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SCAPS-1D Simulation Study on Effect of Absorption Layer Thickness on the Performance of p-CuI/n-InSe Near-Infrared Photodetectors

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Photodetectors based on van der Waals semiconductors are promising candidates for next-generation optoelectronics due to their tunable bandgaps and environmental stability. In this work, the performance of a p-CuI/n-InSe heterostructure photodetector was systematically investigated using SCAPS-1D simulations. The effect of varying InSe absorber thickness (0.40–0.60 μm) was analyzed in terms of dark current, quantum efficiency (QE), spectral responsivity (R_λ), and specific detectivity (D^*). The results reveal that increasing InSe thickness suppresses dark current, improves carrier collection, and enhances sensitivity in the near-infrared (NIR) region. A peak responsivity of ~0.62 A/W was achieved at 864 nm, corresponding to the bandgap of InSe (~1.25 eV). Better noise performance was confirmed by the QE exceeding 96% for thicker layers and the rise in D^* values over the 300–1100 nm spectral region. These results demonstrate how important it is to optimize absorber thickness while creating reliable, lead-free NIR photodetectors.

Keyword: Photodetectors; Optoelectronics; Heterojunctions; Indium selenide
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1. Introduction

Photodetectors are crucial optoelectronic components that transform incoming light into electrical signals. They are used in industrial sensing, medicinal imaging, communication systems, and environmental monitoring. Typically, they fall into one of two primary categories: photonic detectors, which work by using the photoelectric effect, or thermal detectors, which depend on heat-induced changes in material characteristics. Modern technologies make extensive use of photonic detectors because of their wavelength selectivity and rapid response [1,2].

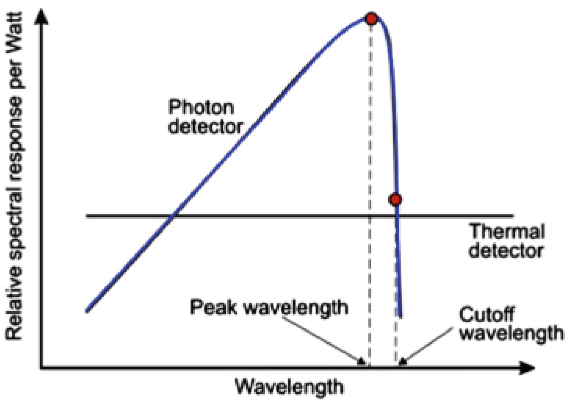

Fig. (1) Ideal spectral response of photonic and thermal detectors [14]

Indium selenide (InSe), a layered van der Waals III–VI combination, has garnered a lot of attention among new semiconductors for photodetector applications. With a straight bandgap (E_g) of around 1.25 eV, InSe is very sensitive to both visible and near-infrared (NIR) light [3-5]. This bandgap is particularly suitable for NIR detection, as it enables efficient absorption of photons with energies matching the spectral range of 800–1000 nm, which is vital for applications such as optical communication, agricultural monitoring, and humidity sensing [6-8]. Additionally, InSe provides effective charge transfer in nanoscale devices, has great carrier mobility, and is inherently n-type [9].

The higher chemical and environmental stability is one of the main advantages of InSe over lead-halide perovskites. InSe exhibits resilience in ambient settings, while perovskites often deteriorate when exposed to oxygen and moisture, limiting their long-term performance [10,11]. InSe is positioned as a possible environmentally acceptable substitute for sustainable optoelectronics because of its stability and lead-free composition.

In this work, we examine the performance of a heterojunction photodetector made of n-type InSe (E_g = 1.25 eV) and p-type copper iodide (CuI, $E_g \approx 3.1$ eV). InSe acts as the primary absorbing layer, while CuI acts as a transparent hole-transport layer with a broad bandgap. Using one-dimensional simulations using SCAPS-1D software, device performance was examined, with an emphasis on how absorber thickness affected dark current, quantum efficiency, responsivity, and specific detectivity. The results provide light on optimizing the absorber layer to create stable, high-performing, lead-free NIR photodetectors.

