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Research Article

Optical, thermal, mechanical and dielectric studies of L Alaine Potassium iodide single crystal by conventional solution growthtechnique

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ABSTRACT

L Alaine Pottassium (AL) single crystal was successfully grown using slow evaporation solution growth technique.The lattice parameter and crystal system was identified grown crystal from the powder X-ray diffraction (PXRD) measurement. The absorbance optical transmittance and optical band gap of grown crystal were identified using UV-Vis-NIR studies and the cut off wavelength is 234 nm. The optical band gap of the crystal was calculated, and it is 4.8ev. The dielectric constant and dielectric loss was measured in the room temperature for grown AL single crystal. Vickers microhardness investigationwas done to recognize the mechanical stability of the grown crystal.Fluorescence was analysis and it is possesses the blue emission the grown crystal.

Key words: Single crystal; UV-Vis-NIR: Microharness; Dielectric;

1. Introduction

Most recently, the second and third order non-linear optical materials enticing the attention of many researchers due to its prime usage in the field of storage technology, optical switching, image reconstruction, holography recording etc. [1–3]. Organic single crystals possess various significant features which includes high optical quality, superior orientation, high packing densities, and larger photochemical stabilities [4, 5]. The organic non-linear optical materials (NLO) retain several superior properties like small dielectric constant, large electro-optic (EO) coefficient and short-response time [6], which attracts the attention of many researchers when compared to inorganic optical materials. However at the same time the majority NLO materials have poor mechanical and thermal properties, and it is exposing the damage during the crystal processing. The researcher to avoid this draw back another kind of NLO materials has been developed from organic- inorganic combination. These semi organic materials having more optical stability, optical nonlinearity of a organic compound with the mechanical and thermal properties of inorganic materials [7]. Amino acids have pulled in a wide enthusiasm of the scientists, since all the mixes in the class comprise of an optically dynamic property. Consequently, amino acids have extraordinary physical properties which make them an perfect contender for their NLO applications [8] the L Alaine single crystal having great deal with photo induced nonlinear optical effects and dispersion of the linear and

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nonlinear optical susceptibilities [9]. In this present investigation we have reported the dielectric, UV-Vis- NIR, Powder X-RD, TG-DTA and Hardness studies.

2. Growth

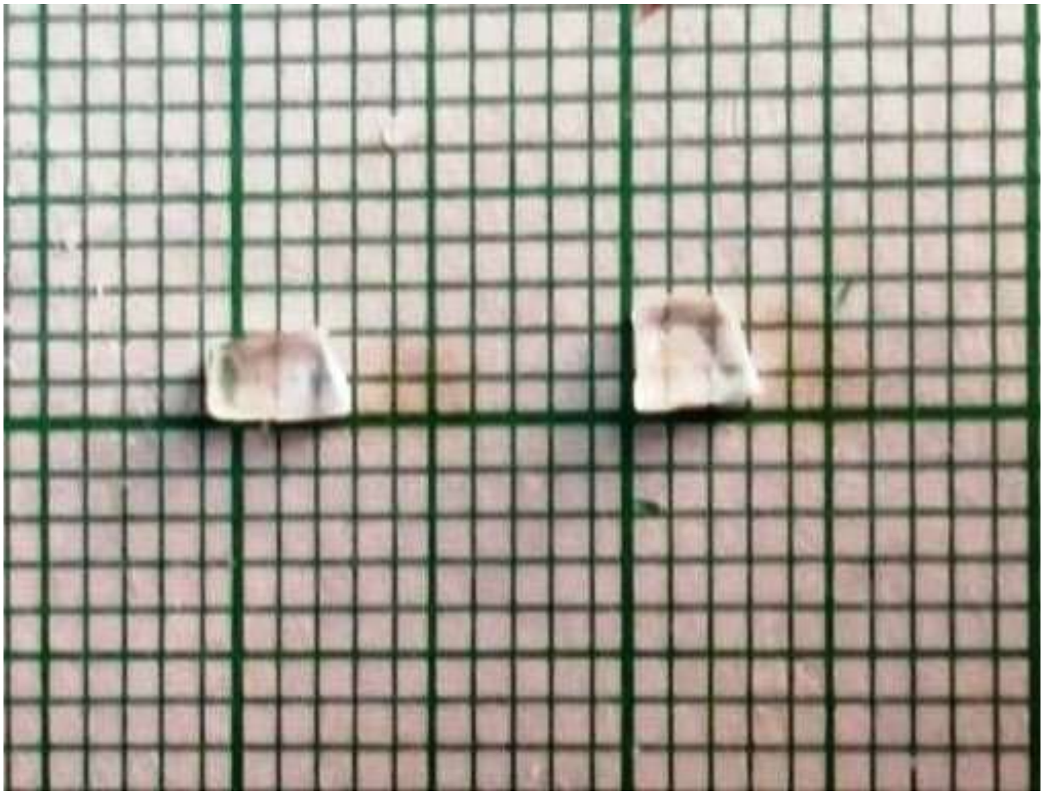

Fig 1. As grown AL single crystal

The AL single crystal was developed by slow evaporation technique using the water as the solvent. The virtue of materials is significant on the grounds that even a modest quantity of pollutions can goes about as undesired added substances repressing specific intermolecular communications and the high optical quality single gems with low imperfection thickness are for the most part dependant on the immaculateness of beginning materials.Initiallythe AL crystal added water and stirred 2 hour after that added with potassium iodide. The solution was then stirred well for 5h to attain homogeneity and filtered using Whatman No. 45 filter paper. The filtrate was collected in a beaker and optimally closed by using a thin perforated plastic paper to control the evaporation of solvent. The nucleation and growth process of ALwas monitored 30 days frequently. Single crystals of AL were found to be grown in 40 days. The as-grown crystals of AL are shown in Fig. 1.

