Optical Materials 57 (2016) 163–168

Contents lists available at ScienceDirect

Optical Materials

journal homepage: www.elsevier.com/locate/optmat

Studies on crystal growth and physical properties of 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline single crystal

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ARTICLE INFO

Article history:
Received 2 February 2016
Received in revised form
30 March 2016
Accepted 18 April 2016
Available online 7 May 2016

Keywords:
Organic compounds
Crystal growth
Differential thermal analysis (DTA)
Optical properties

ABSTRACT

The organic material 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline has been grown by slow evaporation technique. Single crystal and Powder X-ray diffraction studies have been carried out to conform the grown crystal. FTIR and FT-Raman spectra were recorded to identify the functional groups present in the crystal. The optical property of the grown crystal was analysed by UV–Vis–NIR measurement. The thermal property of the grown crystal was analysed by thermogravimetric (TG) and differential thermal analyses (DTA). Thermal diffusivity of the grown crystal was analysed by Photo acoustic spectroscopic (PAS) studies. The third order nonlinear optical properties of 4-(dimethylamino) benzaldehyde-2,4-dinitroaniline was measured by the Z-scan technique using 532 nm diode pumped continuous wave (CW) Nd:YAG laser. The mechanical property of the grown crystal was analysed by using microhardness studies.

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1. Introduction

The growth of nonlinear optical (NLO) materials has received a great deal of attention in developing commercial applications in the fields of optical communication, signal processing, sensing, optical information storage, optical logic gates, laser radiation protection, and locked laser mode [1–3]. Organic molecules that possess nonlinear optical properties have emerged as interesting construction blocks for a new generation of photonic applications [4–7]. The important goal for designing the molecules with large third order nonlinearities is to incorporate them into devices used in the optical signals processing [8,9]. Search for new materials with high optical nonlinearities has been the important task because of their practical application in harmonics generation, amplitude and phase modulation, switching and other signal processing devices [10,11]. The third order response governed by the second hyperpolarizability offers more varied and richer behaviour than the second-order NLO process due to the higher dimensionality of the frequency space [12]. In the light of wide applications of NLO effects, a large number of materials have been synthesized and their NLO properties have been explored using Z-scan and third-harmonic generation (THG). THG measurements are particularly interesting since they are strongly related to electronic processes [13]. In both molecules, the aldehyde and dimethylamino groups are essentially coplanar with the attached benzene ring [14]. Intermolecular hydrogen bonds are an effective tool for organizing organic molecules, very well typified by nitroaniline compounds, which associate via intermolecular H-bonds between the amino and nitro groups [15]. In the present study organic material 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline single crystals have been successfully grown by slow evaporation technique using acetone as a solvent. The grown crystal were characterized by single crystal X-ray diffraction, powder XRD, FTIR, FT-Raman, UV–Vis–NIR, TG/DTA, Photo acoustic spectroscopic (PAS) studies, third order nonlinear optic studies and microhardness measurements.

2. Experimental

The organic material 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline was successfully synthesized using commercially

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http://dx.doi.org/10.1016/j.optmat.2016.04.030
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available AR grade 4-dimethylaminobenzaldehyde and 2,4-dinitroaniline substances in the equimolar ratio (1:1). The synthesized material was dissolved in acetone as solvent. The solubility curve of 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline at different temperatures range from 30 °C to 55 °C is shown in Fig. 1. The solubility curve increases linearly with increase in temperature. For the crystal growth the solvent was allowed to evaporate slowly at room temperature. The solution was closed using a finely perforated polyethylene sheet. The synthesized material was further purified by repeated recrystallization process. Transparent optical quality single crystals were harvested within few days. The photograph of the grown 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline single crystal is shown in Fig. 2.

3. Result and discussion

3.1. Single crystal XRD analysis

The 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline single crystal were estimated using BRUKER ENRAF NONIUS CAD4 MV31 single crystal X-ray diffractometer with MoKα (λ = 0.717073 Å) radiation to identify the structure and to estimate the lattice parameter values. Suitable size single crystal was selected for the X-ray diffraction analysis. The obtained lattice parameters are shown in Table 1. The single crystal XRD result shows that the grown crystal belongs to monoclinic crystal system and the centrosymmetric space group $P2_1/n$. The observed unit cell parameters have good agreement with the reported values [16].

3.2. Powder XRD analysis

Powder X-ray diffraction pattern were recorded using powder X-ray diffractometer with CuKα_1 radiation (λ = 1.54060 Å). The powdered sample was scanned in the range from 10 to 70°. The powder X-ray diffraction pattern of the grown 4-(dimethylamino) benzaldehyde-2,4-dinitroaniline crystal is shown in Fig. 3. The observed (h k l) values are indexed using the homely designed two theta software [17,18]. The well defined sharp Bragg's peaks observed at specific 2θ angles show the high crystallinity of the grown crystal.