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2. Modeling and Simulation

The Solar Cell Capacitance Simulator (SCAPS-1D), a numerical tool created at Ghent University [12,13], was used to carry out the simulations. The basic semiconductor equations, such as Poisson's equation, carrier continuity, drift-diffusion transport, and recombination dynamics, are resolved using SCAPS-1D. It is often used to simulate thin-film devices because it provides flexibility in changing material and structural factors.

In this study, the p-CuI/n-InSe heterostructure was simulated at a standard temperature of 300 K, under AM 1.5G solar spectrum illumination with a power density of 100 mW/cm². The absorber thickness of InSe was varied between 0.40–0.60 µm to investigate its effect on device performance. The front contact was assumed to be transparent (indium tin oxide, ITO), while the back contact was metallic (aluminum, Al).

The following simulation considerations were applied:

- Defect states: bulk defect density in InSe was set to ~1×10^{15} cm^{-3} with mid-gap energy level; interface defect density at CuI/InSe junction ~1×10^{12} cm^{-2}.
- Recombination model: Shockley–Read–Hall (SRH) recombination was included.
- Series resistance: 1 Ω·cm², Shunt resistance: 1×10^{5} Ω·cm^{2}.
- Optical absorption: wavelength-dependent absorption coefficient α(λ) was imported from literature [14,15].

Figure (2) illustrates the configuration of the p-CuI/n-InSe photodetector in its fundamental form, including a transparent layer of p-type copper iodide (CuI) with a substantial energy gap of 3.1 eV, and a primary absorption layer of n-type InSe with a minimal energy gap of 1.25 eV. Table (1) shows the most important detector parameters in the SCAPS-1D simulation.

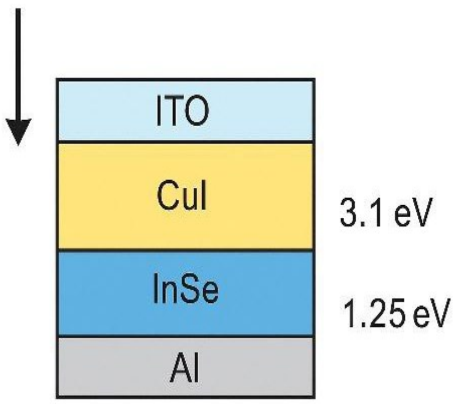

Fig. (2) Schematic diagram of the p-CuI/n-Inse detector

3. Results and Discussion

Figure (3) presents the simulated dark current–voltage (I–V) characteristics of the p-CuI/n-InSe photodetector for absorber thicknesses of 0.40, 0.50, and 0.60 µm under bias ranging from −0.7 to +0.7 V. The results show that the dark current decreases as the InSe thickness increases. At a reverse bias of −0.5 V, the dark current reduces from 1.97×10^{-1} mA/cm² (0.40 µm) to 8.4×10^{-2} mA/cm² (0.60 µm).

Table (1) The detector parameters

Layers Parameter	p-CuI	n-InSe	Units	Ref.
Thickness	0.05	0.40-0.60	µm	[6,9]
Relative permittivity (ε_r)	6.5	11-12	-	[6]
Electron mobility (μ_n)	100	1000	cm²/V.s	[6]
Hole mobility (μ_p)	50	100	cm²/Vs	[6]
Donor density (N_d)	0	$1*10^{15}$	cm^{-3}	[9]
Acceptor density (N_a)	$1*10^{18}$	0	cm^{-3}	[9]
Optical band gap (E_g)	3.1	1.25	eV	[9,10]
Effective density (N_c)	$2.8*10^{19}$	$1.57*10^{18}$	cm^{-3}	[9,10]
Effective density (N_v)	$1*10^{19}$	$3.63*10^{19}$	cm^{-3}	[9,10]
Electron affinity (χ)	2.1	4.7	eV	[9,10]