3. Results and discussions

3.1 XRD analysis

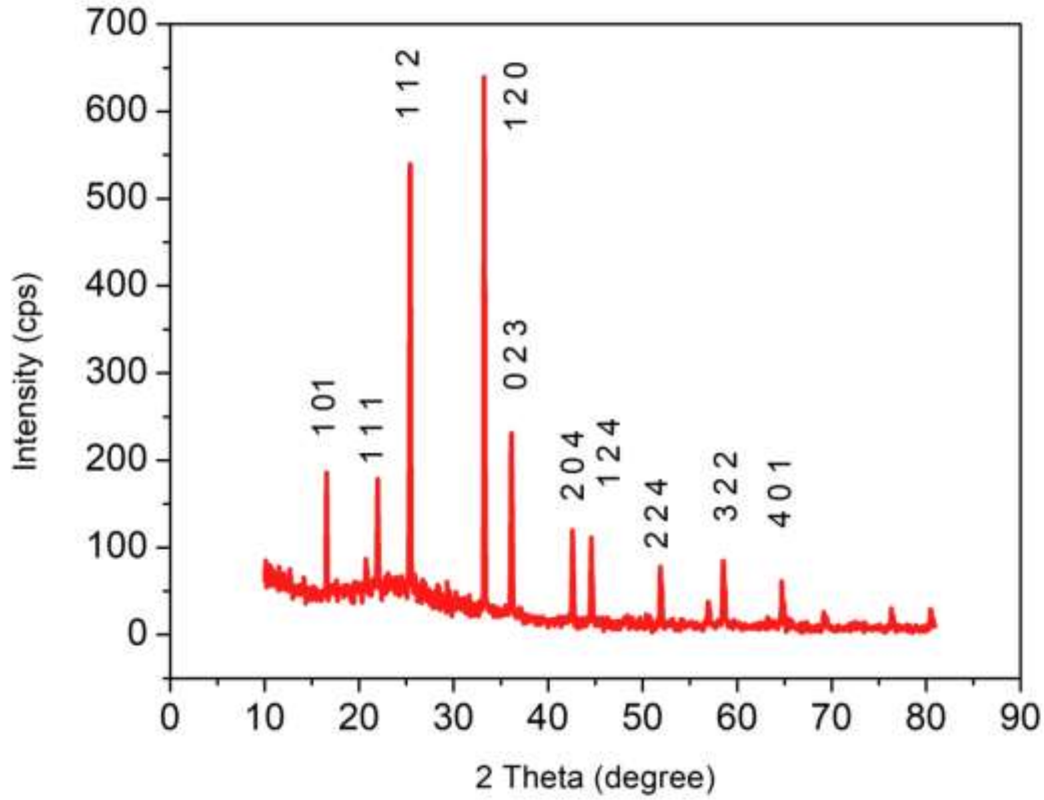

Fig 2. Powder X-rd diffraction

Single crystal and powder XRD examination were done on the grown AL single crystal. AL crystal systemunder in monoclinic. The unit cell boundaries are a = 5.788å, b = 6.030 å, c = 12.325å and α=β= γ =90˚. The lattice parameterare in acceptable concurrence with the reported value [10]. Powder XRD study was completed to show the crystalline of the developed AL crystal. The developed single crystal was finely crushed into the powder and utilized for the investigation. The X-beam powder information were gathered utilizing X-Ray Diffract meter (X'Pert Pro PAnalytic diffractometer) with the Cu Ka radiation (k = 1.5418 Å). The powder XRD pattern of AL is appeared in Fig. 2.

Table. 1. Unit cell parameters of AL single crystal

3.2 UV-Vis-NIR analysis

The optical transmittance and lower UV cut off frequency plays a significant job in recognizing the capability of NLO materials [11]. The optical transmittance spectrum of grown

Lattice parameters	Single crystal XRD	Reported [10]
a (Å)	5.788	5.790
b (Å)	6.030	6.386
c (Å)	12.325	12.157
Crystal system	Monoclinic	Monoclinic
Space group		

crystal is usingPerkin Elemer Lambda 35. The Uv-vis transmittance spectrum was recorded in the range of 100-1200 nm and it is shown in Fig 3. Analysis is made between 190 and 1100 nm, which covers near – ultraviolet (200 – 400 nm), visible (400–800 nm) and then far-infrared(800–1200 nm) regions.The lower cutoff wavelength is found to be 234 nm from transmittance spectrum. The AL crystal has more transmittance in the entire visible region. A cut and well polished 1mm crystal was used in the measurement. The increasing the transmittance may be crystal surface policing.

