IJISET - International Journal of Innovative Science, Engineering & Technology, Vol. 6 Issue 10,October 2019
ISSN (Online) 2348 – 7968 | Impact Factor (2019) – 6.248
www.ijiset.com

Growth and Optical, Mechanical Studies of Semi Organic NLO Active L-Threonine Potassium Iodide Crystal

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Abstract:

A novel semi-organic NLO material L-Threonine Potassium Iodide (LTPI) has been synthesized by slow evaporation method. Single X-ray diffraction study shows that the grown crystal is orthorhombic structure with the noncentro symmetry space group $P2_12_12_1$. The FT-IR spectra are carried out for reveals various functional groups in the crystal have been derived. UV-vis-NIR studying has been performed within 200-1100 nm to determine the optical transparency of the grown LTPI crystal. The fluorescence spectra studies recorded of wavelength 300-700 nm and colour of emission, region reported. The micro hardness test was carried out to mechanical property and from the results strength with stiffness constant characteristics evaluated. Second harmonic generation efficiency of the grown sample was evaluating by Kurtz-Perry method, which yield an efficiency of 1.4 times better than KDP.

Keywords

Crystal growth, L-Threonine Potassium Iodide crystal, XRD, FT-IR, UV-vis-NIR, FL, micro hardness, SHG study

1. Introduction

The optical material is technological powerful tools that laser generation typically advantage in Photonics and an electronics industry. L-Threonine is a secondary hydroxyl in polarisable with α amino acid unchanged side chain and chirallity [1].The important potential applications of the nonlinear crystal are optical parametric frequency conversion, electro-optic phase modulator, to generate switching and in amplitude modulation of other signal processing devices [2]. All this favourable property paved the way for the invention of new amino acid crystals such as L-Threonine and L-Alanine etc. Semi-organic compound shows the highest SHG efficient some over those other materials. In particular, the polar amino acid is an important material which shows higher NLO efficiency other than amino acids materials. L-Threonine was reported the carrier with very few more details [3]. The technologically importance of L-Threonine is relevantly present that derived material and also which shows optical property greater than among related to KDP [4]. Here, this material reported the growth and investigation by many researchers [5]. In recent years, organic compound molecular nonlinear optical materials have been intensely investigative due to their high nonlinearities [6].NLO materials Organic compound has attracted a great deals of attentions, as they have large optical susceptibilities and Ultra speed response time and higher optical threshold gate for laser disc power as compared with other compound inorganic materials. For example, the Proton donor carboxylic -COO group and proton acceptor aminophylline NH_2. L-Threonine picrate and L-Threonine acetate shown very higher SHG efficiency [7]. L-Threonine is an important polarity amino acid and its dipole moment is nearby similar to water [8]. High power visible laser has been no ways, widely known various field such as the display, deep sea communication, bio photonics, optical storage, medicine, making and precision micro fabrications [9]. Intense Research in inorganic and organic on functionalized NLO optical materials play a crucially role because their bond strength, molecular interactions, east incorporating of Ionic etc [10].One of the major advantageous of organic material is that their structure can be modify with the proper doping to get the desired SHG properties [11].

In the present investigation focused mainly towards linearly and nonlinear optical performance of LTPI using single crystal XRD, powder XRD, FT-IR, Fluorescence, UV-visible-NIR, SHG, micro hardness, [12].

2. Experimental procedures

L-Threonine potassium iodide crystals were synthesized by dissolving L-Threonine potassium iodide within molar ratio 1:1 in mixed with water solvent. The solution was stirred continuously, then filter in the prepare solution and fixed in grown of crystal by the slow evaporation method at room temperature. After around 25 days, good quality mono crystallomancy was harvested from the mother solution with the LTPI of dimensions of 0.27 x 0.27 x 0.3 mm^3.The grown crystals are found to be optically transparent an non-hygroscopic. Figure.1 shows the photographs of as grown LTPI crystal. The following chemical reaction for the synthesis of the material was expected to take place.

