REDVET - Revista electrónica de Veterinaria - ISSN 1695-7504
Vol 24, No.4(2024)
http://www.veterinaria.org
Received: 25-07-2023 Revised:13-08-2023 Accepted: 24-08-2023

Investigation of CsPbBr3: DC Electrical Properties, Complex Impedance Study, and Optoelectronic Behavior

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ABSTRACT
$CsPbBr_3$ perovskite was investigated for its structural, optical, electrical, dielectric, and optoelectronic properties. X-ray diffraction confirmed nthe orthorhombic crystal structure, while FESEM analysis revealed well-defined cubic microstructures. ED-XRF measurements verified the presence of Cs, Pb, and Br elements. Optical studies showed a direct band gap of 2.19 eV and a strong photoluminescence emission at 554 nm. Dielectric properties exhibited frequency- and temperature-dependent behavior, with AC conductivity following Jonscher's power law and DC conductivity obeying Arrhenius behavior with an activation energy of 0.517 eV. Impedance analysis confirmed semiconducting characteristics through negative temperature coefficient resistance (NTCR) behavior. Under 100 mW cm^{-2} illumination, the material demonstrated a tenfold increase in photocurrent, with responsivity and detectivity reaching 1.73 mA W^{-1} and 3.27×10^4 Jones, respectively. Furthermore, reduced grain and grain-boundary resistance under illumination indicated enhanced charge-carrier transport. These results highlight the potential of $CsPbBr_3$ as a promising material for photodetectors and other optoelectronic applications.

Keywords: $CsPbBr_3$, perovskite, dielectric properties, impedance spectroscopy, optoelectronic properties, photo detector.

Introduction

This research focuses on $CsPbBr_3$ perovskite, a material with superior electrical, dielectric, and optoelectronic properties. The research focuses on its microstructure, impedance properties, and photo response with a view to understanding how it would be applicable in photo detectors, solar cells, and LEDs.1-4

Perovskite materials, and specifically $CsPbBr_3$, have received considerable research interest owing to their high dielectric constant, tunable band gap, and improved stability over other conventional organic-inorganic perovskite. Their orthorhombic phase structure is significant in determining their properties in charge transport and in how they absorb light, and they are compatible with next-generation optoelectronic devices.5,6 In spite of their potential, nevertheless, more research is needed to understand how external conditions, i.e., temperature and light intensity, influence their electrical and optical properties. By addressing these gaps in knowledge, in this study, we aim to drive the utility and performance improvement of $CsPbBr_3$-based devices.7-11

Therefore, the present work focuses on the synthesis and comprehensive characterization of $CsPbBr_3$ perovskite.12 Structural analysis is carried out using X-ray diffraction (XRD), while field emission scanning electron microscopy (FESEM) is employed to investigate the surface morphology and microstructure. Elemental composition is examined through energy-dispersive X-ray fluorescence (ED-XRF) spectroscopy.13-17 Optical properties are analyzed using UV–Visible absorption and photoluminescence spectroscopy. The dielectric, electrical, and impedance characteristics are studied as functions of frequency and temperature to understand the conduction and relaxation mechanisms. Furthermore, photoresponse measurements are performed under different illumination conditions to evaluate the photodetection capability of the material.18-21 The obtained results provide valuable insights into the charge transport dynamics, dielectric behavior, and optoelectronic performance of $CsPbBr_3$, highlighting its potential for future applications in photodetectors, solar cells, LEDs, and other advanced semiconductor devices.22-25

2. Experimental

The synthesis of CsPbBr3 was carried out via a solution-based method, ensuring phase purity. Structural analysis was performed using XRD, followed by morphological characterization via FESEM. Elemental composition was verified using ED-XRF spectroscopy. Optical properties were studied using UV-Vis spectroscopy and photoluminescence (PL) measurements. Dielectric behavior was analyzed through impedance spectroscopy across different temperatures and frequencies. Finally, the optoelectronic properties were evaluated using a two-probe method under varying light intensities.

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Synthesis of Cesiumleadbromide (CsPbBr3)

CsPbBr3 has been synthesized by reacting equimolar amount of cesiumbromide (CsBr) and leadbromide (PbBr2) at room temperature in ambient environment. In a typical synthesis, 3 mM of CsBr was dissolved in 1.5 mM de-ionized water by ultrasanitation for 2 hour. Hence, 3 mM of PbBr2 was add with 4.5 ml of aqueous hydrobromicacid (HBr) top repare PbBr2 precursor. Top recipitate CsPbBr3, aqueous CsBr was quickly mixed with PbBr2 precursor and orangecol or CsPbBr3 was collected by filtration very carefully. Thenas-synthesized material was washed seve raltimes with ethanol and collected by centrifugations. Finally, the sample was dried overnight in vacuum top repare powder sample for further characterizations.