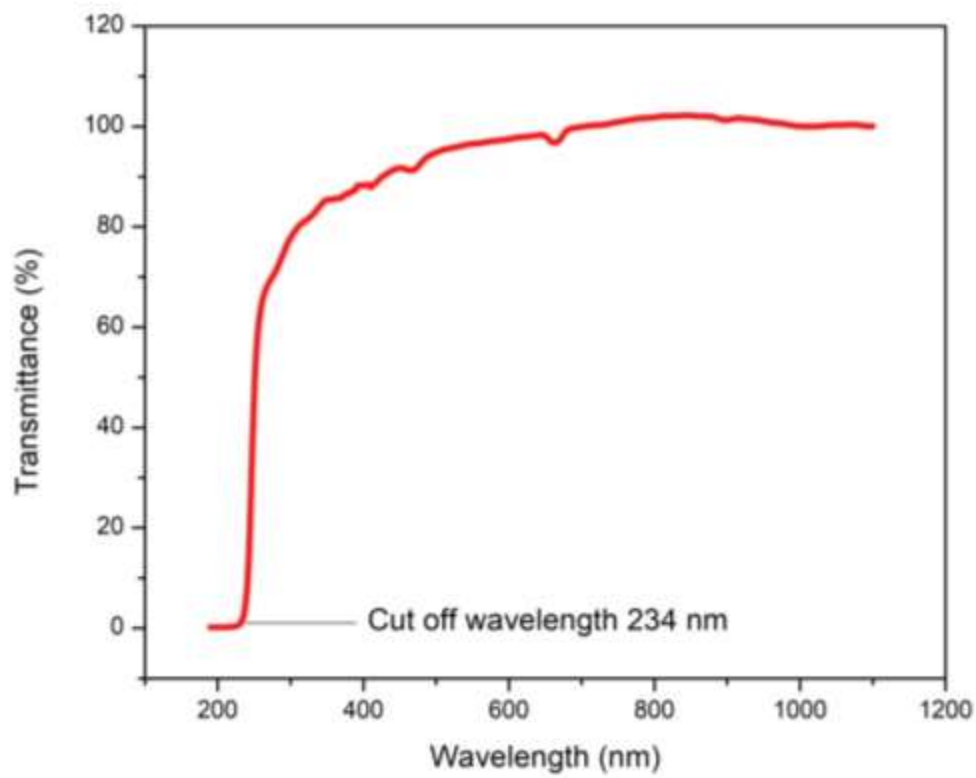

Fig. 3.Transmittance spectrum of AL

The optical absorption coefficient has derived using the relation;

$\alpha = 2.3026(1/t)/t$

Where T is the transmittance and t is the thickness of the crystal. The grown crystal has shown more transparency properties in the visible region, which is suitable material for opto electronic applications. [12]

The optical band gap (Eg) has computed from the transmission spectra and the optical absorption coefficient (a) in close proximity to the absorption edge is specified by

$H\nu\alpha = A(h\nu - Eg)1/2$

Where A is a constant, Eg is the optical band gap, h is the Planck's constant, and v is the frequency of the incident photons. The optical band gap has calculated and plotted in the Fig.4. The band gap energy of AL crystal is 4.8 eV. The variation of the refractive index of AL single crystal with respect to the photon energy is shown in Fig.5. The refractive index of the AL single crystal of optical band gap is 2.33.

