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Modeling and Optimization of Graphene/GaAs Structured Solar Cells Toward Improved Energy Efficiency

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ABSTRACT

The rising global demand for energy, coupled with environmental concerns associated with fossil fuels, has intensified the need for the development of novel technologies based on renewable energy sources. This study focuses on the modeling and optimization of a graphene/gallium arsenide (GaAs) Schottky junction solar cell to enhance power-conversion efficiency (PCE). The proposed structure consists of graphene, GaAs, and silicon oxide layers, simulated using Silvaco software along with advanced physical models, including thermionic emission, Auger recombination, and drift–diffusion mechanisms. The effects of key parameters—such as GaAs substrate thickness, number of graphene layers, graphene work function, and nanograting structures—on critical performance metrics, including open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and PCE were systematically investigated. In addition, the overall stability of the photovoltaic (PV) system was evaluated to ensure consistent and reliable energy conversion performance under continuous illumination. The results indicate that the optimal GaAs substrate thickness is approximately 4 µm, and increasing the number of graphene layers up to three improves the efficiency by about 1.196%. The implementation of rectangular nanogratings enhances light absorption, achieving a final efficiency of nearly 2.05%. Furthermore, employing graphene with a work function of 4.55 eV significantly improves Voc and FF, yielding the best overall performance balance. These findings highlight the pivotal role of precise nanostructure design and the optimal selection of optical and electrical material properties in advancing next-generation graphene-based solar cells.

1. Introduction

The growing reliance on clean energy resources worldwide stems from the depletion of fossil fuels and their detrimental environmental impacts. Among the various renewable energy options, solar energy holds the largest share, thereby becoming the focal point of research aimed at enhancing the power conversion efficiency (PCE) of solar cells [1, 2].

Within the broad spectrum of photovoltaic technologies, group III–V solar cells—particularly gallium arsenide (GaAs)—offer significant advantages over silicon (Si)-based devices. These benefits include the potential for high efficiency, a direct bandgap, superior carrier mobility, suitability for thin-film designs, a high absorption coefficient, and stable operation across a wide temperature range [3, 4]. As a key semiconductor material, GaAs with its 1.42 eV bandgap is recognized as one of the most efficient, demonstrating the highest reported efficiency among single-junction solar cells [5, 6]. Despite these advantages, GaAs devices face the critical challenge of high surface recombination rates, which can be partially mitigated by applying AlxGa1−x surface layers. Nevertheless, relying solely on GaAs junctions is insufficient for achieving higher efficiencies, and the incorporation of complementary layers above or below the junction structure can lead to significant performance improvements [7, 8].

In recent years, two-dimensional (2D) materials have attracted considerable attention due to their unique properties and potential applications in photovoltaic

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technologies [9]. Among these, graphene (Gr) has emerged as a highly promising candidate for solar cells, owing to its exceptional characteristics such as ultra-high electron mobility (exceeding 200,000 $cm^2/V\cdot s$), remarkable optical transparency of nearly 97.7%, low sheet resistance, high carrier density, outstanding mechanical strength, excellent crystalline quality, and stability under large-scale synthesis. Moreover, Bernardi et al. [10] demonstrated that monolayer two-dimensional materials can achieve extraordinary sunlight absorption, highlighting their strong potential for application in ultra-thin photovoltaic devices [10-12]. The excellent transparency of graphene in the visible and near-infrared regions significantly reduces photon losses [12]. Furthermore, the integration of graphene with semiconductors in the form of graphene/semiconductor Schottky heterojunction solar cells have recently gained substantial interest among researchers, primarily due to their relatively simple fabrication process and low production cost [13, 14].

The power conversion efficiency (PCE) of heterojunction Schottky solar cells is directly dependent on the number of photons absorbed within the active absorber layer. However, the efficiency is often constrained by the limited absorption capacity of the active layer as well as by from the material interfaces [1]. Optical losses remain a major bottleneck in the advancement of such devices [15]. Studies indicate that more than 30% of the incident solar radiation is lost due to surface reflection, with the most pronounced losses occurring in the short-wavelength (blue light) region. Additionally, insufficient absorption in the long-wavelength range and excessive reflection at shorter wavelengths further limit the fraction of solar energy that can be effectively converted into electricity [16].

