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Investigation on Growth, Structural, Optical, Dielectric and Surface Properties of Organic Nonlinear Optical Material: DAPSH

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Abstract: The organic nonlinear optical salt *trans* – 4' – (dimethylamino) – N – phenyl – 4 – stilbazolium hexafluorophosphate (DAPSH) was synthesized and single crystals of DAPSH were grown by slow evaporation method using acetonitrile as solvent. The structure of the crystal was studied using single crystal X - ray diffraction. FTIR analysis were carried out to confirm the functional groups present in the crystal. From UV – vis –NIR studies, the crystal was found to be transparent in the region 400 -1100 nm. Dielectric constant and dielectric loss of DAPSH were measured in the frequency range from 50 Hz – 5 MHz at different temperatures. The surface features of the DAPSH crystal were analyzed by scanning electron microscope.
Keywords: DAPSH, THz, SEM

Introduction

Recently organic NLO material has drawn the attention of researchers due to its enhanced properties and applications [1-3]. Numerous investigations have been carried out on organic THz materials because of their high SHG (Second harmonic Generation) efficiency which make them a potential candidate for device fabrication [4]. Terahertz (THz) electromagnetic waves have been expected to be utilized in various practical applications in nondestructive imaging, see-through analysis, non-invasive inspection and so on. A second order nonlinear optical (NLO) process can effectively generate THz waves. Organic ionic single crystals with high second order optical nonlinearities have attracted a lot of attention because of their potential for THz generation. Though DAST is a well-known THz generating material, it shows some absorption peaks in its THz spectrum and growing good quality and prominent sized crystal is challenging one. In order to overcome these drawbacks, search for new derivatives of DAST crystal has become an area of interest. In this paper a DAST derivative crystal *trans* – 4' – (dimethylamino) – N – phenyl – 4 – stilbazolium hexafluorophosphate has been synthesized and the characterization analysis were done for the first time.

Synthesis and Growth

DAPSH was synthesized using Dean –Stark apparatus. The synthesis process was carried by the base-catalyzed condensation of N-Phenyl -4-Picolinium chloride(which was prepared from the starting material of 4-picoline , chloro-2,4-Dimethylbenzene and aniline) with 4-N-N-dimethylamino benzaldehyde and the product was metathesised to the *trans* – 4' – (dimethylamino) – N – phenyl – 4 – stilbazoliumhexafluorophosphate (DAPSH) by precipitation from aqueous NH_4PF_6 [5]. Fig.1 shows the as-grown crystal of DAPSH with dimensions $23 \times 2 \times 1$ mm^3.

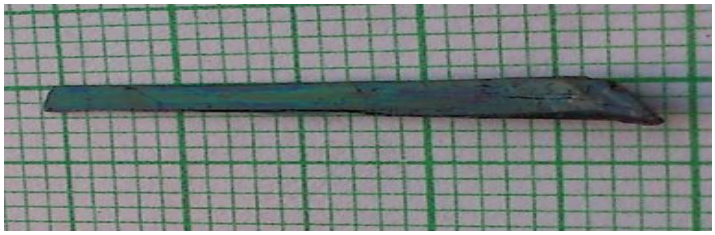

Fig. 1 As-grown crystal DAPSH

Result and discussion

1. Single crystal XRD.

The crystalline compound DAPSH grown by slow evaporation method belongs to monoclinic structure with space group Cc. The cell parameters and interfacial angles are: a =19.4 Å, b = 10.7Å, c = 11.9Å, β = 125.86° and V = 2026.9 $Å^3$. The XRD data are in good agreement with earlier reported data [5].

2. FTIR Spectral analysis

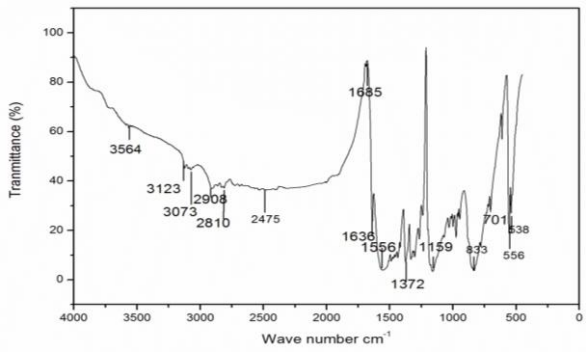

Fig. 2 FTIR spectrum of DAPSH

The FT-IR spectrum was recorded in the wavelength range 450-400 cm^{-1}. FTIR spectrum of DAPSH single crystal is shown in Fig. 2. The peak at 3073 cm^{-1} is assigned to the aromatic C-H stretch. The alkene bond stretching vibrations in conjugated systems without a center of symmetry interact to produce C=C stretching bonds near 1556 cm^{-1} and 1636 cm^{-1}. The peak at 1372 cm^{-1} corresponds to CH_2 bending. The peak at 1159 cm^{-1} corresponds to C-N stretching mode.