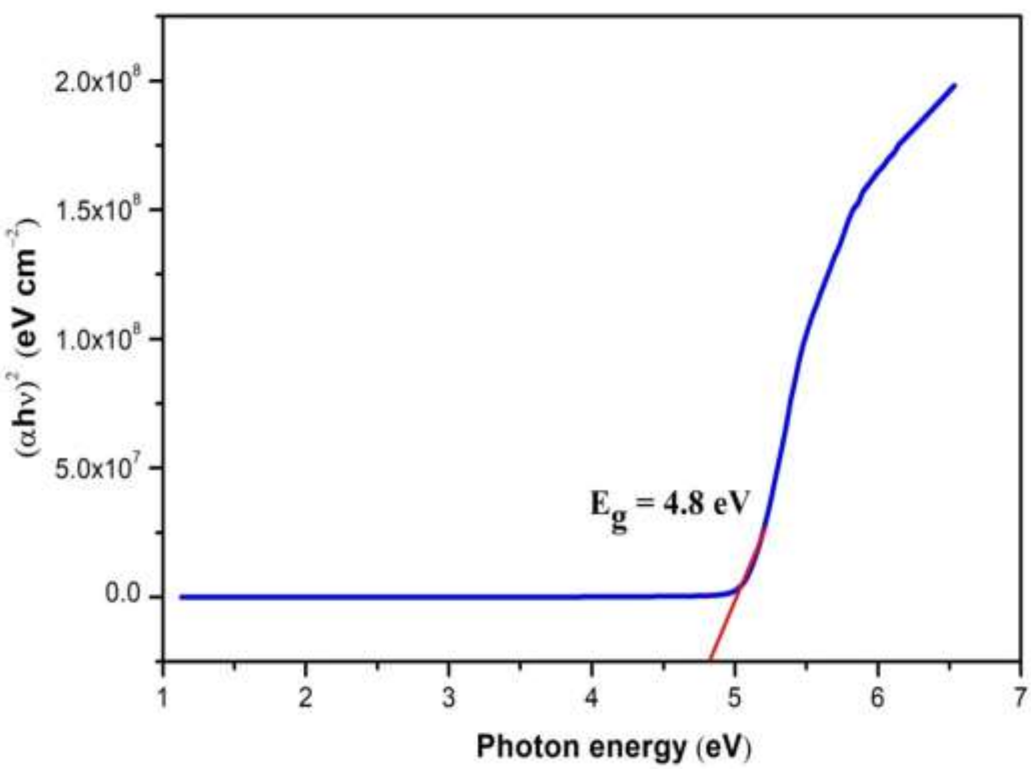

Fig.4. Plot of ht vs. ***(αhν)*****^{½}**

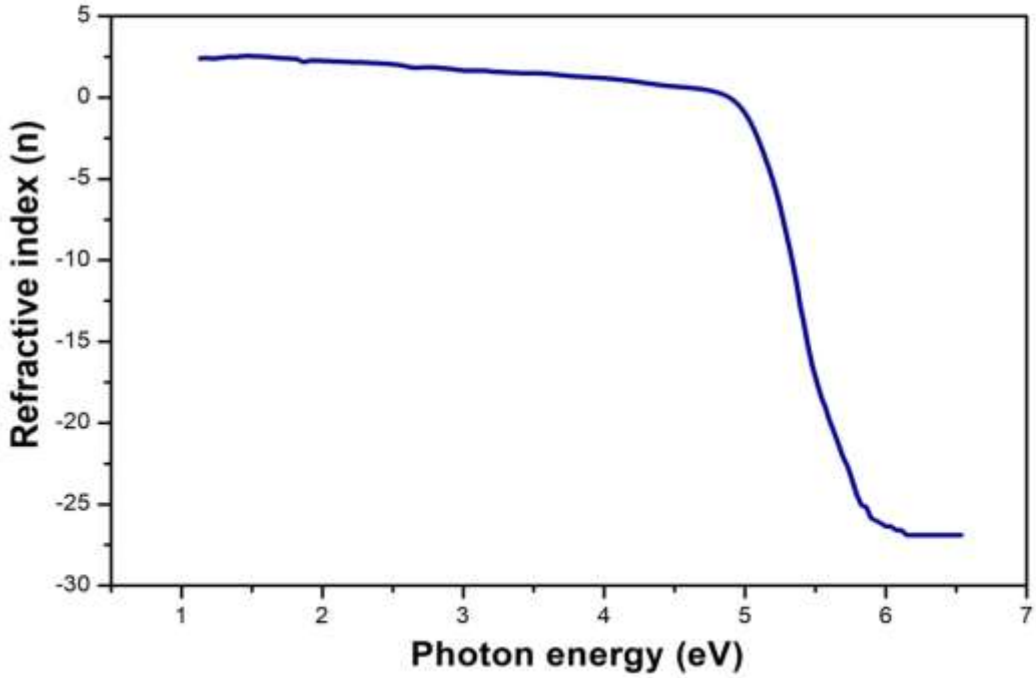

Fig. 5.Refractive index spectrum of AL

3.3 Vickers Microhardness Test

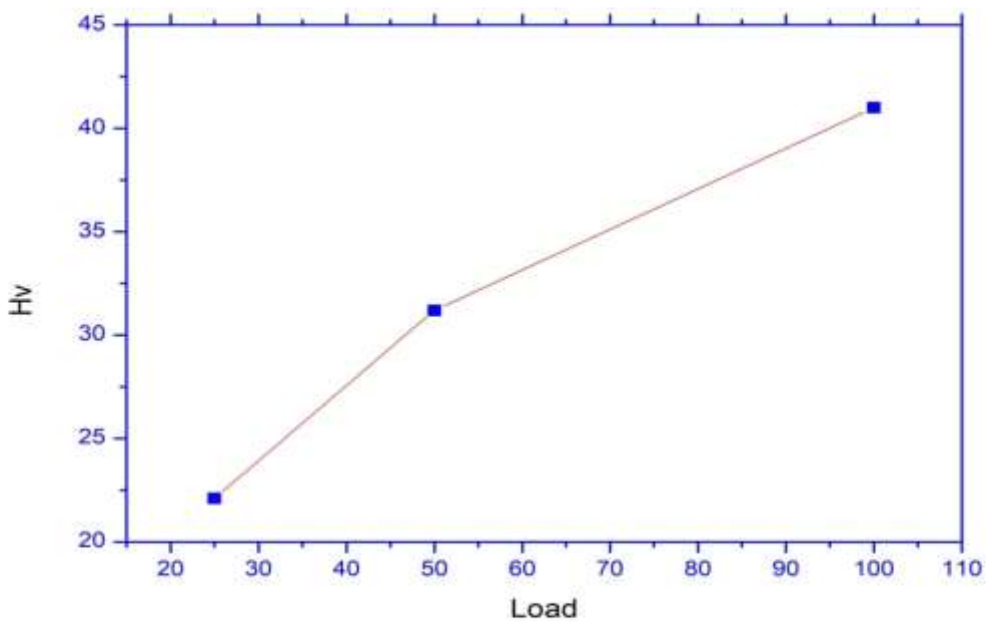

Fig.6. Plot of Load vs. *Hv*

Microhardness testing is one of the best techniques to comprehend the mechanical properties of materials, such as fracture behaviour, yield strength, brittleness index and temperature of cracking [13]. The crack free crystal was selected to analysis for microhardess measurements.

