EFFECT OF BIS THIOUREA ZINC CHLORIDE ON OPTICAL PROPERTIES OF POTTASSIUM DIHYDROGEN PHOSPHATE (KDP) CRYSTAL

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ABSTRACT:
The single crystal of bisthiourea zinc chloride doped potassium dihydrogen phosphate was grown by slow evaporation solution technique. The UV-visible study was carried out using UV-Vis-NIR spectrophotometer in the range of 200-900 nm. The optical band gap of grown crystal was found to be 3.84 eV. The linear optical constants such as reflectance, refractive index and extinction coefficient were also estimated. The results of optical studies suggest that 2 mole% BTZC doped KDP crystal possesses slightly improved transparency than pure KDP.

KEYWORDS: crystal growth; optical constant; optical device

1 INTRODUCTION
Potassium dihydrogen phosphate and its isomorphs are representatives of hydrogen bonded material that posses important piezoelectric, ferroelectric, electro-optic and nonlinear properties. They have attracted the interest of many theoretical and experimental researchers probably because of their comparatively simple structure and very fascinating properties associated with a hydrogen bond system involving a large isotopic effect, broad transparency range and relatively low production cost. Improvement in the quality of KDP crystal and performance of KDP based devices can be realized with suitable dopants [1, 2]. During recent years the performance of KDP is improved with Di and Trivalent metal, rare earth elements, amino acids as dopants in appropriate percentage [3-7]. Thiourea molecule play an important role in the growth of non linear optic crystals such as bis thiourea zinc chloride, bis thiourea zinc sulphate, bismuth thiourea chloride, bis thiourea cadmium formate [8-12].

The effect of bis thiourea zinc chloride [13] and Copper thiourea complex [14] on the performance of KDP was studied. This paper reports the optical band gap and the linear optical constants of bis thiourea zinc chloride doped KDP through optical spectral analysis.

2. EXPERIMENTAL
CRYSTAL GROWTH

The 1 and 2 Mole (M) % BTZC salt were doped in the supersaturated solution of KDP and kept for slow evaporation in constant temperature bath of accuracy ±0.01 °C. Good quality transparent single crystals of 1M and 2M BTZC doped in KDP were grown within 15-20 days as shown in fig.1 and fig. 2 respectively.

![Fig. 1KDP+1M%BTZC](image1.png)

![Fig. 2KDP+2M%BTZC](image2.png)

3. RESULT AND DISCUSSION

UV-Vis STUDIES

The UV-Vis studies of 1M% and 2M% BTZC doped KDP crystal was carried out using Shimadzu UV-2450 spectrophotometer in the range 200nm and 900 nm. From the transmission spectrum, the 2mole% BTZC doped KDP crystal shows high transparency in entire visible region, shown in fig.3. The transmittance of 2M% BTZC doped KDP is found to be 75% in entire visible region. The values of band gap of the grown crystals were calculated from the Tauck’s plot depicted in Fig. 4. The band gap is found to be 3.84 eV and 3.68eV for 1M% and 2M% BTZC doped KDP crystal respectively, indicating lower defect which is essential for fabrication of optoelectronic devices [15]. The variation of refractive index and reflectance with wavelength are shown in Fig. 5 and 6 respectively. The low refractive index and reflectance of doped KDP crystals in the entire UV-VIS region makes it prominent for antireflection coating in solar thermal devices and nonlinear optical applications [16]. The optical conductivity and susceptibility are shown in Fig. 7 and 8. It reveals for lower wavelengths optical conductivity and susceptibility becomes constant value. The extinction curve shows exponential decay initially and then rise up curve as shown in fig.9. The lower values of extinction coefficient 7.21*10^-5 and optical dielectrics (Fig. 10 and 11) are responsible for high conversion efficiency. The comparative optical parameters of pure KDP and 1M% and 2M% BTZC doped KDP crystal are shown in table 1. The absorption coefficient was calculated by using the transmittance spectrum,

\[ \alpha = \frac{2.303 \log \left( \frac{1}{T} \right)}{d} \]  

Where T is the transmittance, \( \alpha \) is the absorption coefficient, \( d \) is the thickness of the crystal

Optical band gap (Eg) depicted in fig. 3 was calculated by

\[ \alpha = \frac{A(h\nu - E_g)^{\frac{1}{2}}}{\lambda} \]  

Extinction coefficient can be obtained by the following relation,

\[ K = \frac{\alpha}{4\pi} \]  

![Fig. 3 Transmittance Spectrum](image3.png)
Reflectance in terms of refractive index (n) is given by relations respectively,

$$R = \frac{(n-1)^2}{(n+1)^2}$$  \hspace{1cm} (4)

The electrical susceptibility was calculated using the relation,

$$\chi_c = n^2 - 1$$  \hspace{1cm} (5)

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Fig. 4 \((ahv)^2\) vs. Photon Energy

Fig. 5 Refractive Index vs. Photon energy

Fig. 6 Reflectance vs. Photon energy

Fig. 7 Optical conductivity vs. Photon Energy

Fig. 8 Electrical susceptibility vs. Photon Energy

Fig. 9 Extinction Coefficient vs. Photon energy
Table 1 Optical parameters

<table>
<thead>
<tr>
<th>Sr.No.</th>
<th>Physical Quantity</th>
<th>KDP</th>
<th>KDP+1MBTZC</th>
<th>KDP+2MBTZC</th>
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<tbody>
<tr>
<td>1</td>
<td>Band gap</td>
<td>3.64 eV</td>
<td>3.84 eV</td>
<td>3.68 eV</td>
</tr>
<tr>
<td>2</td>
<td>Cutoff wavelength</td>
<td>407 nm</td>
<td>437 nm</td>
<td>449 nm</td>
</tr>
<tr>
<td>3</td>
<td>Refractive index (at 407 nm)</td>
<td>1.70</td>
<td>1.70</td>
<td>1.70</td>
</tr>
<tr>
<td>4</td>
<td>Reflectance(at 407 nm)</td>
<td>32.66</td>
<td>39.40</td>
<td>37.15</td>
</tr>
<tr>
<td>5</td>
<td>Extinction coefficient(at 407 nm)</td>
<td>2.46*10&lt;sup&gt;-6&lt;/sup&gt;</td>
<td>7.21*10&lt;sup&gt;-5&lt;/sup&gt;</td>
<td>6.42*10&lt;sup&gt;-5&lt;/sup&gt;</td>
</tr>
<tr>
<td>6</td>
<td>Complex dielectric</td>
<td>4.35</td>
<td>4.35</td>
<td>4.35</td>
</tr>
<tr>
<td>7</td>
<td>Optical Conductivity</td>
<td>2.6*10&lt;sup&gt;10&lt;/sup&gt;</td>
<td>2.6*10&lt;sup&gt;10&lt;/sup&gt;</td>
<td>2.6*10&lt;sup&gt;10&lt;/sup&gt;</td>
</tr>
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Fig. 1 Plot of ε<sub>i</sub> vs. Photon Energy

4. CONCLUSIONS

BTZC doped KDP crystals were successfully grown by slow solution evaporation technique. The optical studies of grown crystal were comparatively investigated. The optical transparency of 2 mole% BTZC doped KDP crystal is higher than KDP while the large enhancement in band gap of KDP was observed with 1 mole% BTZC. The comparative study confirmed that the grown crystal may be exploited for optical device applications.

REFERENCES


