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GROWTH, STRUCTURAL AND OPTICAL PROPERTIES OF NONLINEAR OPTICAL POTASSIUM DIAMMONIUM CHLORIDE (PDAC) SINGLE CRYSTAL

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Abstract
Inorganic good quality single crystal of potassium diammonium chloride (PDAC) has been grown from solution by slow evaporation technique with dimensions of 3 x 3 x 2 mm^3 in a period of 27 days. The powder X-ray diffraction was used to determine its cell parameters. The cut off wavelength and band gap energy of PDAC crystal were determined from UV-visible spectral analysis. The Kurtz and Perry SHG test shows the suitability of grown PDAC crystal for nonlinear optical applications.

Keywords: Slow Evaporation Technique, Powder X-ray Diffraction, UV-Visible, Kurtz and Perry Test.

1. Introduction

Nonlinear optical (NLO) materials play a major role in nonlinear optics and in particular they have a great impact on information technology and industrial applications. In the last decade, however, this effort has also brought its fruits in applied aspects of nonlinear optics. This can be essentially traced to the improvement of the performances of the NLO materials [1-7] Inorganic crystals find widespread application as non-linear optical materials in high performance devices. In the past two decades, researchers have generated several new materials and achieved advances both in materials processing and in engineering devices [8-11]. In this paper, Potassium Diammonium Chloride (PDAC) single crystal was grown by the solution growth method using slow evaporation (SE) technique. The grown crystal has been subjected to powder X-ray diffraction analysis, UV- Visible studies and nonlinear optical test.

2. Experimental Procedure

Potassium Diammonium Chloride (PDAC) single crystal was grown by the solution growth method with slow solvent evaporation technique. Analar grade potassium hydroxide and ammonium chloride in stoichiometric ratio 1:2 in double distilled water and stirred well at room temperature for about 3 hours using magnetic stirrer to yield a homogeneous mixture of solution. The adduct is formed according to the reaction,

$$KOH + 2NH_4Cl \rightarrow (NH_2OH)_2\,KCl + HCl + 2H^+.$$

The prepared solution was filtered using WHATMAN filter paper to the impurities. The filtered solution was taken in vessel and closed with perforated covers and kept in dust free atmosphere. A good quality of optically transparent with clear morphology crystal of size 3 x 3 x 2 mm^3 was harvested in the growth period of 27 days and is shown in the fig.1.

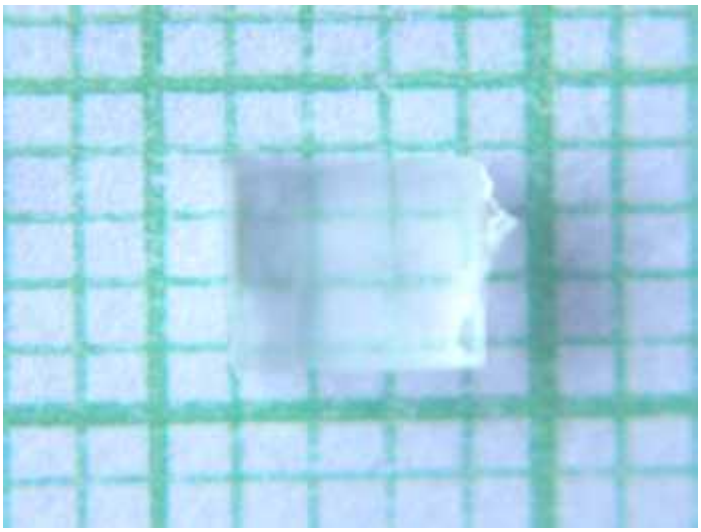

Fig.1: Photograph of PDAC crystal

3. Result and Discussions

3.1 Powder X-Ray Diffraction Studies

The powder crystal X-ray diffraction has been carried out using powder X-ray diffractometer with Cu – Kα radiation of wavelength 1.5405 A˚. The sample was scanned over the range of 10˚ to 90˚ at a scanning rate of 1˚/ min. The indexed powder diffraction pattern of PDAC crystal using JCPDS software as shown in fig.2

The diffraction data are given in the well-defined Bragg's peaks at specific 2θ angles in the diffraction pattern shows that the samples are crystalline nature. The unit cell parameters obtained are a = 11.53 Å, b = 11.53 Å, c = 6.21Å, α = β = γ = 90˚ and volume = 825.562 $Å^3$. Hence the crystal is belongs to tetragonal crystal system.