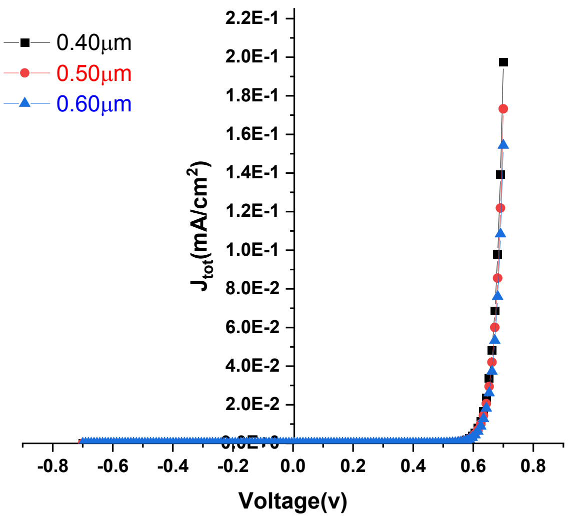

Fig. (3) The I-V characteristics in dark for different thicknesses of InSe absorption layer (0.40, 0.50, 0.60 µm)

This reduction can be attributed to the increase in depletion region width and enhanced photon absorption, which suppresses thermally generated carriers and recombination processes. Thicker absorbers provide improved carrier separation, lowering leakage currents and enhancing junction stability. Similar trends have been reported in other van der Waals photodetectors [11].

The quantum efficiency (QE) is defined as [2]:

$$\eta(\lambda) = \frac{(I_{ph}/q)}{(P_s/h\nu)} \quad (1)$$

Figure (4) shows that QE increases with absorber thickness. For 0.60 µm, QE reaches ~96.9% at short wavelengths (<600 nm) and maintains 80% at ~990 nm, close to the InSe band edge (E_g ≈ 1.25 eV). The improvement is due to enhanced absorption length and reduced surface recombination, which improve electron–hole pair generation. These results align with recent experimental studies on InSe photodetectors [13,14].

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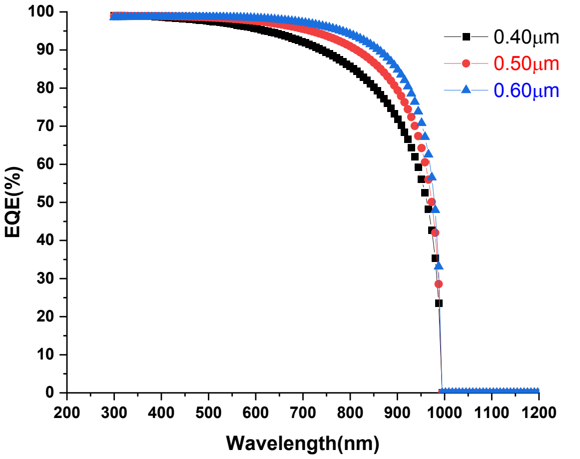

Fig. (4) Variation of quantum efficiency (QE) as a function of wavelength for different thicknesses of n-InSe layer at a reverse bias voltage of -0.5V

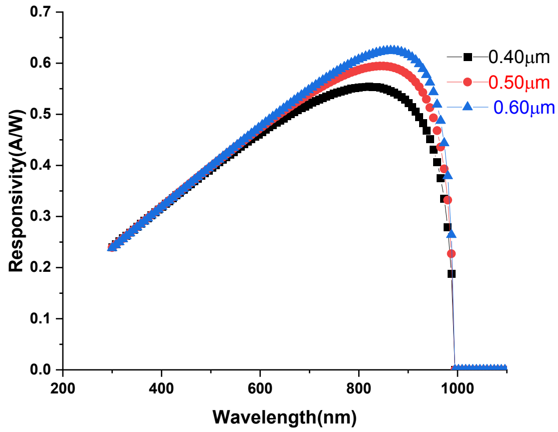

Fig. (6) Variation of spectral responsivity as a function of wavelength for different thicknesses of n-InSe layer at a reverse bias voltage of -0.5V