Consequently, strategies aimed at improving solar-cell performance have increasingly shifted toward optical engineering rather than relying solely on material optimization or fabrication processes [17]. These approaches are primarily based on two optical principles: (i) enhancing light transmission through anti-reflection (AR) effects, and (ii) increasing the photon absorption rate in the active layer by extending the optical path length [1]. Various light-management structures have been proposed for GaAs solar cells, including front-side nanostructures such as plasmonic scattering nanoparticles, textured window layers, dielectric coatings, and metallic back reflectors [18].

Anti-reflection coatings (ARCs) and textured surfaces are among the most common tools for reducing reflection and improving light absorption. ARC materials function by introducing a gradual refractive index transition between air and the solar cell surface, thereby minimizing reflection at optimized thicknesses [5, 17]. However, ARCs typically operate effectively only over a limited wavelength range and at specific incident angles. Moreover, issues such as thermal instability, poor adhesion, and sensitivity to thickness variations present additional challenges [5]. By contrast, textured surfaces not only suppress reflection but also scatter incoming light, thereby increasing its path length within the absorber layer and enhancing the probability of photon absorption [18]. These advantages make textured surfaces a promising strategy for improving short-circuit current density (JSC) and overall device efficiency in heterojunction Schottky solar cells [1, 19, 20]. By extending the optical path length, textured interfaces allow ultrathin solar cells to behave optically like thicker devices, enabling JSC values comparable to those of conventional thin-film GaAs cells with absorber thicknesses of 2–3 μm [18]. Among the efficient methods for achieving such surface modifications, ultraviolet nanoimprint lithography (UV-NIL) has emerged as a cost-effective, low-energy, and highly reproducible technique suitable for large-area fabrication of nanostructured surfaces [17].

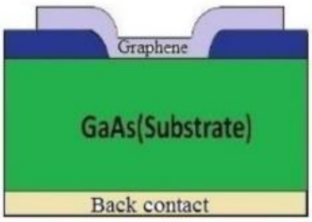
The interaction of light with textured surfaces strongly depends on the ratio between the structural dimensions and the incident wavelength. When the surface features are larger than the wavelength, reflection and diffraction dominate; conversely, for subwavelength structures, the textured interface behaves as an effective refractive index medium, where a gradual index transition reduces reflection and enhances light transmission [19].

Numerous studies have highlighted the effectiveness of these approaches. Abdullah et al. demonstrated that introducing conical textures on multicrystalline silicon significantly reduced surface reflection and improved JSC [16]. Similarly, Salman et al. reported that porous silicon (PS) provided superior reflection suppression compared with conventional pyramid structures, thereby enhancing the performance of crystalline silicon (c-Si) solar cells [21]. In another study, van der Wood et al. incorporated a GaP scattering layer into ultrathin GaAs solar cells, achieving a 6.7% increase in JSC relative to flat counterparts [18]. Song et al. further showed that employing nanotube and nanohole structures on the emitter surface of GaAs cells reduced surface reflection by up to 11%, boosting device efficiency from 4.25% to 7.15% [5]. In addition, Shoji et al. developed self-organized back-surface textures in InGaAs/GaAs quantum cells, enabling enhanced light trapping and extended optical path lengths, which significantly improved photovoltaic performance [22].

Despite extensive research on textured structures, the majority of studies have focused on silicon-based solar cells, leaving a notable research gap regarding nanostructures in GaAs devices. Given that experimental fabrication and testing of these cells are costly and time-intensive [5], numerical simulations offer a practical and efficient alternative for design optimization. In this work, we address the existing challenges in graphene/GaAs solar cells by designing and simulating novel structures using Silvaco TCAD software. Specifically, we investigate the effects of GaAs substrate thickness, graphene work function and layer number, as well as textured nanostructure configurations on device performance. The primary objective is to identify an optimized combination of material and structural parameters capable of enhancing power conversion efficiency (PCE), short-circuit current density (JSC), open-circuit voltage (VOC), and fill factor (FF). The outcomes of this study are expected to contribute to the development of a new generation of high-efficiency, low-cost graphene/GaAs solar cells.