3. UV-vis-NIR spectrum

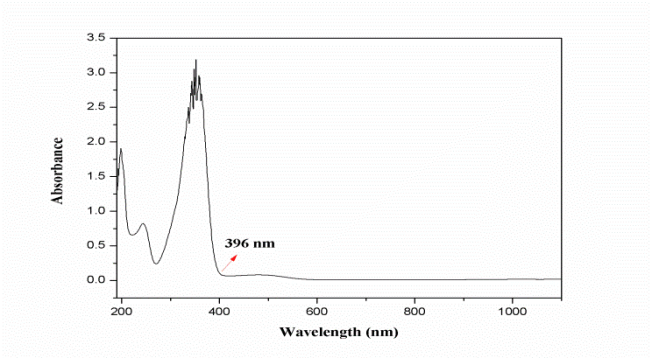

Fig. 3 UV-vis-NIR spectrum of DAPSH

The absorbance spectrum of DAPSH crystal was recorded in the range 190 nm-1200 nm. The lower cut of region of the crystal DAPSH lies around 396 nm. The crystal has high transparency in the vis-NIR region. There is no absorption in the range 400 nm – 1100 nm which can be further exploited for second order harmonic generation as well third order harmonic generation.

4. SEM

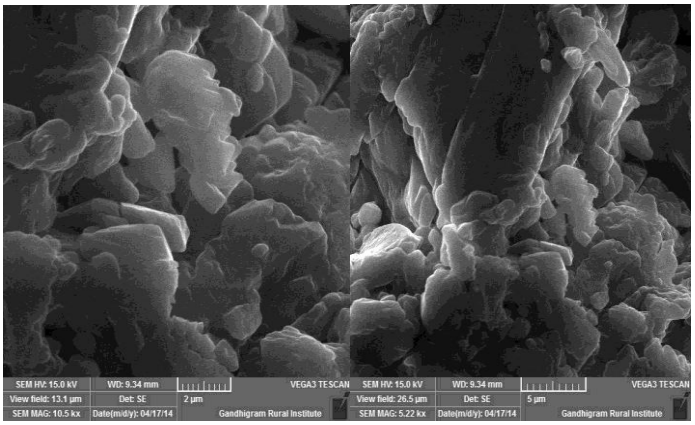

Fig. 4 (a) & (b) SEM photographs of DAPSH crystal

Figs. 4(a) and (b) show SEM images with two different resolutions. Highly transparent region was chosen for the analysis. 2 μm resolution exhibits waxy like smooth surface with grain boundaries. Lower resolution shows inclusions of smooth inter-grown microcrystals on to the surface with no pits.

5. Dielectric studies

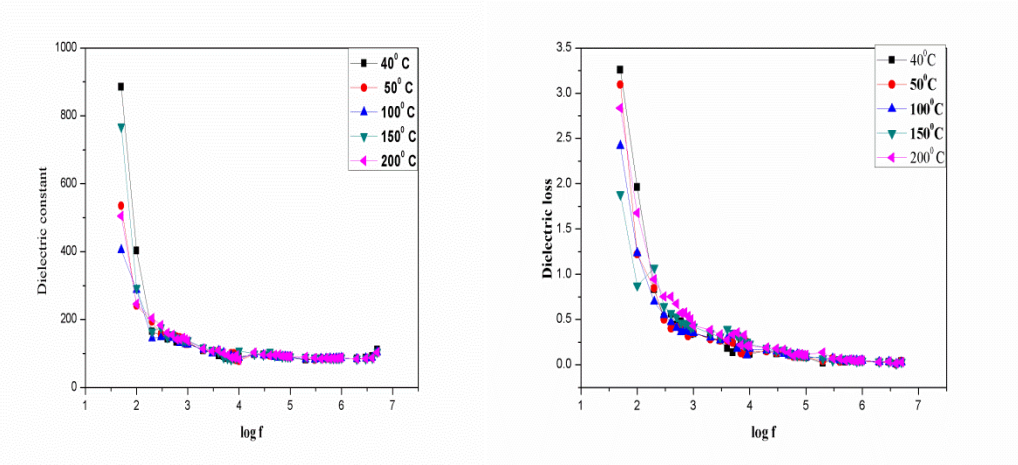

Fig. 5(a) & (b) frequency dependence of dielectric constant and loss of DAPSH

The different polarization mechanisms in solids can be well understood by the dielectric constant. Fig. 4(a) shows the variation of dielectric constant with frequency of the terahertz material DAPSH. The dielectric constant was calculated using the relation,

$$\varepsilon_r = \frac{Ct}{\varepsilon o A}$$

With increasing frequency the dielectric constant decreases. The high values of dielectric constant at low frequency are due to presence of all four types of polarization. The low value of dielectric loss in Fig. 4(b) suggests that the material possess high optical quality with minimum defects.

Conclusion

Lattice parameter and crystal system were confirmed using single crystal X-Ray diffraction analysis. The optical absorption spectrum was analyzed using UV-vis-NIR spectral studies. Various functional groups present in the DAPSH crystal were confirmed using FTIR spectral analysis. SEM micrographs show waxy nature. Dielectric loss and dielectric constant were calculated using dielectric studies. The low dielectric constant at high frequency region suggests the suitability of the material for photonics and electro-optic applications.

Acknowledgement

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