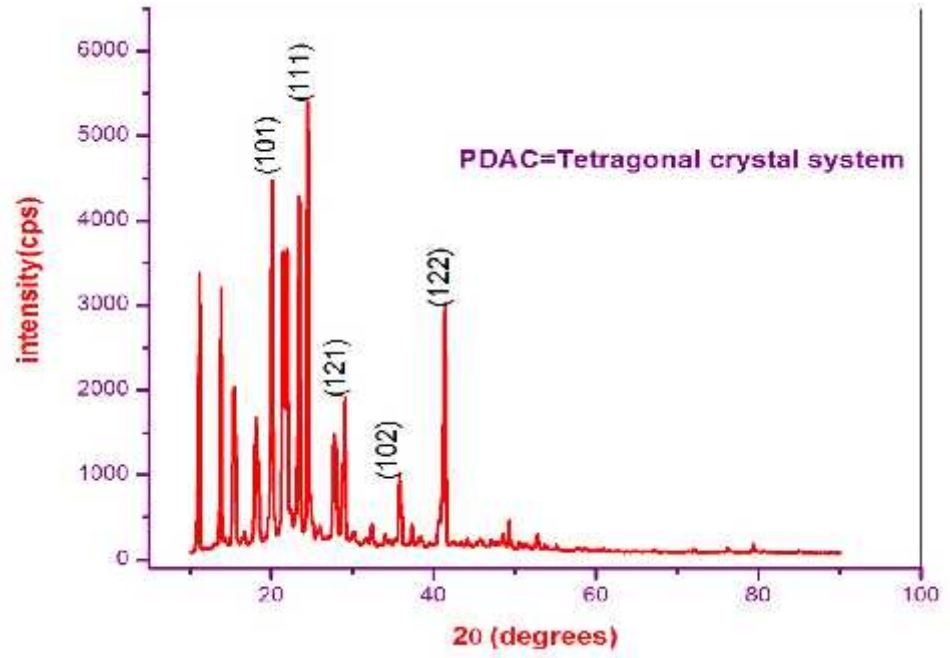

Fig.2. Powder X-ray diffraction Pattern of PDAC

3.2 UV – Visible Studies

The optical absorption spectra of PDAC crystal were recorded in the range of 200 to 800 nm using by LAMBDA 35 UV-Visible spectrophotometer. The recorded spectrum is shown in the fig.3. From the UV-Visible spectrum, it is observed that the cut off wavelength of grown crystal is 212 nm. The calculated cut-off wavelength was used to calculate the energy gap (E_g) of DAPC crystal by the following relation,

$$E_g = h\, c/\lambda$$

Where h is the Planck's constant (6.625×10^{-34} JS $^{-1}$), c is a velocity of light (3×10^8 ms $^{-1}$) and λ is the cut-off wavelength of grown crystal.

$$Eg = 6.625 \times 10^{-34} \times 3 \times 10^8 / 212 \times 10^{-9}$$
$$= 9.375 \times 10^{-19}\ J$$

Energy gap Eg in eV

$$Eg = 5.859\ eV$$

The estimated forbidden energy gap (E_g) is 5.89 eV and this value indicates that the grown crystal belonging to the category of typical insulating material [12]

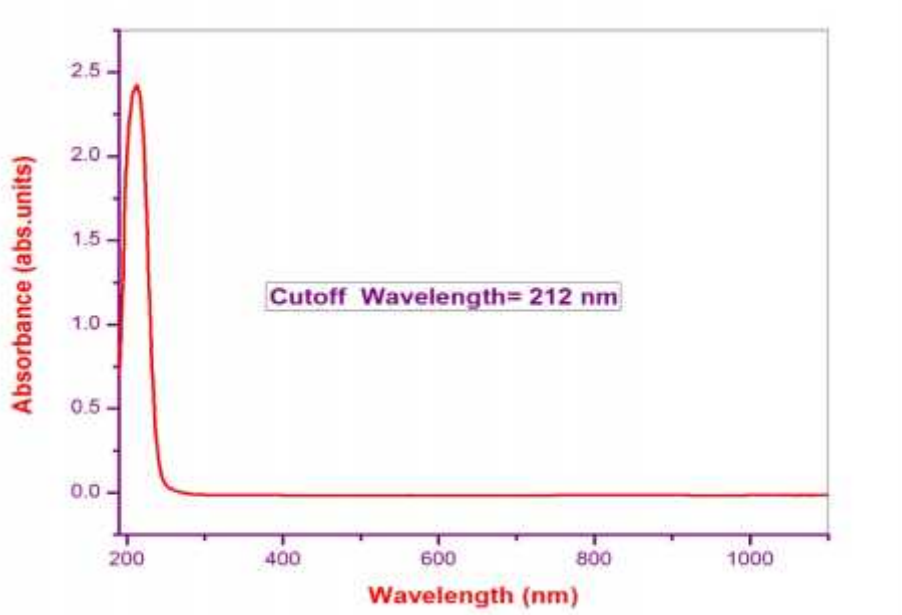

Fig.3. UV-Visible absorption spectrum of PDAC

3.3. NLO Test

The second harmonic generation efficiency of grown material was detected using Kurtz and Perry technique. [13].Generally the micro crystalline sample of potassium dihydrogen ortho phosphate was used for correlation in the calculation of nonlinear efficiency of grown PDAC crystal. The sample was light radiated using Q-switched Nd: YAG laser with input energy pulse of 0.685J. The release of green light from the sample confirms the second harmonic generation in the crystal [14,15]

Conclusion

In the present work, good quality PDAC single crystals were successfully grown by slow evaporation technique. The powder X-ray diffraction studies confirmed that the title compound belongs to tetragonal crystal system. From absorption spectra, it is evident that PDAC crystal has a lower cut-off wavelength at 212nm and its band gap is found to be 5.859 eV. All these studies indicate that the potassium diammonium chloride crystal can consider being a potential candidate for the fabrication of opto-electronic devices.

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