The mechanical property, the Vickers microhardness studies were carried out on the grown AL crystals. 1 mm thick plate of AL crystal was used. Vickers microhardness indentationswere made on the as grown surface of the grown AL crystal with the load ranging from 25 g to 100 g for a dwell period of 10s using Shimadzu HMV-2T Vickers microhardness tester.
$H_v = 1.8544\ P/d^2$

Where, P is the applied load in kg and d is the diagonal length of indentation impression in mm and 1.854 is a constant of a geometrical factor for the diamond pyramid. The crack was observed in the crystal beyond the 100g. Fig 6 shownthe HV vs Load with various load 25g to 100g. The various loads it is showing Reverse indentation size effect (RISE) in the crystal.

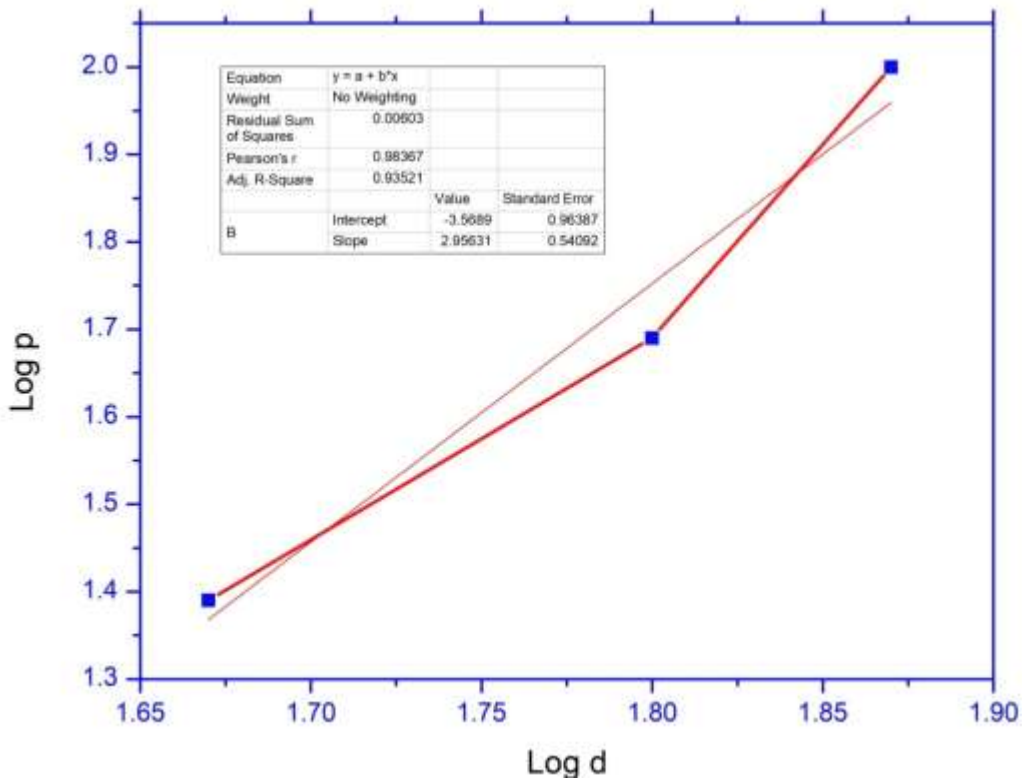

Fig.7. Log D vs. Log P

The relation connecting the appliedload “P” and diagonal length “d” of the indenter is given by Meyer’slaw [14]
$P = ad^n$,
where ‘n’ is the Meyer’s index or work hardening coefficient. According to Onitsch[15] and Hannemann [16] should lie between 1 and 1.6 for harder materials and above 1.6 for softer materials. The value of AL single crystal is 2.9 and it is belongs to the soft material category.

Fig 7 shown the Log D vs. Log P.

Stiffness is a measure of the resistance offered by an elastic body to deformation.Theelastic stiffness constant (C_{11}) for different loads are calculated using Wooster's empirical formula [17].

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$C_{11} = H_v^{7/4}$

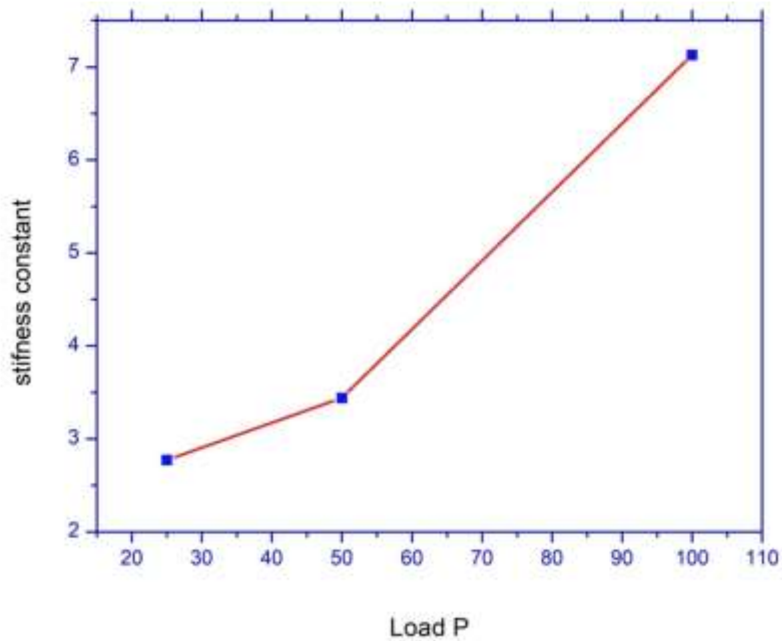

Fig.8. Load vs. stiffness constant

The plot of load vs. stiffness constant is shown in Fig.8.The values of stiffness constant are observed to be increasing with the increase of applied load to the sample. The high value of the stiffness constent has shown the strong binding force in the ions and lattice. [18]