$$C_4H_9NO_3 + KI \rightarrow C_4H_9KNO_3^+ I^-$$

Fig.1. Photograph of as grown LTPI crystal

3. Characterization Techniques

Single crystal XRD data have also been recorded using an ENRAF NONIUS CAD4-MV31 single crystal X-ray diffractometery with MoKα λ=0.71073nm. The presence of functional groups and the bond assignments, nature of the bonds presently in the title materials were assessed by the FTIR spectral analysis using in PERKIN ELMER FTIR spectrophotometry. The optical characters of the sample were examined by subjects in to linear opticals analysis. The absorption and transmission spectrum were obtained within the wavelength range of 200 nm to 1100 nm with the help of PERKIN ELEMER LAMBDA 365 UV visible spectrometer. Fluorescence spectrometer using analysis PERKIN ELMER LS45 evaluated the spectrum between the range 300-700 nm. Vickers micro hardness measurements for LTPI single crystal were carried out using SHIMADZU HMV hardness testers fitted with a diamond indenter. The second Harmonic generation efficiency of LTPI crystals were tested by an AQ switched high energy Nd: YAG laser λ=1064 nm QUANTA RAY MODEL LAB-170-10 using a light source, with the input energy of 3.2 mJ, pulse width of 8ns and repetitions rate of 10Hz.

4. Results and Discussion

4.1 Single Crystal XRD

The phase purity of the as grown LTPI sample is analysed by performing single crystals X-ray diffraction. The analysed results confirm that the grown LTPI is mono crystalline belongs to the orthorhombic crystal systems within the space group $P2_12_12_1$. The lattice parameters were calculated from the collected data and found to be a=5.20 Å,b=7.75 Å, c =13.6 Å α =90º, β =90º, γ=90º, and V=560Å^3 .The morphology of the grown LTPI crystal was indexed by a winxmorph software program. The indexed morphology of LTPI is presented in figure.2.

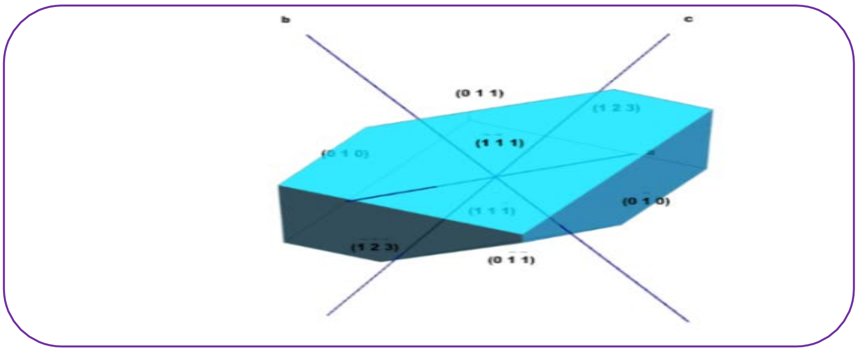

Fig.2. Morphology of LTPI crystal indexed by winxmorph software

4.2 FTIR studies

The FTIR spectrum is presented in figure.3.The frequency of various assignments has been listed in table.1. CH_2 scissoring vibrations are revealed due to the peak 1339 cm^{-1} [13]. The NH_3^+ group absorbed 1427 cm^{-1}and1623 $cm^{-1}$and strong 1427 cm^{-1} and 1623 cm^{-1} strong symmetrical bending and weak asymmetrical bending. The peak at 2050 cm^{-1} and 2215 cm^{-1} due to asymmetrical NH_3^+ bending. The NH_3^+ bending observed at wave number 2511cm^{-1}. The peak observed strong NH_3^+ stretching band in the region at wave number 2714 cm^{-1}. The O-H stretching observed set 2876cm^{-1}. The sharp peak observed at 3175 cm^{-1} was assigned to N-H stretching of primary amino group in LTPI. The NH_3^+ group is nearly observed by 3724 $cm^{-1}$and 3893 cm^{-1}, which assigned NH_3^+ stretching bonds. The carboxylic groups and amine are coordination confirmed due to the presence of functional group in the FTIR spectra [11].