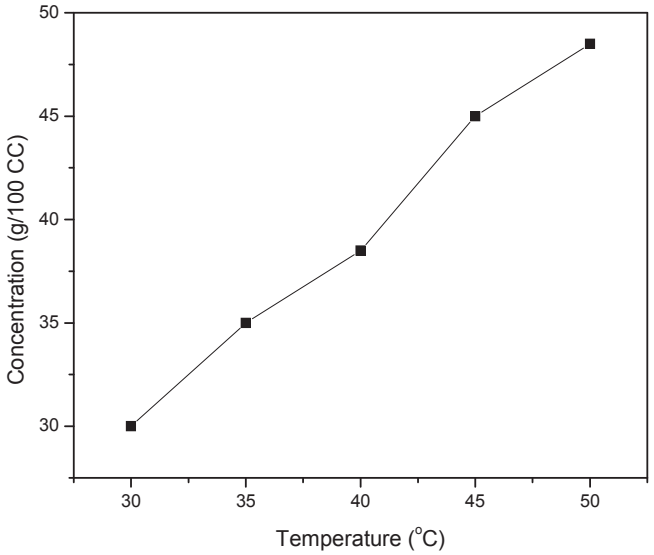

Fig. 1. Solubility curve of 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline.

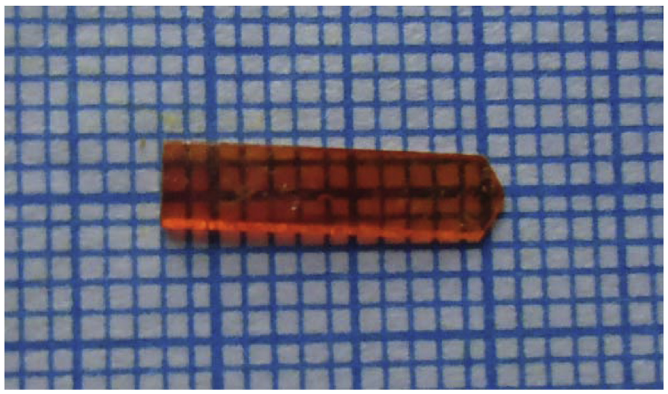

Fig. 2. Photograph of 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline single crystal.

Table 1
Single crystal XRD data for grown 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline.

Parameter	Literature [16]	Present study
a (Å)	18.7512 (18)	18.73
b (Å)	7.3182 (6)	7.32
c (Å)	24.338 (2)	24.38
α (°)	90	90
β (°)	109.493	109.52
γ (°)	90	90
Volume Å^3	3148.4 (5)	3151
System	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$

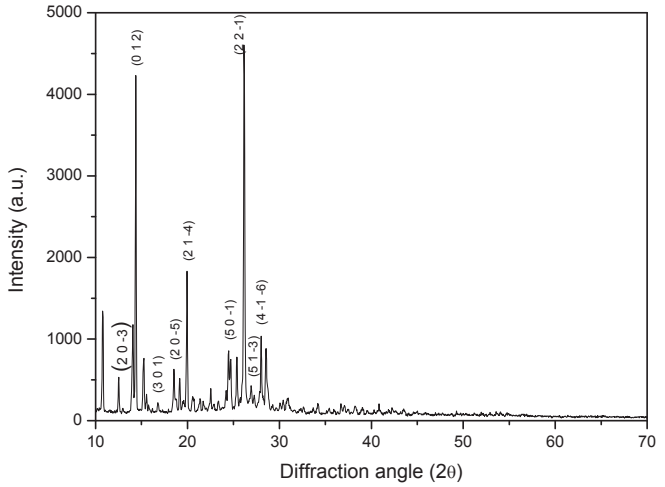

Fig. 3. Powder X-ray diffraction pattern of 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline.

3.3. FTIR and FT-Raman spectral analyses

The functional groups of the grown 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline single crystal were analysed using FTIR and FT-Raman spectral analyses. FTIR was recorded using Perkin–Elmer spectrophotometer using the KBr pellet technique in the frequency range 4000–400 cm^{-1}. The FTIR spectrum of 4-(dimethylamino)benzaldehyde-2,4-dinitroaniline crystal is shown in Fig. 4. The FT-Raman spectrum was recorded by using BRUKER-RFS 27 FT-Raman spectrometer in the range 3500–50 cm^{-1}. The FT-Raman spectrum of 4-(dimethylamino)benzaldehyde-2,4-

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