Robert, S. Arumugam, C. Inmozhi, Opt. Mater. 51, 139. (2015).
5. K. Manimekalai, R. Rajasekaran, Intern. Res. J. Engine. Technol. 04, (2017).
6. Nabeel A, A. M. Funde, V. S. Waman, M. M. Kamble, R. R. Hawaldar, D. P. Amalnerkar, S. W.Gosavi, S. R. Jadkar, Pramana J. phys.76, 519-531(2011).
7. E. F.Schubert, J. K. Kim, J. Q. Xi, Phys. Stat. Sol. 244, 3002-3008 (2007).
8. Chuang-tian Chen, Guang-Zhao liu, Annu. Rev. Mater. Sci. 16, 203-243 (1986).
9. S.K. Kurtz and T.T. Perry, J. of Appl. Phys. 39 3798-3813 (1968).
10. Podder, J. of Cry. Growth 237,70-75(2002).
11. K. D. Parikh, D. J. Dave, B. B. Parekh, M. J. Joshi, Cry. Res. Technol. 45, 603-610 (2010).
12. N. Kanagathara, G. Anbalagan, Intern. J. Optics 2012, 1-6 (2012).
13. P. Jagdish, N. P. Rajesh, J. Optoele. Adv. Mater. 13, 962-966 (2011).
14. Abbas J. Jinia and Jyotsna R. Pandey RJC 8,167 - 171 (2015).
15. G. G. Muley, Science and Technology, 2, 109-113 (2012).
16. S.Vetrivel, P. Anandan, K. Kanagasabapathy, Suman Bhattacharya, S. Gopinath, R. Rajasekaran spectrochimica Acta A 110, 317-323 (2013).
17. N. Zaitseva, L. Carman, I. Smolsky, R. Torres, M. Yan, J. of Cry. Growth 204, 512-524 (1999).