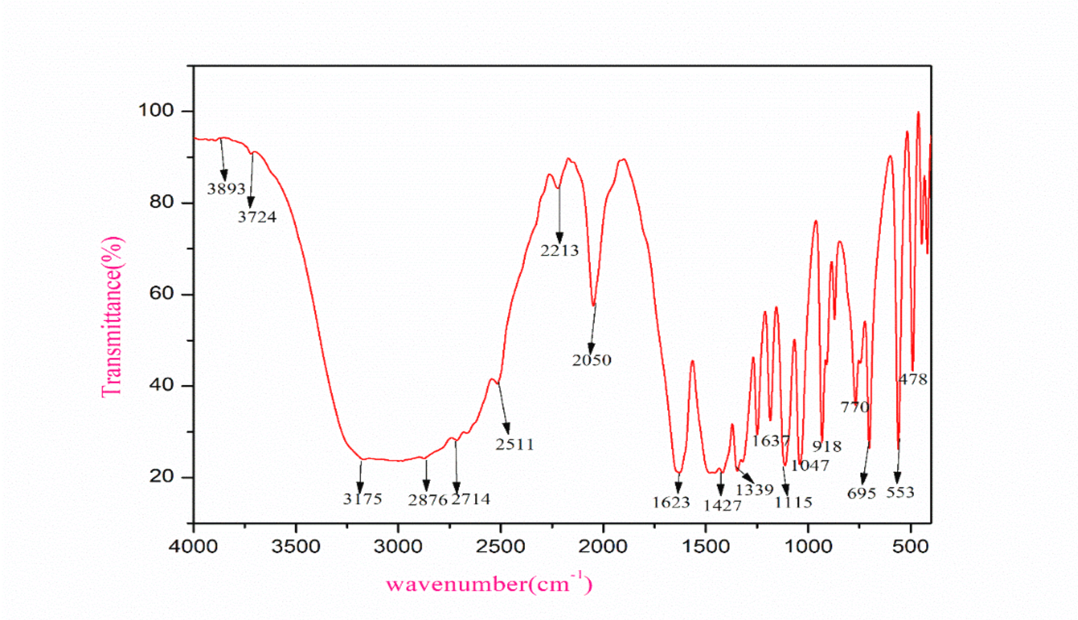

Fig 3. FT-IR spectrum of LTPI crystal

Table.1. FT- IR Assignments of LTPI crystal

wave number(cm^{-1})	Assignments
3893,3724	NH_3^+ stretching band
3175	N-H stretching
2876	O-H stretching
2714	strong NH_3^+ stretching band
2511	NH_3^+ bending
2213, 2050	asymmetrical NH_3^+ bending
1623	NH_3^+ week asymmetric bending
1427	strong symmetrical NH_3^+ banding
1339	CH_2 scissoring
1367	C-N stretching
1115	NH_3 rocking
1047	CH_2 wagging
918	CH_2 rocking
770	C-C stretching
695	KI mode

4.3 Optical studies

The UV-vis-NIR spectrum of LTPI was shown in fig.4 of thickness of the sample is 1.5cm.The cut off wave length was found to be lower than 275 nm. The cut off wavelength of LTPI was relatively lower compared with other standard organic NLO crystal; such good transparency of LTPI was highly useful for NLO application and optoelectronics. The wavelength of UV radiation causing electronic transition n-π^* at about 275nm depend orbital originally occupied. The transmittance measured T optical using absorption spectrum was calculated the coefficient α using the relation formula.

$$\alpha = \frac{2.3026}{t} \log (1/T)$$

Where, T is the transmittance and t are the thickness of the crystal. The optical absorptions coefficient α and opticals band gap E_g has been evaluates from the transmissions spectrum absorption edges as given by, $h\upsilon\alpha = A(h\upsilon-E_{g)})^{1/2}$, where E_g is the optical band gap, A is the constants h is the Plank constant is frequency of incident photons. The LTPI crystal band gap was estimating by plotting $\alpha h\upsilon^2$ versus hυ as shown Figure.5. The band width of LTPI crystals confirms the transmittance in the visible region and the opticals band gap was estimating by plotting $\alpha h\upsilon^2$ vs hυ. The plot was known as Taučs plot from which the optical band gap was estimated and it was found to be 4.5 eV. Since the material possesses excellent qualities like lower cut-off wavelength 275 nm, LTPI crystal can be utilized as a potential material in the fabrications like LASER and LED [13].

