Effect of Potassium Thiourea Chloride on Structural and Optical Properties of Potassium Dihydrogen Phosphate crystal

Y.B. Rasal[a] , R.N. Shaikh[a] , Mohd Anis[c], Mohd Azher[d], M.D. Shirsat[b], S.S. Hussaini[a]*
[a] Crystal Growth Laboratory, Department of Physics, Milliya Arts, Science and Management Science College, Beed-431122, Maharashtra, India.
[b]Intelligent Materials Research Laboratory, Department of Physics, Dr.Babasaheb Ambedkar Marathwada University, Aurangabad-431005, Maharashtra, India.
[c]Department of Physics, Sant Gadge Baba Amravati University, Amravati-444602, Maharashtra, India.
Sir Syed College, Aurangbad (M.S.)
* Corresponding author. Mobile: +91 9325710500.
E-mail address: shuakionline@yahoo.co.in

Abstract– Crystals of Potassium thiourea chloride doped Potassium dihydrogen phosphate have been grown by slow evaporation method at room temperature. The single crystal X-ray diffraction studies confirm that the crystal belongs to Tetragonal structure. The second harmonic generation (SHG) efficiency of the grown crystal was found to be 1.25 times higher than that of KDP. The incorporation of potassium thiourea chloride in KDP was identified using Fourier transform infra-red (FT-IR) analysis. The cut off wavelength of the grown crystal was found to be 390 nm with optical band gap 4.15eV.

Keywords– Crystal growth, Optical studies, Slow evaporation method

INTRODUCTION

During the last few years, the semi-organic nonlinear optical (NLO) crystals have attracted much interest due to their superior properties. Potassium Dihydrogen Phosphate (KDP) is well known transparent dielectric material and having good optical properties. Due to its NLO properties it has various applications like optical switching, communication, optical frequency conversion devices etc. The doping of thiourea and thiourea metal complex improves the qualities of inorganic material such as KDP, ADP so as to have their wide NLO applications [1-6]. P. Kumaresan et al have reported the effect of copper thiourea complex of KDP on structural, optical and thermal behavior [7].The present investigation reports growth and characterization of Potassium Thiourea Chloride doped KDP crystal.

EXPERIMENTAL DETAILS

The potassium chloride and thiourea of AR grade are mixed together in the molar ratio 4:1in the deionized water to synthesize Tetra Kis Thiourea KCL (TKTKCL). The impurities of the crystal were removed by successive recrystallization. The 0.2 mole% TKTKCL is doped in the saturated solution of KDP. After well stirring solution was filtered by Whatmann no.1 filter paper and kept for slow evaporation. The seed crystals were produced within 7-8 days.

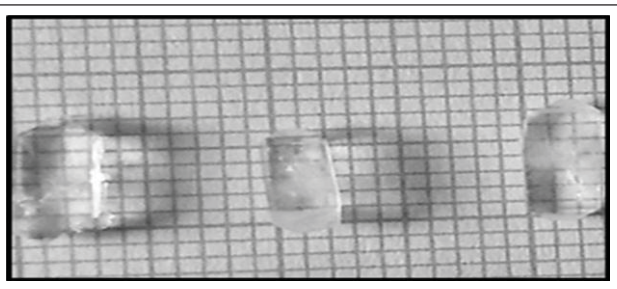

Fig. 1. Photograph of TKTKCL doped KDP crystal

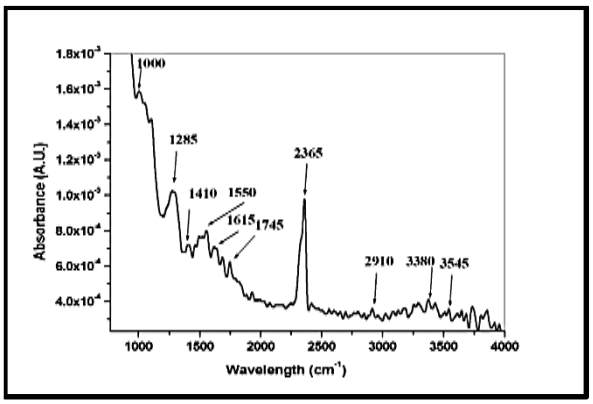

Fig. 2. FTIR spectrum of doped KDP crystal

RESULTS AND DISCUSSION

SINGLE CRYSTAL X-RAY DIFFRACTION ANALYSIS

The single crystal analysis of grown crystal was carried out using Enraf Nonius CAD4-MV31 crystal X-ray diffractometer. The unit cell parameters are a=b= 7.48Å, c = 7.00Å and cell volume is 391 Å^3.The crystal belongs to tetragonal system and determined cell parameters are as shown in table 1. From single crystal X-ray analysis it is confirmed that the dopant does not change the basic structure of the crystal. The slight change in unit cell parameters

confirm the lattice strain on KDP crystal reinforced due to incorporation of dopant TKTKCL.

