

Analyzing the Optical, Structural, Mechanical, Thermal, and Dielectric Properties of a ZTS Single Crystal Through Its Growth and Characterization

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ABSTRACT:

This research examines the development of Zinc Thiourea Sulfate (ZTS) single crystals. A method known as slow evaporation was used to grow the crystals. The produced grown crystals validate the ZTS crystal structure, according to the X-Ray diffractions research. Single crystals measuring 12x5x7mm³ were developed in the good grade crystals. Fourier transform infrared research has pinpointed the existence of sulfur-to-zinc links in the complex. The generated crystal with ZTS crystal exhibits a low UV cutoff of 220 nm and high transparency in the visible range, according to the optical characterization. Zinc thiourea sulfate may be exfoliated at temperatures up to 240°C in ZTS single crystal, according to the thermal study. Investigating the mechanical stability of the produced crystal, ZTS crystal was discovered to have an increased Vicker's microhardness number. As a function of frequency (80 kHz) and room temperature, the dielectric constant of ZTS single crystal electro-optic modulators is studied.

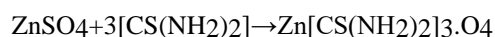
Key word: FTIR, UV-Visible, Micro hardness test, PowderXRD, Thermal analysis, electrical studies.

1. INTRODUCTION:

Zinc thiourea sulphate, or ZTS for short, is an NLO that is semi-organic [1-2]. Thiourea metal complexes with low ultraviolet (UV) cutoff wavelengths and high power frequency conversion are used in semi-organic nonlinear optical materials [3]. The thermal stability of ZTS crystals is low, but their over-all efficiency is great. Despite their great thermal stability, inorganic crystals have a negligible NLO composition [4]. Aside from having excellent mechanical hardness, low angular sensitivity, and laser-induced damage, semi-organic NLO materials have very high non-linearity. With 1.2 times better SHG efficiency than KDP, the ZTS has what it takes to succeed [5]. Laser technology is greatly affected by nonlinear optical crystals. The use of light for transmission and electrical modification of light waves [6]. Dielectric measurements, thermal gravimetric analysis, powder X-ray diffraction, FTIR, UV-Visible spectroscopy, and the Vickers hardness test were all used to characterize the generated crystal.

2. MATERIALS AND METHODS:

A stoichiometric ratio of 1:3 is used in the synthesis of the chemical from purified zinc thiourea sulphate. The produced substance is refined by recrystallization, which employs water as a solvent.



To create a consistent solution, the purified substance is dissolved in two parts of distilled water. To achieve seed crystals by spontaneous nucleation, the solution is maintained at a constant temperature. As the temperature was lowered by 0.05 to 0.5 degrees Celsius every day, the growth process continued. The seeds that were collected by gradual evaporation were used for the planting. The time it took for the plant to mature was 40-60 days. Imperfect crystals measuring 12x5x7mm³ were successfully produced.

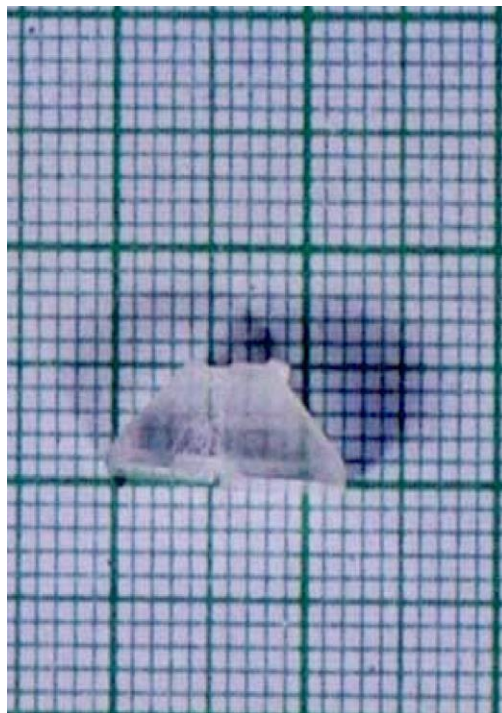


Fig1. The Photograph of ZTS single crystal.