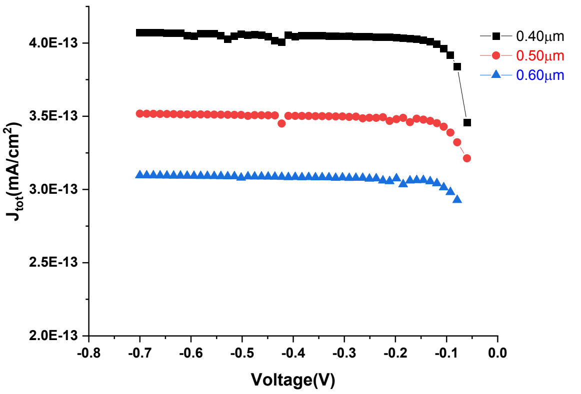

Fig. (5) The J-V characteristics under illumination for different thicknesses of n-InSe absorption layer at a reverse bias voltage of -0.5V

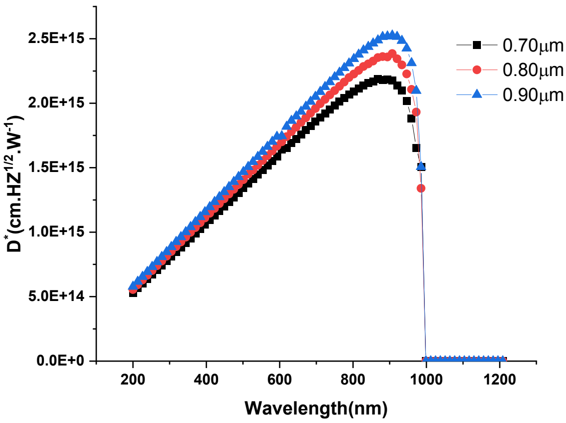

Fig. (7) Specific detectivity as a function of wavelength for the p-CuI/n-InSe photodetector for different thicknesses of n-InSe layer at a reverse bias voltage of -0.5V

The spectral responsivity is defined as [1]:

$$\mathcal{R} = \frac{(\eta(\lambda)\, q\, \lambda)}{(h\, c)} \quad (2)$$

As shown in Fig. (6), responsivity increases with absorber thickness, reaching a maximum of 0.62 A/W at 864 nm for 0.60 μm thickness. The peak corresponds closely to the InSe bandgap energy (1.25 eV ≈ 992 nm), confirming efficient absorption near the band edge. This peak responsivity indicates the suitability of CuI/InSe heterostructures for NIR applications such as optical communication (850–900 nm window) and environmental monitoring.

The specific detectivity (D^*) is defined as [10]:

$$D^* = R(\lambda)\sqrt{\frac{A.\Delta f}{2qI_d}} \quad (3)$$

Figure (7) shows that D^* increases with absorber thickness across the 300–1100 nm spectral range. At 0.60 μm, D^* reaches 10^{12}–10^{13} cm·Hz$^{1/2}$·W^{-1}, demonstrating significant noise suppression. The improvement is mainly attributed to the lower dark current and enhanced responsivity, consistent with shot-noise-limited performance models [15,16].

3. Conclusions

This study highlights the crucial role of absorber thickness in optimizing the performance of p-CuI/n-InSe photodetectors. SCAPS-1D simulations demonstrated that increasing the InSe thickness from 0.40 to 0.60 μm significantly reduced dark current, enhanced quantum efficiency (up to 97%), and improved responsivity, achieving a peak of 0.62 A/W at 864 nm. Specific detectivity (D^*) also increased across the 300-1100 nm range, confirming improved noise suppression. These results emphasize that absorber-layer optimization is essential for developing high-sensitivity, lead-free, and environmentally stable near-infrared photodetectors.

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