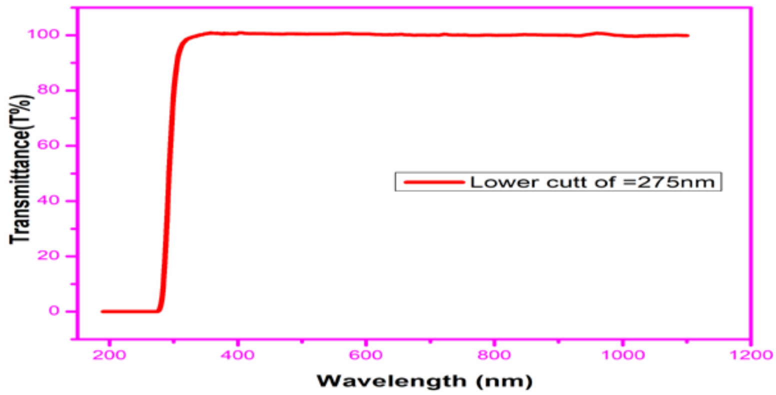

Fig.4.UV-vis-NIR transmittances spectrum of LTPI crystal

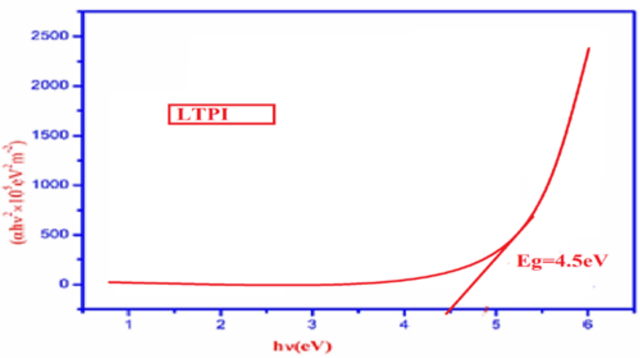

Fig.5. Tauċs plot $\alpha h\upsilon^2$ versus, hυ for LTPI crystal

4.4 Fluorescence study

Fluorescence spectrograph was recorded the wave length range between 300 to 700 nm was measured and the results are displayed, electrons are excited from low energy level to high energy level and due to this emission peak as shown figure.6.The complex synthesized show that peak at 530 nm in the emission spectrum and peak observed indicates that the complex exhibits green emission [14].

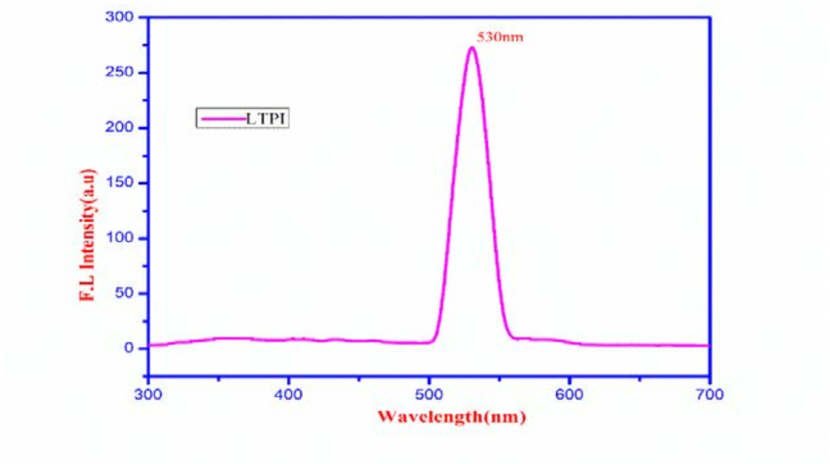

Fig.6.Fluorescence spectrum recorded emission of the LTPI crystal

4.5 Microhardness studies

The hardness of LTPI was measured used to molecular binding, yields strength, the elastic constant are the mechanical properties that can be evaluated from the results. These mechanical property are very sensitive have phase transitionally and lattice perfection prevented. The hardness material was determined by heat formation of Debye temperature, lattice energy, and interatomic spacing [9]. From the hardnesses of the grown sample, the applied load was varied from 25, 50, and 100g for a constant indentation period of 10s.The Vickers hardnesses number Hv was calculated use the relation. $H_V = 1.8544(p/d^2)$ kg/mm^3 where, p is the applied loads and d is average diagonal length of the impressions .The Vickers hardness variations of Hv with in applied loads was shown in figure.9. As shown in the results, microhardness value decreased with applied load increases, which was in agreement with normal indentations size effect (ISE). The microhardness coefficient n was found by take the slope in the line of the graph, log p versus log d as presented in figure.10. The work hardening coefficient n is greater than from the microhardness, which increases with increasing load. The coefficient work hardening for LTPI crystallized less than 2, which shows hardness decrease with increased load confirmed. Since the work hardened coefficient is according to ostrich relation, LTPI crystal belong the soft material category [10].The yield strength (σy) LTPI of the material could be calculated by $\sigma y = \frac{Hv}{2.9}[1-(n-2)(\frac{12.5(n-2)}{1-(n-2)})]^{n-2}$ and $C_{11=}\ H_v^{7/4}$.The elastic stiffness coefficient was first order C_{11} derived using Wooster empirical relation[9]. According figure.11 represents the results, it was observed that both stiffness constant and yield strength increases with increase of applied load for LTPI crystal.

