Growth and study of dielectric behavior of organic single crystal: Furfurylaminium 2-chloro-5-nitrobenzoate

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Abstract. Fine quality organic crystals of Furfurylaminium 2-chloro-5-nitrobenzoate (FC) have been favorably utilizing slow evaporation technique. The cell parameter was measured by powder XRD method and the crystallographic data were found to be a=11.77 ´, b = 6.84 ´, c = 16.33 ´ and $\alpha = \gamma = 90^{\circ}$, $\beta = 91.12^{\circ}$ and certifies the crystal system as Monoclinic. The dependence of dielectric constant as well as dielectric loss of FC crystal on temperature has been examined within the range of 50-80 °C. The dielectric properties show the normal behavior and the enhanced quality of the material gives the low dielectric loss.

INTRODUCTION

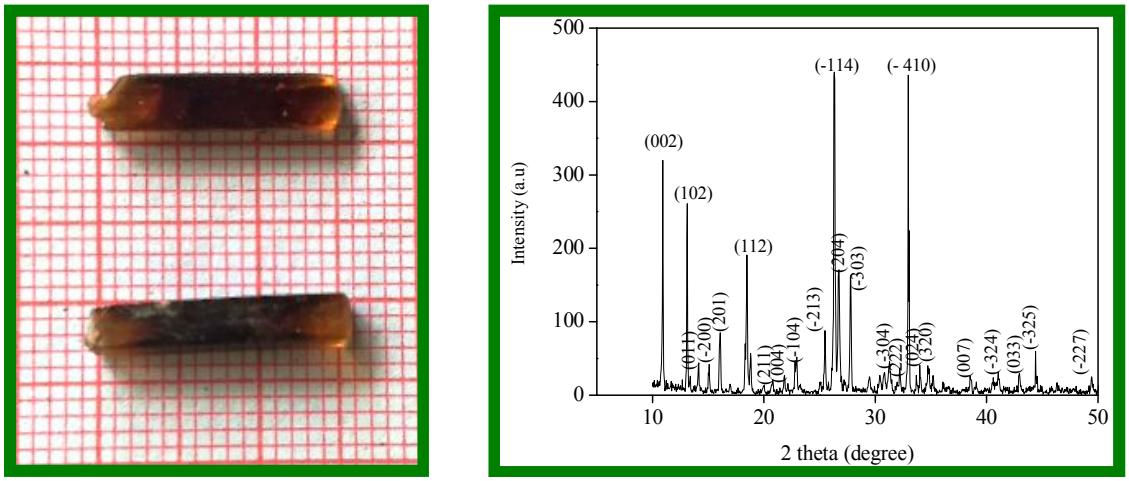
In contemporary years reasonable attention is being dedicated to the materials that have unique NLO, piezoelectric as well as pyroelectric properties. The discovery of different types of nonlinear materials and their applications in enormous area of science made research more advanced in developing our technology. Growth of NLO crystals are increasing interest due to its rapid advances in various technological applications. Advanced NLO functional materials have been used in Laser technology, Fibre optics, Optical communication, frequency conversion, optical data storage, frequency mixing and optical parametric oscillations [1-5]. Organic materials are appealing because of their nonlinearities, ultra fast response and high laser damage threshold [6-7]. The 2-chloro-5-nitrobenzoic acid is a simple organic compound which can be used as a chemical building block. Furfurylamine is an amine and a of fusion of furfural. Furfurylamine is yellow color liquous with an ammonia odor. It is an intermediary in the manufacturing many pharmaceutical, industrial chemicals and agricultural products. It is admired to have unique characteristics in engine cleaning formulations. Supramolecular assemblies, observed in micelles, liposomes and many biological membranes act as ion channels for nano scale objects. The hydrogen bonding tune the intermolecular spaces in the self assemblies of supramolecules creating appropriate medium for ion transfer [8]. Self assemblies of 2-chloro-5-nitro benzoic acid with various organic bases containing nitro, amino groups pave way for supramolecular helical structures [9]. The title compound, Furfurylaminium 2-chloro-5-nitrobenzoate (FC) exhibits interesting supramolecular features with active non-covalent interactions of nitro and carboxyl groups and the π electron cloud. In the present study, we report the thermal and laser damage threshold studies of furfurylaminium 2-chloro-5- nitrobenzoate single crystals.

MATERIALS AND METHODS

Synthesis and Growth of single crystals

Furfurylaminium 2-chloro-5-nitrobenzoate (FC) is obtained by mixing an aqueous solution of commercially available furfurylamine (Merck) and 2-chloro-5-nitrobenzoic acid (SRL) in 1:1 ratio. The resulting material was stirred well about 5 h at room temperature. The prepared homogeneous solution was carefully filtered off in an

experimental beaker without any impurities and kept in a dust free chamber for slow evaporation at room temperature. After a few weeks, a good transparent crystal with a cell volume of 15 x 4 x 3 mm^3 was harvested from the mother solution. The grown crystal of FC is shown in the Fig.1 (a).



