



OPTICAL PROPERTIES OF POTASSIUM NITRATE DOPED L-THREONINE SINGLE CRYSTAL

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ABSTRACT:

A nonlinear optical crystal- potassium nitrate doped L-threonine was grown by slow evaporation of solution growth method and its optical properties were studied. The presence of dopant potassium element was confirmed by atomic absorption spectroscopy. The optical properties were studied by means of transmission and reflectance in the wavelength region 200-1083nm. Optical band gap of the crystal was found to be 5.15 eV. Extinction coefficient was also determined.

KEYWORDS: Crystal Growth, Band Gap, Atomic Absorption Spectroscopy.

1. INTRODUCTION

Nonlinear optical (NLO) materials find practical applications in second harmonic generation (SHG), sum or difference frequency mixing, optical parametric oscillation, switching and in other optical processing devices [1]. Now a day, many amino acids crystals have been investigated due to their favourable NLO properties in real applications. Although, many NLO materials including inorganic, organic, semiorganic, organo-metallic have been synthesized and studied for NLO activities. Organic NLO active materials have extensively been studied owing to higher SHG efficiency, high laser damage threshold, ultrafast response, and easily synthesis [2]. Recently, organic amino acid attracts the attention of scientific society as they possess proton donor carboxylic group (-COO) and proton acceptor group (-NH₂). L-threonine is an important amino acid among other family members as it has higher SHG efficiency than other family members do. [3]. L-threonine can form hydrogen bonding with many inorganic and organic compounds. This ability of L-threonine was used to synthesis new hybrid crystals viz. L-threonine acetate and L-

threonine picrate, L-threonine formate [4, 5]. Sekar et al. reported the improvement in optical properties of glycine by silver nitrate doping. [6]. However, until now, there is no report on the combination of L-threonine with potassium nitrate. As potassium nitrate is an ionic salt of potassium ions (K⁺) and nitrate ions (NO₃⁻). Therefore, we first tried to synthesize and grow the single crystal of complex combining potassium nitrate and L-threonine but it is found that the complex cannot be formed and potassium and nitrate ions enter as a dopant.

In the present work, single crystals of pure and potassium nitrate doped L-threonine were grown by slow evaporation of solvent at a constant temperature from aqueous solution. The grown crystals were subjected to the ultraviolet-visible-infrared (UV-vis-NIR) absorption and transmission study and atomic absorption spectroscopy. Optical parameters such as lower cut-off wavelength, optical band gap, extinction coefficient and percent reflectance have been determined. The concentration of potassium element in a crystal has been estimated by using atomic absorption spectroscopy (AAS).

1. EXPERIMENTAL

1.1 CRYSTAL GROWTH

Single crystal of L-threonine doped with potassium nitrate was grown by low temperature solution growth method adopting slow solvent evaporation technique. L-threonine and potassium nitrate were taken in equimolar ratio and dissolved in double distilled water. The mixture was continuously stirred for two to three hours to form homogeneous solution. Prepared solution then filtered using membrane filter papers and kept for spontaneous crystallization to grow crystal in constant temperature water bath at 35°C, maintained at constant temperature with an accuracy of $\pm 0.1^\circ\text{C}$. Good optical quality crystal was harvested within 15-20 days (Fig. 1).

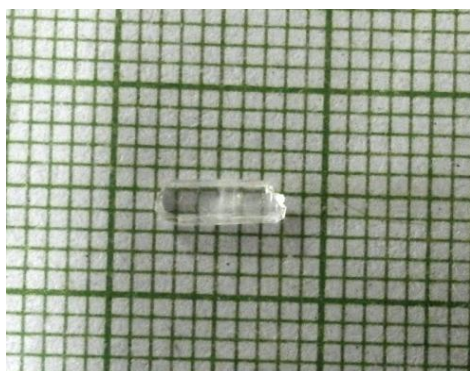


Fig. 1. Photograph of grown LTKN crystals.