Table 1 - Single crystal XRD data

Crystal	*Cell parameters(Å)*	*Volume (Å)^3*	*Crystal system*
KDP	a=b= 7.44, c = 6.94	384	Tetragonal
TKTKCL-KDP	a=b= 7.48, c = 7.00	391	Tetragonal

Fourier Transform Infrared Spectroscopy (FT-IR) Analysis

The FT-IR spectra of TKTKCL doped KDP crystal are as shown in Fig.2. The C-Cl symmetric bond stretching vibration is attributed at 1000 cm-1. The N-C-N bond stretching vibration associated with TKTKCL is observed at 1410 cm-1. The C=C and C=O bond stretching vibration is attributed at 1615 and 1745 cm^{-1} respectively. The C=N-OH bond stretching vibration is observed at 1745 cm^{-1}. The P-H stretching vibration is attributed at 2365 cm^{-1}.The absorption observed at 2910 and 3380 cm^{-1} corresponds to C-H stretching. Similarly the absorption observed at 3545 and 3645 cm^{-1} corresponds to O-H stretching [8].

NLO STUDIES

The Kurtz–Perry powder test was performed to determine second harmonic efficiency of grown crystal [9].The 0.2 mole % TKTKCL doped in KDP were subjected to SHG test. The crystalline powder was illuminated by Q switched Nd- YAG laser operating at 1064 nm having input beam energy of 4.7 mJ/pulse, repetition rate of 10 Hz and pulse width of 10 ns. The collected green emission from the powdered sample at the output confirmed the nonlinear behavior of the doped KDP crystals. The measured output signals for pure and doped KDP crystals were 114 mV and 141 mV, respectively. The 0.2 mole % TKTKCL doped in KDP has SHG efficiency 1.25 times higher than that of KDP. Thus grown crystal may be efficient NLO material for applications in Second harmonic generation and electro-optic devices [10].

OPTICAL STUDIES

The Optical transparency of pure and TKTKCL doped KDP single crystal of thickness 2mm is obtained by using Shimadzu UV-2450 spectrophotometer in the range 200 to 900 nm. The recorded transmittance spectrum (Fig. 3) reveals that KDP crystal is optically transparent up to 87% while the increased transmittance of TKTKCL doped KDP crystal is up to 89 % in entire visible region. The high optical transparency of TKTKCL doped KDP crystal is most essential parameter for designing NLO devices[11].The cut off wavelength of the grown crystal was found to be 390 nm with optical band gap 4.15eV.The refractive index is determined by using formula $n=1/T+\sqrt{(1/[T-1])}$ where T is Transmittance and reflectance is calculated in terms of the refractive index as $R = (n-1)^2/(n+1)^2$.The reflectance and refractive index plot is as shown in Fig. 4.It is observed that the refractive index and reflectance of doped crystal is lower in entire visible region. The lower refractive index and reflectance of doped crystal pronounces its potential candidature for calibrating filters, resonators and reflectors which are vital components of photonic devices [12].

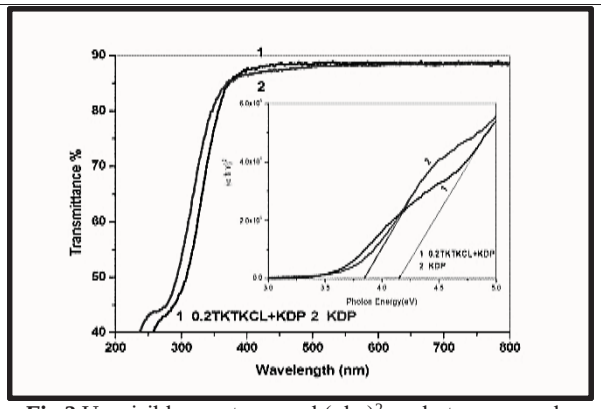

Fig.3.Uv-visible spectrum and $(\alpha h\nu)^2$vs.photon energy hν

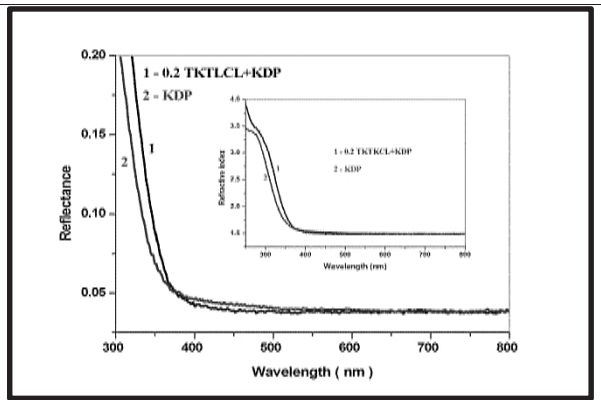

Fig.4. Reflectance and Refractive index vs. wavelength.

CONCLUSIONS

The TKTKCL doped KDP crystals have been grown by slow evaporation method at room temperature. The single crystal XRD confirmed the tetragonal symmetry. The FT-IR analysis established the incorporation of TKTKCL in KDP crystal. The SHG efficiency of doped crystal is enhanced than that of pure KDP. The optical parameters of doped KDP crystal were improved. The optical band gap of grown crystal is found to be 4.15 eV therefore it is concluded

that grown crystal has potential NLO applications for lasers and photonic devices.

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