Another mechanical parameter viz., yield strength was calculated using relation $\sigma_y=H_v/3$ where H_v is the Vickers microhardness number .

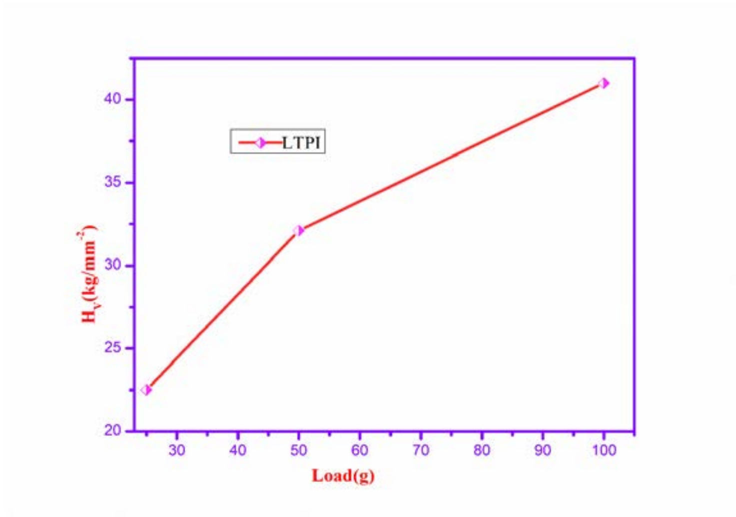

Fig.9. The Vickers hardness of LTPI as versus of applied load

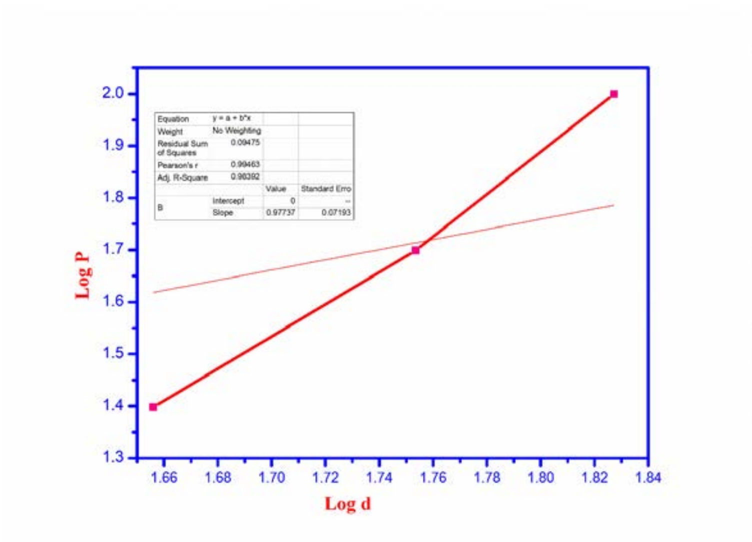

Fig.10.The curve of Log d versus Log p for LTPI crystal

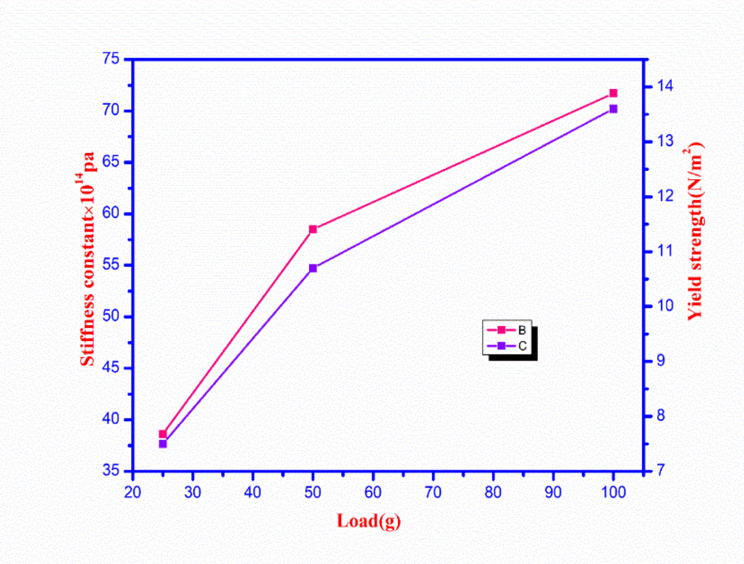

Fig.11. Applied load with variation of stiffness constant and yield strength

4.6 NLO Studies

SHG Powder measurement was the crystallized sample confirms the SHG activities of LTPI crystal. The converter output was displayed on a digital storage oscilloscope. From the SHG efficiency obtained data the of LTPI samples was 1.4 time higher than that of potassium dihydrogen phosphate. This property of enhancing the frequency makes LTPI crystal can eligible candidate in doubling applications [15].

5 .Conclusion

Semi-organic crystal LTPI was grown by a slow solvent evaporation method at room temperature. Single crystal XRD confirms the orthorhombic crystal system and unit cell parameter with a non Centro symmetric space group. The FTIR Spectra prove the presence of functional groups in LTPI crystal. The optical studies exhibit that the energy gap is about 4.5 eV. The transmission was lower cut off wavelengths 275 nm. Fluorescence spectra were emitted at 530 nm emission of green colour region. The Vickers microhardness proved that a mechanical strength of LTPI crystal to the soft material. The second harmonics generation efficiency is due to powder sample of LTPI crystal which is 1.4 times higher than of KDP crystal. Among all the studies used in for the sample suitable at the fabrication of laser based device.