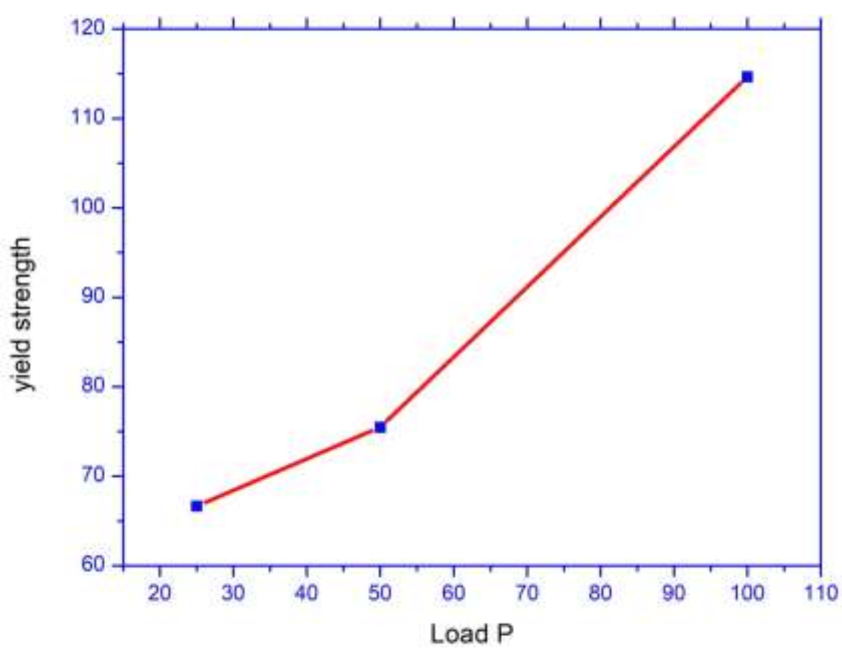

Fig.9.Load vs. Yield strength.

Yield strength (σ_y) of the material can be found out using the relation

$\sigma_y = H_v/3$

The plot of load vs. yield strength is shown in Fig. 9. Yield strength increases with the increase in load.

3.4 Dielectric studies

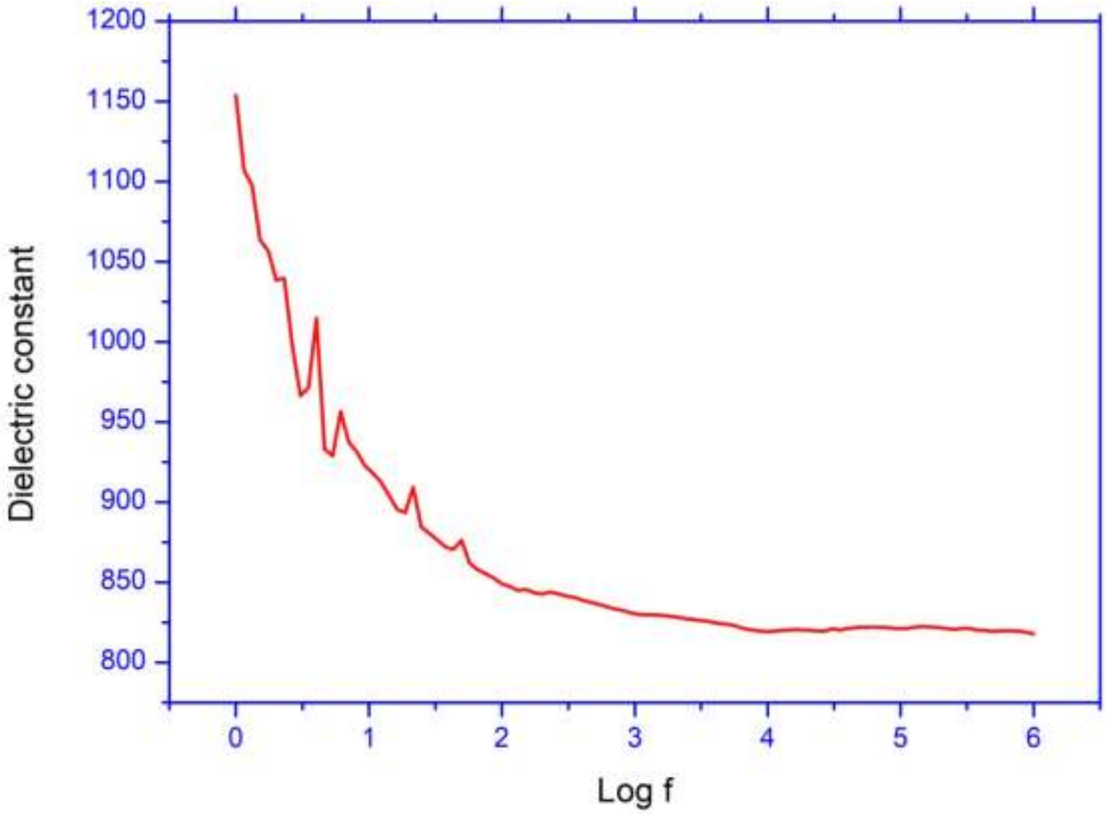

Fig. 10.Log F vs Dielectric constant

The dielectric properties are related with the electro-optic property of materials, especially when they are non-conductingmaterials [19]Dielectric steady is one of the fundamental electrical properties of the solids. [20]The dielectric study of grown AL single crystal were carried out using PSM 1735 LCR meter in the frequency range from in the room temperature. Fig 10 and Fig 11.Showed the dielectric constant and dielectric loss of the grown crystals. Form the plot it is observed that the dielectric constant decreasing with increasing the frequency. From the analysis it is observed the saturated constant value in the higher frequency. The low dielectric value at higher frequency may be due to that these materials have more optical quality withless defects which is a significant parameter for nonlinear optical materials and their applications [21]