3. CHARACTERIZATION:

3.1 Powder X-Ray Diffraction:

A study using powder X-ray diffraction was conducted on pure ZTS. The range of 11 to 52 (2θ) was used to scan the samples. Figure 2(a) displays the X-ray spectra that were acquired for pure ZTS. Using Bragg's equation, we were able to determine the interplaner d spacing. All of the reflections' hkl values were calculated using the value of d. Tables 1 and 2 show the computed and experimental d-values for pure ZTS crystals, together with the hkl indices of the matching reflecting planes. The ZTS crystal has cell characteristics $a=11.12\text{\AA}$, $b=7.773\text{\AA}$, and $c=15.49\text{\AA}$, all of which point to an orthorhombic structure.

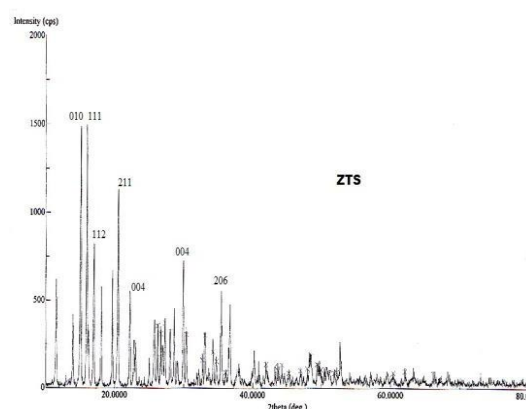


Fig 2(a) Powder X-Ray spectrum of ZTS

3.2 UV-Visible Transmittance Study:

Using a LAMBDA-35 uv-visible spectrophotometer, the UV-Visible spectra of pure ZTS crystals were obtained within the 190nm-1100nm range. Figure 2(b) shows that ZTS exhibits high transparency in the 200–1100 nm range of its optical transmission spectra. At 220 nm, pure ZTS crystals have a lower cutoff frequency. In the

visible light spectrum, a pure ZTS single crystal has a minimum transmission of 55%.

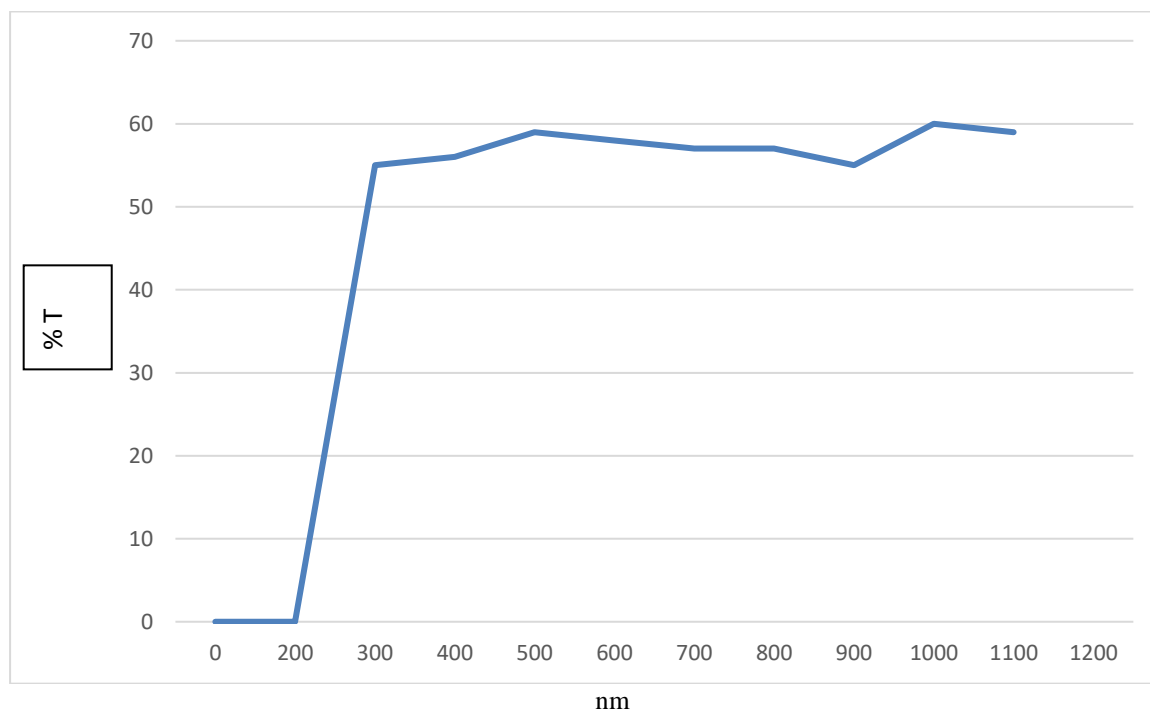


Fig 2(b) UV-Visible spectrum of ZTS

FTIR Analysis:

The existence of ZTS crystal was examined by comparing the FTIR spectra of the produced crystals. Figure 2(c) shows the FTIR spectra of crystals made entirely of ZTS. The PERKIN ELMER fourier transform infrared spectrometer was used to record the spectra in the frequency range of 400–4000 cm^{-1} , utilizing the KBr pellet method. Various molecular groups found in the sample are represented as bands in the FTIR spectrum. Zinc coordinated thiourea's symmetric and asymmetric modes emerge from the ZTS's wide envelope, which lies between 2712 cm^{-1} and 3585 cm^{-1} . The NH_2 bending vibration absorption band is located in the spectra at around 1626 cm^{-1} . The stretching vibration of N-C-N is correlated with the absorption at around 1508 cm^{-1} . The stretching vibration of N-H is reflected in the absorption band somewhere between 1,746 cm^{-1} and 1,948 cm^{-1} . The sulfate ion's existence in the coordination sphere of pure ZTS as shown by the FTIR spectra's frequency region peaks.

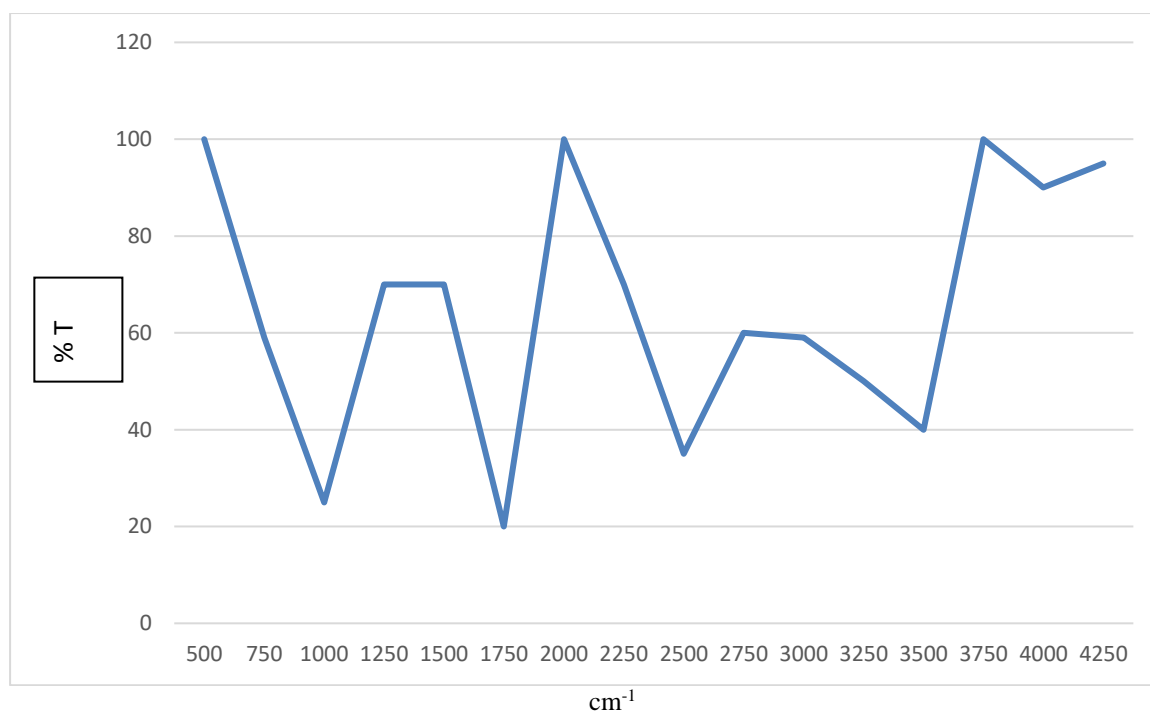


Fig 2(c) FTIR Spectrum of ZTS

Table1: Wavenumber for FTIR Spectrum of ZTS

| Thiourea | Pure ZTS | Assignment |
|----------|----------|-----------------------------|
| 3616 | 2841 | NH ₂ stretching |
| 1535 | 1614 | Asymmetric N-C-N stretching |
| 1311 | 1151 | N-H stretching |
| 936 | 749 | N-H stretching |