2.2 CHARACTERIZATIONS

The grown crystal was subjected to the linear optical properties and AAS studies. Optical transmission of the grown crystals in UV-vis-NIR spectral range was measured with UV-visible spectrophotometer (Black-Comet-SR, Stellarnet Inc., USA). In the present study, crystal was cut in to small plate of thickness 1mm, polished it and used for the transmission and absorption measurement. The quantitative determination of chemical elements in the sample has been done with Atomic Absorption Spectrometer (AA300, Perkin Elmer, USA).

3. RESULTS AND DISCUSSION

3.1 ATOMIC ABSORPTION SPECTROSCOPY

The exact concentration of element in a given sample is determined by using atomic absorption spectroscopy. 0.01 mg of fine powder of the LTKN crystal was dissolved in

10 ml of double distilled water and the prepared solutions were subjected to atomic absorption spectroscopy (AAS) analysis. The exact concentration of the potassium present in the respective doped crystals is determined. The results show that 2.42 mg/L concentration of potassium is present in the respective samples, while the expected concentration is 8.49 mg/L.

3.2 TRANSMISSION AND ABSORPTION STUDY

It is mandatory to study the linear optical properties of the crystal, especially transmission at fundamental and second harmonic wavelength of laser before deciding applicability of the crystal for NLO applications. The SHG application need a transparent crystal at both fundamental (1064 nm) and second harmonic wavelength (532 nm) of Nd:YAG laser. In the present study, we used a polished thin rectangular thin crystal of thickness 1 mm to record UV-vis-NIR transmission over a spectral range 190-1083 nm. The recorded UV-vis-NIR transmission and absorption spectra of LTKN crystals are shown in Fig. 2 and 3 respectively. It is noticed from the transmission spectra that the crystal show a lower cut-off at around 220 nm and have a high transmission ($\sim 96\%$) over a wide measured spectral range up to 1083 nm attest the usefulness of material for optoelectronic devices. Absorption spectrum indicates no absorption over the visible region suggesting potential candidate for SHG in blue-green region. Low absorption in 240-1083 nm region is mainly attributes to the absence of strong conjugate bonds of amino acid. LTKN crystal indicates lower cutoff wavelength at $\sim 220\text{nm}$ [7].

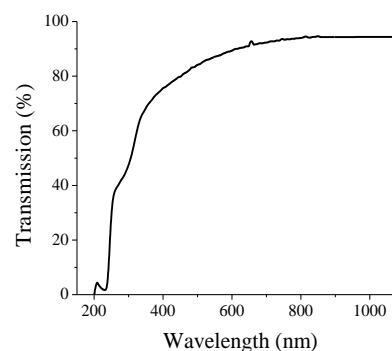


Fig. 2. Transmission spectrum of LTKN.

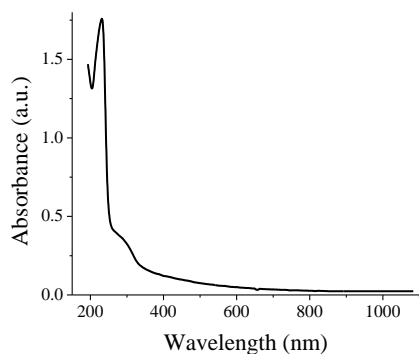


Fig. 3. Absorbance spectrum of LTKN.

3.3 BAND GAP

Optical band gap is an important optical parameter evaluated from UV-vis-NIR transmission spectra. The optical absorption coefficients (α) of LTKN crystal in the wavelength range 190-1083 nm was calculate using the relation;

$$\alpha = \frac{2.303}{d} \log\left(\frac{1}{T}\right) \quad (1)$$

Where T is the transmittance and d is the thickness of the crystal.

The direct band gap of the crystal can be calculated by using relation;

$$(\alpha h\nu)^2 = A(E_g - h\nu) \quad (2)$$

Where, A is a constant.

The optical band gap can be estimated by plotting a graph between $(\alpha h\nu)^2$ and photon energy ($h\nu$), as shown in the Fig. 4, and drawing a tangent to the straight portion of the curve. Intersect on photon energy ($h\nu$) axis gives optical band gap. The estimated optical band gap for LTKN crystal is 5.15 eV.