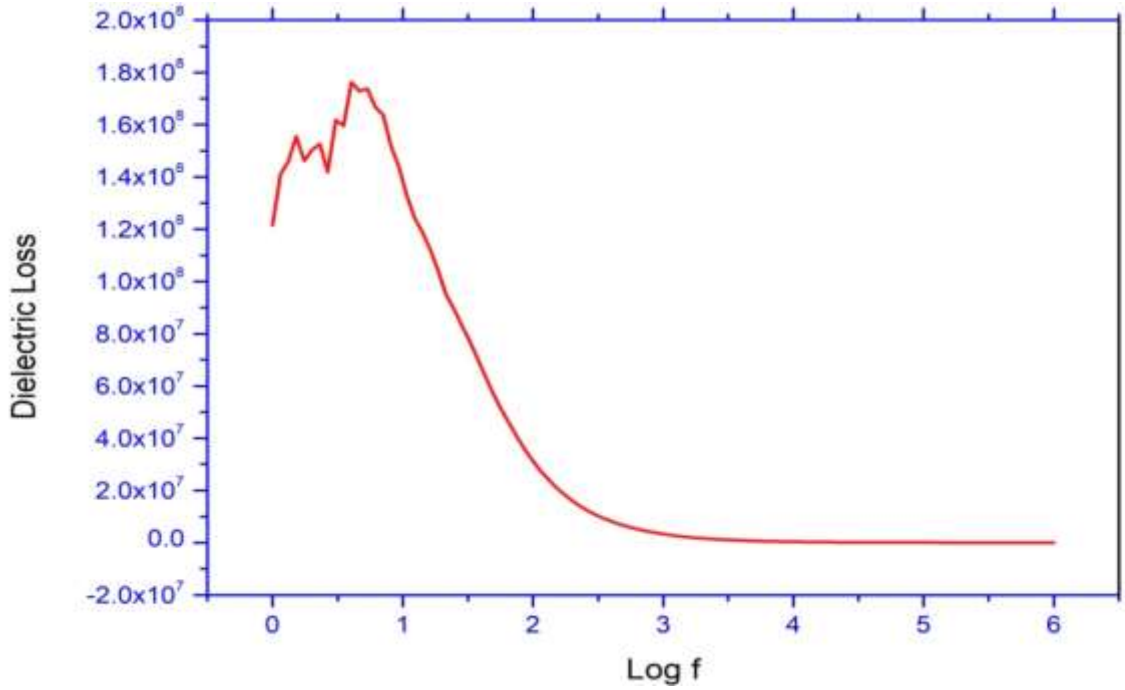

Fig. 11 Log F vs Dielectric Loss

3.5 Fluorescence

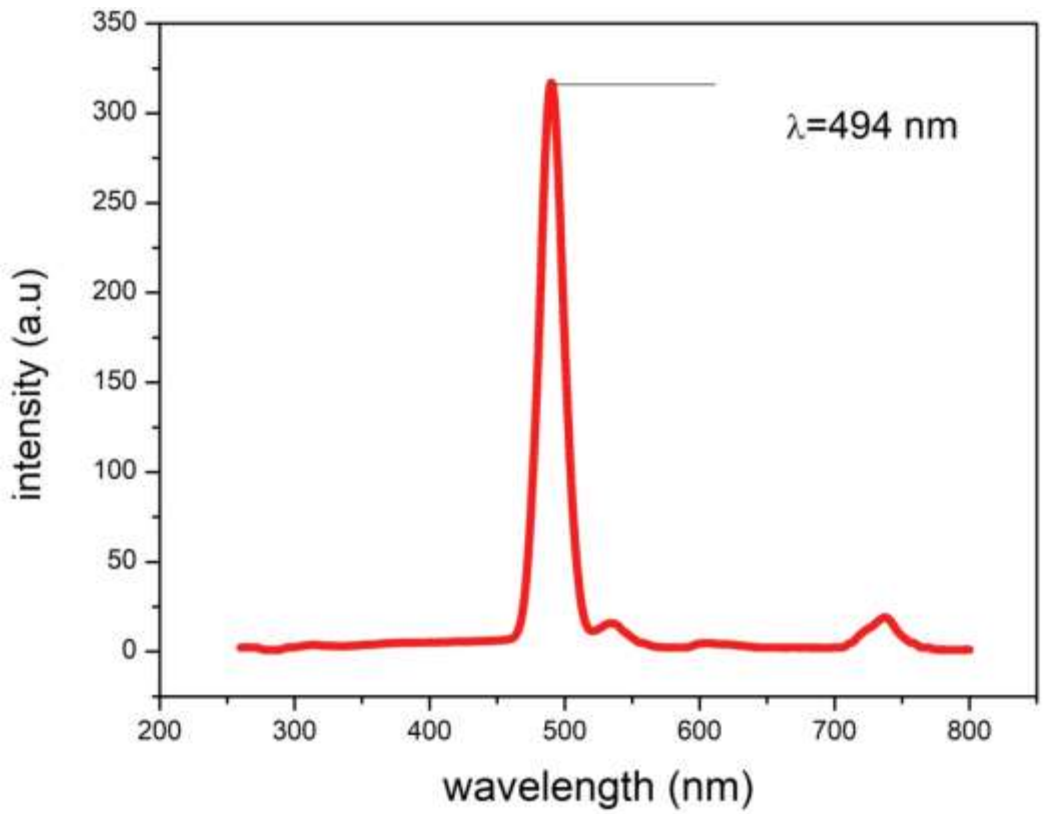

Fig. 12. Fluorescence spectrum of AL

Fluorescencepossesses many characteristics and it is widely preferred in many applications such as biochemistry, medicine, fluorescent lamps, and Light Emitting Diode (LED) lamps. Generally, the fluorescence mainly anticipated in aromatic molecules or the molecules with multiple conjugated double bonds at a high degree of resonance stability [22]. The crystalline and structural perfection of the sample crystal mainly decides the PL Intensity [23]. The Perkin Elmer LS 45(200nm to 900nm) was used to define the fluorescence (PL) spectrum of AL crystal and the values were recorded for the wavelength ranging from 200–800 nm. When the wavelength reaches 390 nm, the input excitationwavelength of PL spectrum happens. The maximum fluorescence peak was detected when the wavelength reached 494 nm which divulges the green emission and it's shown Fig 12. The luminescence in the Blue emission is the vital factor for applications like display and solid-state lighting applications [24].