3.3 Micro hardness Measurement:

By assessing the resistance of the lattice to an applied load, micro hardness testing determines if a material is suitable for use in mechanical applications. This process is carried out on single crystals. Using the Leitz-Wetzler hardness tester, measure the hardness. Figure 2(d) shows the developed ZTS crystal with a weight P ranging from 25 to 100 g and a constant duration of 10 seconds for each experiment. The diagonal length was then measured.

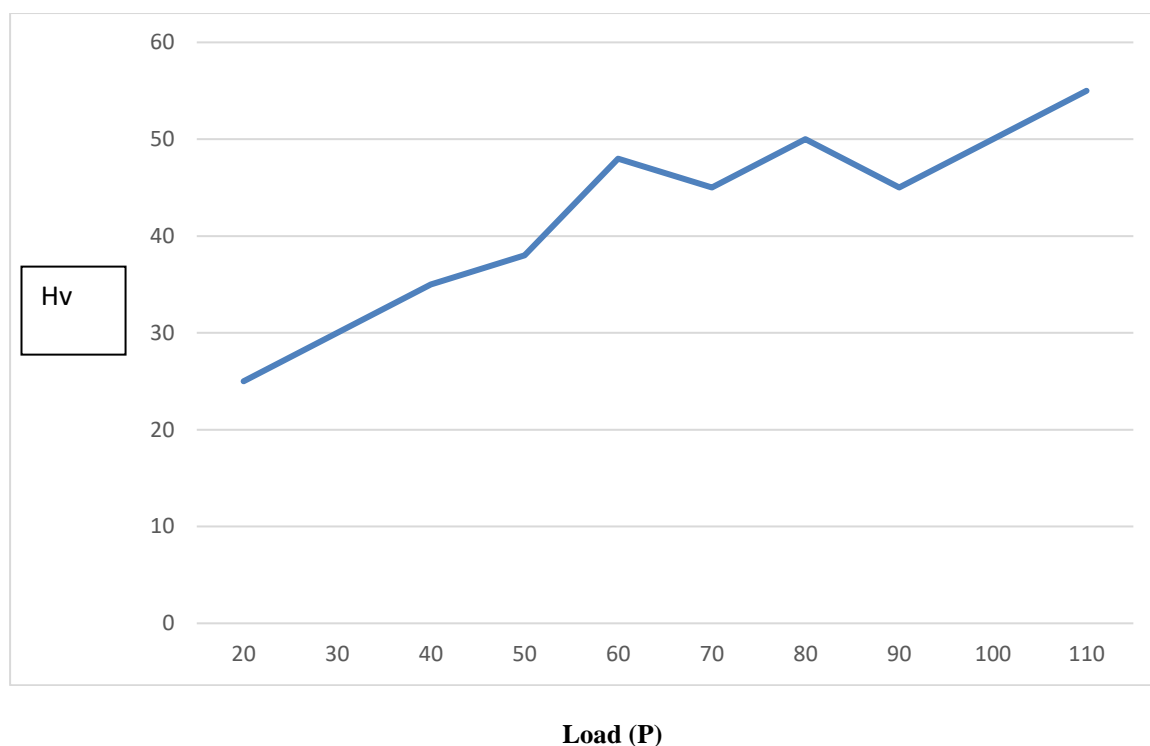


Fig 2(d) Microhardness test of ZTS

3.4 THERMAL ANALYSIS OF ZTS:

Pure ZTS crystals were examined using SDT Q600 thermo gravimetric analysis. The sample of pure ZTS crystals is stable from 25°C to 240°C in a nitrogen environment when heated at a rate of 10°C/min. The weight loss from the second endothermic peak is 37.78%, and the temperature is rising to 347.84°C. In thermal gravimetric analysis, the presence of sulfur from thiourea in zinc coordination results in the formation of this ZTS crystal.

