

High Energy Optical Resistivity Study on Nonlinear Optical Pyrrolidinomethylphthalamide Crystal

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Abstract: PMP crystal shown was synthesized. The PMP single crystal was grown by slow evaporation solution technique. The grown crystals were characterized by powder crystal X-ray diffraction, FTIR spectrum. The crystal structure and unit cell parameters were analyzed from the X-ray diffraction studies. The FTIR spectrum analysis has confirmed the functional group in the PMP crystals. The high energy optical resistivity studies have been carried out on this crystal and the results have been shown here.

Key words: X-ray diffraction, growth from solutions, optical resistivity, PMP, FTIR spectrum crystal

INTRODUCTION

Crystal growth is a frontier area of Science and technology, which plays a major role in the technology of Photonics. The fast developments in the field of optoelectronics and Photonics necessitate the search for New Efficient Nonlinear Optical (NLO) materials which can be utilized for optical computing, optical communications, electro-optic shutters, optical modulations, optical switching, optical logic, frequency shifting and optical data storage for developing technologies in telecommunications, treatment of HIV, signal processing (Kumar *et al.*, 2009). The interesting molecular engineering of these complexes has enabled the crystals growers to develop a new promising class of NLO crystals. The materials combine the high optical nonlinearity and chemical flexibility of organics with physico-chemical raggedness and chemical inertia of inorganics. Nonlinear crystals have proved to be interesting candidates for a number of applications, like Second Harmonic Generation (SHG), frequency mixing, electro optic modulation, optical parametric oscillation, etc. (Senthil *et al.*, 2009). The growth and characterization of Pyrrolidinomethylphthalamide (PMP) crystal was being reported here for the first time, powder X-ray Diffraction (XRD), Fourier Transform Infrared (FT-IR) spectroscopy studies. The high energy optical resistivity study has been carried out results are shown in this study.

MATERIALS AND METHODS

Crystal synthesis: The saturated solution of PMP crystal was shown at room temperature and stirred well to enable

homogenization of the solution. The seed crystals were shown by the slow evaporation method. Good quality seed was chosen and kept suspended into the supersaturated solution. As grown the crystals was subjected to spectral analysis, for the investigation of structural and optical properties. The optical constants were calculated using the theoretical formulae. The structural properties were analyzed using X-ray diffraction data and FTIR spectrum. The high energy optical resistivity study has been carried out results are shown in this study.

RESULTS AND DISCUSSION

XRD analysis: The grown PMP sample was crushed as fine powder for X-ray diffraction studies. The recorded X-ray diffraction pattern for powdered PMP crystal is shown in Fig. 1. The recorded spectrum of the sample was taken at room temperature in a 2θ range of $0-80^\circ$ using $\text{CuK}\alpha 1$ radiation of wavelength 1.54056 \AA . From the diffraction pattern, the d-spacing and hkl values for each diffraction peak in the corresponding spectrum of sample were identified. Using the monoclinic crystallographic equation, the lattice parameter values of PMP were calculated and compared with the shown values from JCPDS. It is confirmed that PMP belongs to monoclinic crystal system, the unit cell parameters were found to be $a = 13.09 \text{ \AA}$, $b = 9.48 \text{ \AA}$, $c = 8.03 \text{ \AA}$ and $V = 952.82(\text{ \AA})^3$, with space group $P21/c$ and $z = 8$.