3. Results and Discussion

The XRD pattern of the as-synthesized CsPbBr3 confirms the formation of a single-phase orthorhombic crystal structure (JCPDS No. 74-2251) with the Pbnm space group. The observed diffraction peaks match the characteristic planes of orthorhombic CsPbBr3. The calculated Goldschmidt tolerance factor (t = 0.939) indicates a stable perovskite lattice with slight distortion from the ideal structure, which can significantly influence its optical and electronic properties. Rietveld refinement using the MAUD software further validates the structural parameters and phase purity of the synthesized sample (Figure 1a). The morphological properties of the as-synthesized $CsPbBr_3$ powder were investigated using field-emission scanning electron microscopy (FESEM). The FESEM images (Figure 1b) confirm the successful formation of predominantly cubic-shaped particles, which is consistent with the crystal structure of $CsPbBr_3$. Most particles exhibit well-defined cubic morphology, while a few slightly deformed particles with comparatively smaller dimensions are also observed. A magnified image of a representative particle (Figure 1c) shows a cube with an edge length of approximately 3 µm. The nearly equal edge lengths in all directions indicate isotropic crystal growth, suggesting that the growth rate was almost uniform along different crystallographic orientations. This uniform growth behavior contributed to the formation of well-faceted cubic crystals.

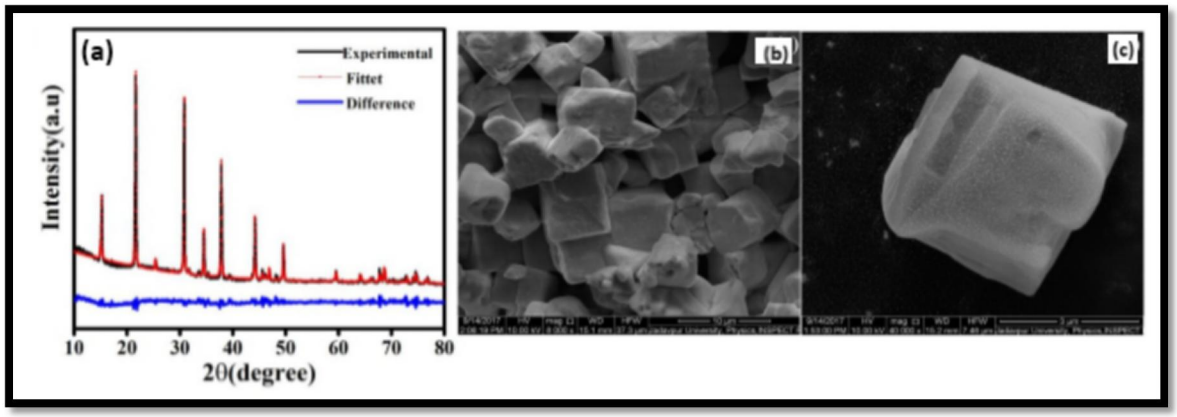

Figure 1: (a) XRD spectra with Rietveld refinement; (b) Cluster of CsPbBr3 micro cube, (c) Single micro structure of CsPbBr3

Optical Properties

Absorbance spectra of the sample have been collected in the wavelength range of 300 nm to 800 nm. It is well known that CsPbBr3 has a direct band gap, which is measured by using Tauc plot. It can be expressed as,

$$\alpha h\nu = (h\nu - E_g)^n$$

Where, α is absorption coefficient, hv represents the energy of the incident photon, Eg is the band gap of respective material and n=½ or 2 for direct and indirect band gap type material. Here (h)2 vs h has been plotted to calculate the band gap from the interpolation as depicted in (Figure 2a). The band gap of CsPbBr3 has been appeared as 2.19eV. (Figure 2b) illustrates the PL emission spectra of the powder sample which is excited at 428 nm. It is evident from the figure that a sharp peak has appeared at 554 nm (2.23eV) which may be a rising from band-to-band transition. Over all emission line width is very broad due to the formation of self-trapped excitons instead of dissociation and collection of excitons within material.

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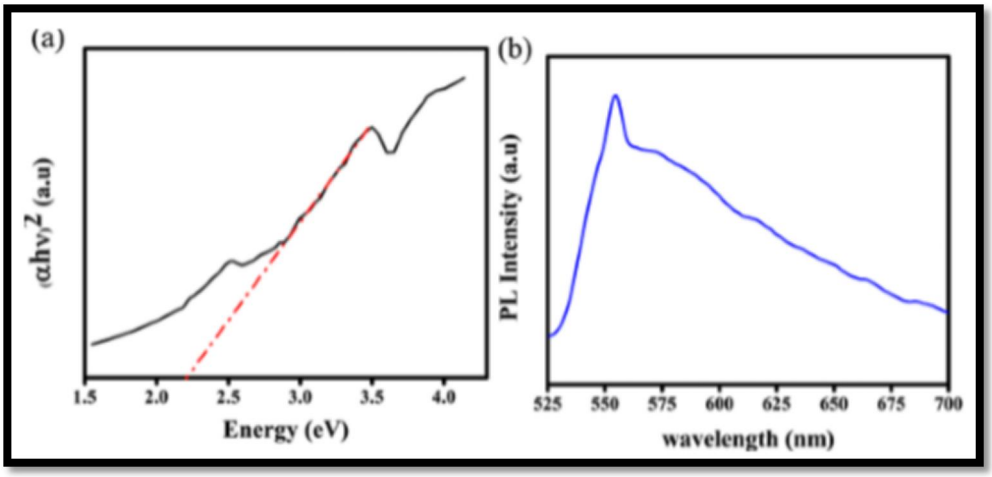