(a) (b

FIGURE 1. (a)As-grown FC crystal and (b) Powder X-Ray Diffraction pattern of FC

RESULTS AND DISCUSSION

Powder X-Ray Diffraction

The X-ray powder diffraction (XRD) study was carried out to demonstrate the crystallinity of title compound crystal. Observed prominent peaks confirm the crystalline nature of the grown FC crystal. It was also confirmed that the grown FC crystal belongs to the monoclinic crystal system and unit cell parameters were found to be a=11.77± 0.012 ˚, b = 6.84 ± 0.012 ˚, c = 16.33 ± 0.028 ˚ and α= γ =90°, β=91.12° with space group P21/c. The powder XRD with well-indexed reflection peaks are shown in Fig.1 (b).

Dielectric Study

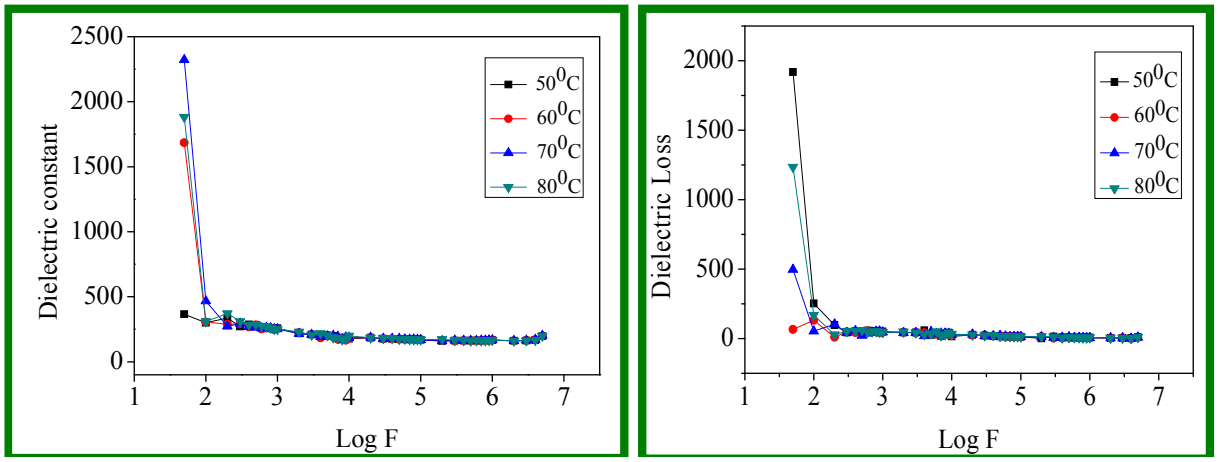
The study of dielectric measurement of FC was carried out to find out the activity of charges in FC crystal on reaction with external electric field applied. Thus makes to understand the nature of various atoms present in the molecule as well as their bonding can be studied. The dielectric measurement was applied using LCR meter in a frequency range 50Hz-5MHz. Silver paste was applied over the cut and polished FC sample and placed in the cell which is connected with a thermocouple. Dielectric constant can be related to dimensions (thickness & area of the sample) and capacitance of the sample (C):

$$\varepsilon' = \frac{Ct}{\varepsilon_0 A} \quad (1)$$

$$\frac{\varepsilon''}{\varepsilon'} = \tan\delta \quad (2)$$

where ε_o is the permittivity of free space. Fig. 2(a) shows that the dielectric constant displays large dispersion at low frequencies while almost constant at high frequencies which is the normal behavior. The dielectric permittivity will be originated from electronic, ionic, orientation and space polarization mechanisms within the material. The high ε' at low frequencies is due the fact that the charge accumulation will follow the applied electric field while the lagging of dipoles with electrical field tends decrease ε' with frequency. Moreover, dielectric constant attains a near constant value due to the disappearance of space charge polarization. The observed low value of dielectric constant

establishes that the as-grown crystal has potential for microwave applications. Similarly, dielectric loss behavior is same as dielectric constant which denotes high value at low frequency region (Fig.2 (b)) which attributes to oscillation of dipoles. The low value of dielectric loss shows the grown crystals are of quality crystals. Thus photonic, electro-optic and NLO devices need this type of good quality crystals [10].



(a) **(b)**

FIGURE 2. (a) Plot between dielectric constant and log frequency (b) Plot between dielectric loss and log frequency

CONCLUSION

The exposed title paper communicates about the grown FC crystal using slow evaporation method. The crystallographic data were calculated using PXRD analysis. The low dielectric permittivity and the low dielectric loss enhance the optical quality of the material with lesser imperfections.

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