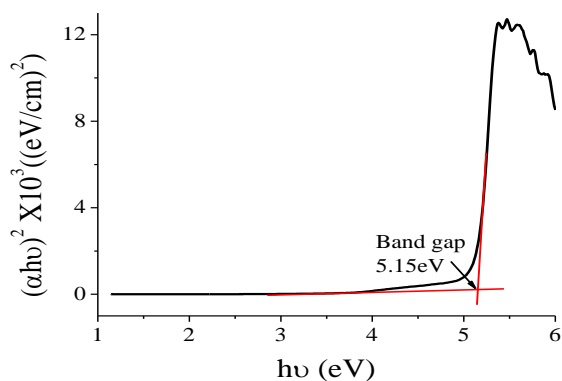


Fig. 4. Band gap measurement.

3.4 EXTINCTION COEFFICIENT AND REFLECTANCE

Another parameter related with absorption coefficient (α) is extinction coefficient (K), which is important in describing propagation of electromagnetic wave through the crystal and are related as follows,

$$K = \frac{\alpha \lambda}{4\pi} \quad (3)$$

The measure of energy loss of electromagnetic wave in crystal due to absorption, scattering phenomenon in the entire wavelength region can be realize with lower extinction coefficient (as shown in Fig. 5).

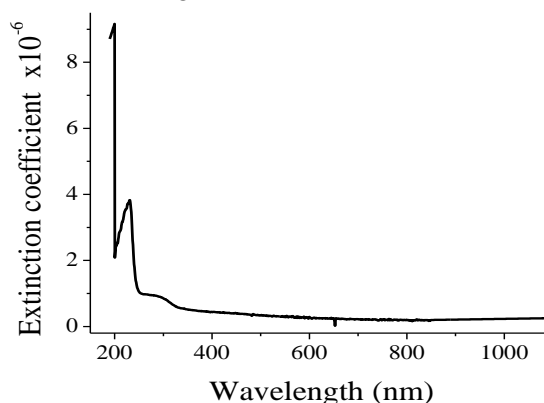


Fig. 5. Extinction coefficients of LTKN crystal.

The reflectance (R) is associated with the transmittance (T) as given below,

$$R = \frac{\exp(-\alpha t) \pm \sqrt{\exp(-\alpha t)T - \exp(-3\alpha t)T + \exp(-2\alpha t)T^2}}{\exp(-\alpha t) + \exp(-2\alpha t)T} \quad (4)$$

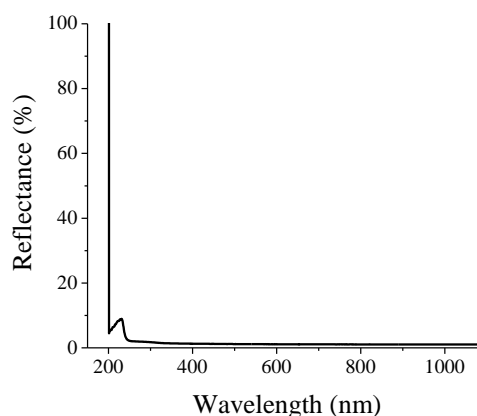


Fig. 6. Reflectance spectrum of LTKN crystal.

Reflectance for wavelength range is shown in Fig. 6. The lower value of reflectance, high transmission of material over a large wavelength range indicates the use of material for anti reflecting coating in solar devices [8].

4. CONCLUSIONS

Good quality single crystal of LTKN was grown by slow solvent evaporation solution growth method at 35°C. AAS study determines the concentration of potassium in LTKN crystal that confirms doping. UV-vis-NIR spectroscopic study indicates very high optical transparency in the wavelength region 230-1083nm. Lower cut-off and optical band gap were estimated to 220 nm and 5.15 eV respectively. Owing to the high transmission in wide range of spectrum, suggest use in NLO applications.

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