Reference

[1]P.Christuraj,S.Anbarasu,P.S.Joseph,D.P.Anand,Optik (2015),http://dx.doi.org/10.1016/j.ijleo.2015.09.090

[2] G. Ramesh Kumar, S. Gokul Raj, R. Shankar, R. Mohan, S.P. Pandi, R. Jayavel, Journal of Crystal Growth 267 (2004) 213-217

[3] G. Ramesh Kumar, S. Gokulraj, R. Mohan, R. Jayavel, Journal Crystal Growth 275(2005) e1947-e1951)

[4]M.RSureshkumar,H.J.Ravindra,A.Jayarama,S.M.Dharamaprakash,Journal.Crystal Growth 286(2006)451-456

[5]G.Rameshkumar,S.GokulRaj,AmitSaxena,A.K.Karnal,ThennetiRaghavalu,R.Mohan, Materials Chemistry and Physics 108 (2008) 359-363

[6] Redrothu HanumanthaRao, S.Kalainathan,Materials.Research .Bulletin 47(2012)987-992

[7] Redrothu. Hanumantharao, S.Kalainathan, Spectrachemica Act Part A (2012)78-83

[8] A. Puhal Raj, I. John David Ebenezar, C. Ramachandra Raj Optick Xxx (2013) xxx-xxx

[9] Subhashini, D. Sathya, V. Siva Shankar, P. S Latha mageshwari, S. Arjunan Optical Material 62(2016) 357-365

[10] Sagadevan Suresh, Synthesis, growth and characterization of L-Threonine Zinc acetate Optick Xxx (2014) Xxx-Xxx

[11] J.ElberinMaryTheras,D.Kalaivani,D.Jayaraman,V.Joseph, Journal of Crystal Growth, http://dx.doi.org/10.1016/j.jcrysgro.2015.06.009

[12] J.H. Joshi, S. Kalainathan, D, K. Kanchan, M, J. Joshi, K.D. Parikh, Arabian Journal of Chemistry (2017) https://doi.org/10.1016/j.arabjc.2017.12.005

[13] Hanumantharao Radrothu, S. Kalainathan, G. Bhagavannarayana, Optick xxx (2013) xxx-xxx

[14] M.Radha Ramanan, R.Radhakrishnan, T.Dhanabal, M.Sivaraju, R.Ashok Kumar, Optick (2015) http://dx.doi.org//10.1016/j.ijleo.2015.09.043

[15] S.K.Kurtz, T.T Perry.J.Apply Phy,39.3798.1968