FTIR analysis: The FTIR spectrum was measured within the $400-4000 \text{ cm}^{-1}$ region using Perkin Elmer FTIR spectrophotometer by Kbr pellet technique. The FTIR

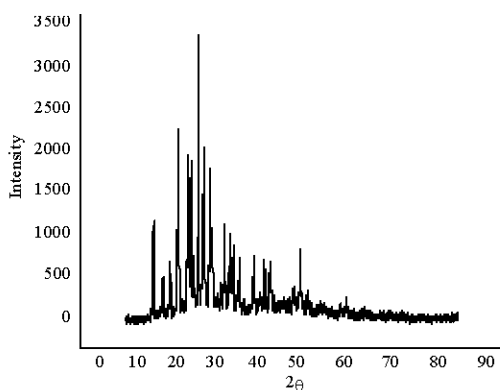


Fig. 1: X-ray diffraction analysis of PMP crystal

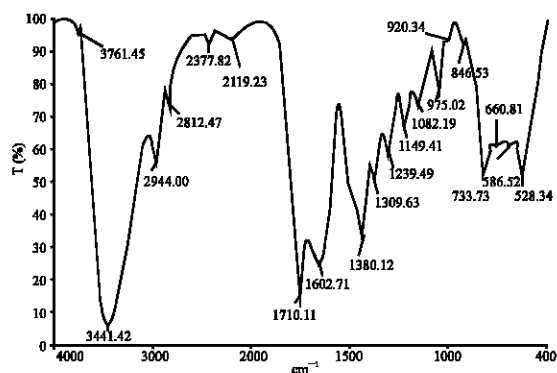


Fig. 2: FTIR analysis of PMP crystal

spectrum of PMP crystal, shown in Fig. 2. In FTIR spectrum of PMP crystal, the N-H stretching vibrational bands of NH₂ was observed at a wave number 3441 cm⁻¹.

The C-N stretching vibrations were observed at wave numbers 1082, 1149 and 1239 cm⁻¹. The in-plane and out-plane vibrations of C-H group are identified at 1082 and 660 cm⁻¹, respectively (Krishnan *et al.*, 2008).

The absorption at 2944 cm⁻¹ is due to stretching vibrations. The sharp intense peak was observed at 1710 cm⁻¹ which is due to the C = O stretching of the benzene ring. The band due to the C = N of PMP crystal was observed as a sharp and intense one at 1602 cm⁻¹ (Arivanandham *et al.*, 2006; Selvaraju *et al.*, 2006).

High energy optical resistivity study: Measurements of high energy optical resistivity (ρ_{opt}) study were carried out in by using the theoretical formula. The variation of log of optical resistivity as a function of Energy (eV) is shown in Fig. 3.

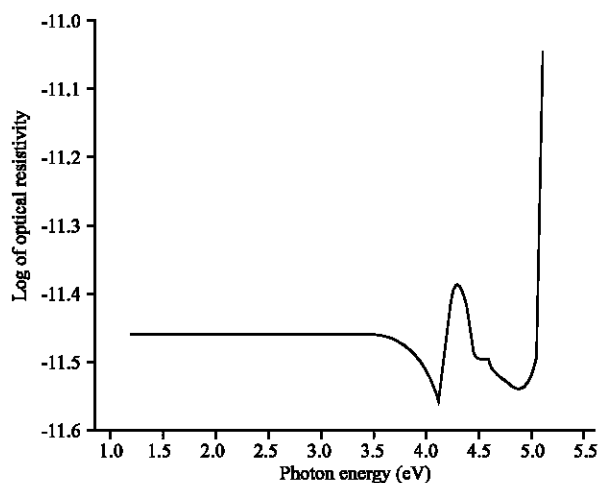


Fig. 3: The log of optical resistivity versus photon energy (eV)

CONCLUSION

Good quality PMP crystal were synthesized and subjected to Powder crystal XRD, FTIR analysis and optical studies. From the X-ray diffraction, it was confirmed that the crystal belongs to monoclinic structure with space group P21/c. FTIR analysis was carried out to confirm the presence of functional groups of the grown crystals.

By tailoring the absorption coefficient and tuning the band gap of the material, achieve the desired material which is suitable for the fabrication of various optoelectric devices because of its wide optical band gap. Those crystals may also be used as a photo luminescent material. The refractive index which is suitable for the fabrication of various photonic devices. The high energy optical resistivity study has been carried out results are shown in this study.

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