3.5 Dielectric Properties:

An object's electro-optic and dielectric characteristics are connected. Figure 2(e) displays the ZTS crystals' relative dielectric constant (ϵ_r). The values of ϵ_r at room temperature decline with increasing frequency, reaching a minimum value of 80 KHz relative to ambient temperature. When the temperature of ZTS rises, its overall polarizability increases, and at low frequencies, the dipolar contribution diminishes, while the electronic contribution increases.

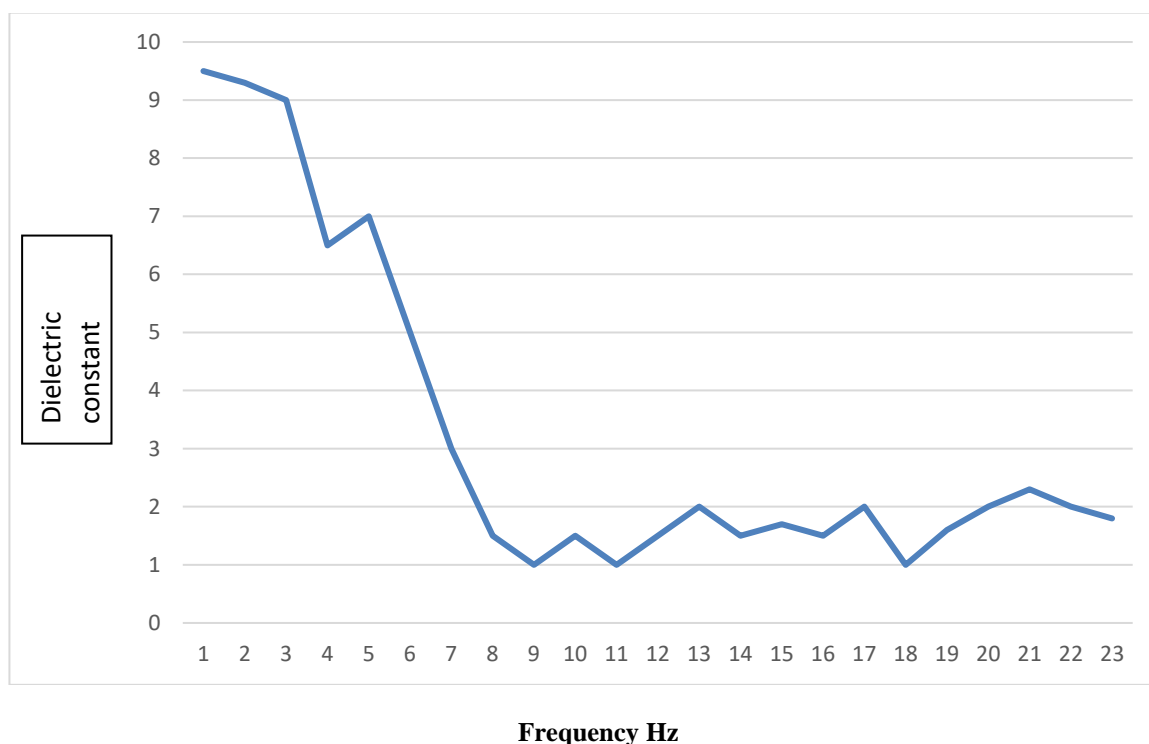


Fig 2(e) dielectric studies of ZTS

CONCLUSION:

Using a slow evaporation approach, pure ZTS crystals were produced and characterized. The crystal was found to be orthorhombic for PC2a1 using X-ray diffraction. Each chemical group in the sample was identified by its distinctive band in the FTIR spectra. The transmission spectra showed that the crystals are transparent all the way down to the UV-Visible spectrometer, demonstrating their wide transparency. This material is more thermodynamically stable than pure ZTS crystal, according to thermo gravimetric (TGA/DSC) research. The mechanical property of the formed crystal has been investigated by measuring the values of the microhardness number. As is typical for normal dielectrics in ZTS single crystals, the frequency-dependent dielectric constant at room temperature and higher decreases with increasing frequency, as shown at 80 kHz.

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