3.6 TG-DTA

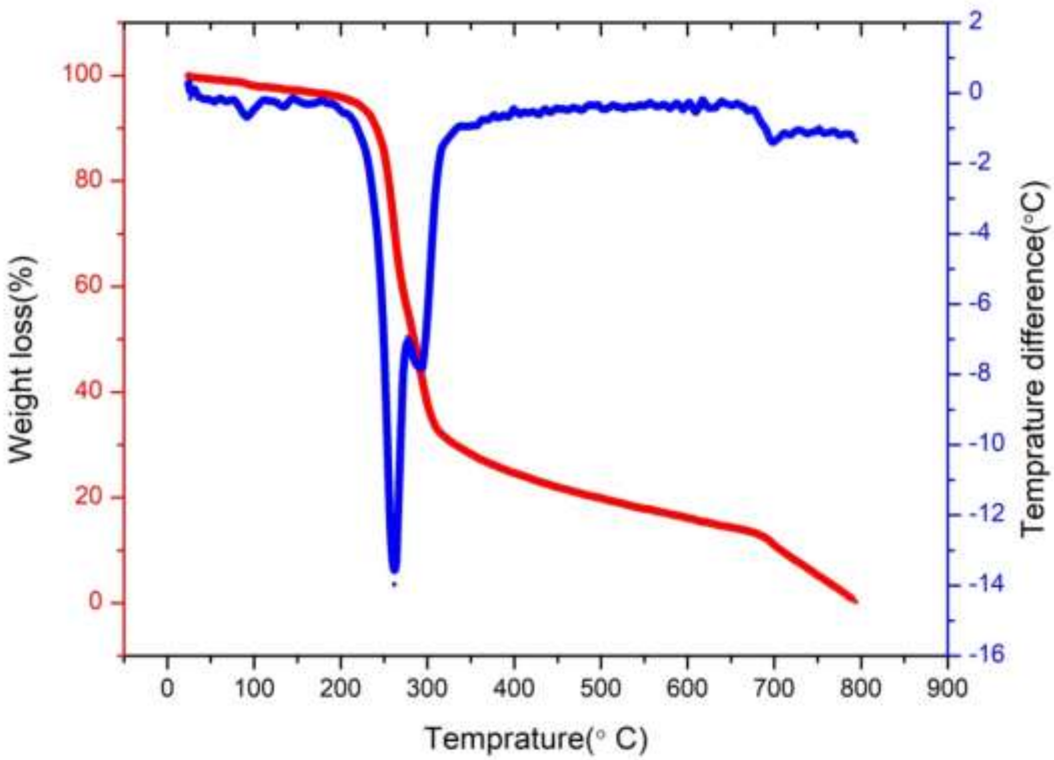

Fig. 13 TG-DTA spectrum of AL

The thermogravimetric analysis (TGA) and differential thermal analysis (DTA) were analyzed in the temperature of room temperature to 800° C by using (instrument name). Through this measurement were determine the melting point and thermal stability of the grown crystals. The thermal properties of AL grown crystal is shown in Fig. 13. The TGA Spectrum shown there is no weight loss up to 200° C may be due to release of internal energy of the sample. The TGA spectrum that the compound starts to weight loss 219°C and it continuously up to 800°C. the DTA shows the sharp peak at 260°C. The AL compound 100 % weight loss occurs between 200° C to

800^{o} C. the thermal analysis reveled the AL compound decompose starts 200^{o} C. Hence the grown AL single crystal is stable up to the 200^{o} C and it can be use for device application up to the constraint of that temperature.

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