Figure 2: (a) Taucplot (from Uv-Vis spectra) CsPbBr3; (b) PL spectra of CsPbBr3

Optoelectronic Properties

To illustrate the photo response capability of CsPbBr3, two probe method has been used for measuring the I-V profile under simulated solar spectrum of different intensity. (Figure 3a) represents the I-V curves of the photo-detector under light illumination ranging from 0 mW cm-2-100 mW cm-2. The I-V curves maintain a non- linear proportionality with applied bias indicating non-Ohmic type of contact between ITO and CsPbBr3. As shown in (Figure 3b), photo current increases up to 10 times compared to dark current at light intensity 100 mW cm-2. The variation of photo current

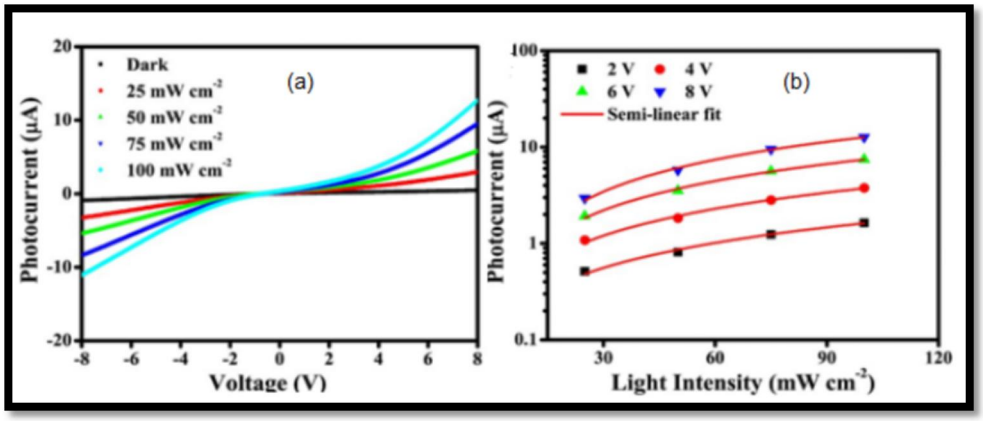

Figure 3: (a) I-V response of the detector; (b) Light dependent photo-current

With light intensity for several applied bias has depicted in (Figure 3b). The light dependence of current can be expressed as Iph= ~Pα, where α signifies the response of current with light intensity. The value of α has been accounted from the linear fit of log- log curve as 0.74. The non-unity value (0.5< α <1) of α indicates that photo-responsivity of CsPbBr3 may be attributed by combined effect of electron-hole pair generation, trapping within material and recombination. When light with high energy compared to band gap (Eg) incidents on the material, photons are absorbed by the material. As a consequences of which electron-hole pairs are generated (h →e-+h+) within semiconducting CsPbBr3. The photo generated electron-hole pairs are the prime essence of this phenomenon which enhance the conductivity of this material and decrease the potential barrier at the same time. Significant number of photo-generated holes recombine with Br-trapped electron. Therefore, unpaired electrons becomes the major charge carrier within material which are mainly contributing to the photo-physical properties.

Conclusion

$CsPbBr_3$ exhibits excellent dielectric and optoelectronic properties, making it a highly promising material for photodetector and semiconductor applications. The structural and morphological investigations confirmed the successful synthesis of well-crystallized $CsPbBr_3$ with predominantly cubic morphology. Electrical studies revealed a strong dependence of dielectric and conductivity parameters on temperature, indicating the thermally activated nature of charge transport within the material. Furthermore, the material demonstrated significant photoresponse under light illumination, with high photodetection efficiency and stable electrical behavior. These characteristics suggest effective generation,

separation, and transport of photogenerated charge carriers. The combination of favorable electrical properties, good crystallinity, and enhanced photoresponse highlights the potential of $CsPbBr_3$ for use in next-generation optoelectronic devices, including photodetectors, light-sensing systems, and semiconductor-based electronic components. Further optimization of synthesis conditions and device fabrication may lead to improved performance and broader practical applications.

Funding
No funding received for this work.

Acknowledgment
The authors express their gratitude to the Department of Chemistry Sheth M. N. Science College, Patan, and Department of Chemistry Amity University, Gwalior for their assistance with experimental work and analysis support.

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