2. Methodology

Fig. 1(a) illustrates a cross-sectional view of a graphene/gallium arsenide (GaAs) solar cell. The device consists of three main components arranged from bottom to top: a GaAs substrate, a silicon dioxide (SiO_2) layer, and a graphene layer. In this structure, a 10 nm-thick graphene layer is placed on top of the GaAs substrate, featuring a window of 1 µm × 12 µm within the oxide layer. The SiO_2 layer on both sides functions as an insulator, preventing direct contact between the top electrode and the GaAs semiconductor.



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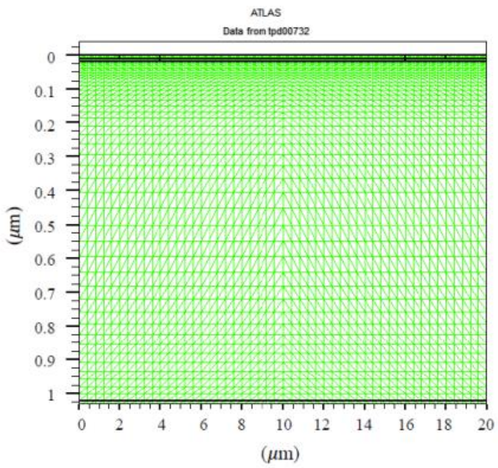


(b)

Fig. 1. (a) Cross-sectional view of the graphene/gallium arsenide (GaAs) Schottky-junction solar cell. (b) The designed mesh model of the structure.

Fig. 1(b) illustrates the simulated structure of the solar cell modeled using TCAD software. In the device modeling process within TCAD, the first step is the-mesh definition. The mesh must be designed to ensure computational accuracy while minimizing simulation time. In this model, a denser mesh is employed in the upper region of the structure, where the interfaces between graphene and GaAs, as well as between graphene and the oxide layer, are located. Simulation results indicate that the graphene–GaAs contact forms a Schottky junction, which is favorable for generating a strong built-in electric field. When sunlight irradiates the graphene/GaAs solar cell, electron–hole pairs are generated and subsequently separated by the electric field at the Schottky junction, eventually collected at the electrodes. Since graphene is recognized as a novel material and is not included as a default entry in the material library of Silvaco Atlas, the simulation of graphene-based solar cells in the TCAD environment is typically carried out in two stages. In the first stage, one of the predefined materials in Silvaco is used as the graphene layer in the device structure.

In the second stage, the properties of this material are redefined to match the physical characteristics of graphene within the Atlas tool. However, in the present study, graphene was directly introduced into Silvaco as a new material, and its absorption coefficient was defined using an n-k file to ensure closer agreement between the simulation results and experimental data. In this modeling, graphene was considered a semi-metal with a carrier mobility of 15,000 $cm^2/V{\cdot}s$.

In this study, the designed solar cell was simulated under standard 1.5 AM illumination with an irradiation intensity of 1000 mW/cm^2. This solar spectrum covers the full range of sunlight wavelengths, thereby providing realistic optical conditions for evaluating device performance. To accurately model the internal physical processes, the thermionic emission (TE) model was employed. In addition, physical models describing electron and hole mobility were incorporated to simulate carrier transport within the structure. To further analyze recombination phenomena, the Auger recombination model was applied to calculate recombination rates in both the bulk and surface regions of the cell. The system of equations for this simulation was solved using Newton's Method, which offers high accuracy for nonlinear systems.

Key parameters that govern solar cell performance include short-circuit current (Isc), open-circuit voltage (Voc), and fill factor (FF). These parameters were extracted using the Atlas simulation code.

Table 1 presents the physical and electrical parameters used in the simulation, specifically related to GaAs substrate.

Table 1. The physical and electrical parameters of gallium arsenide used in the simulation [23].

Parameter	Definition	Value
E_g	Bandgap energy of GaAs semiconductor	$1.42eV$
N_c	Effective density of states in the conduction band	$4.35 \times 10^{17} cm^{-3}$
N_v	Effective density of states in the valence band	$8.16 \times 10^{18} cm^{-3}$
χ	Electron affinity of GaAs	$4.07eV$
μ_e	Electron mobility in GaAs at 300 K	$8000\ cm^2/Vs$
μ_h	Hole mobility in GaAs at 300 K	$400\ cm^2/Vs$

When light irradiates the surface of a solar cell, three phenomena may occur: reflection, absorption, or transmission. In the present structure, the majority of the incident light is absorbed within the barrier region and the semiconductor substrate. In this study, GaAs crystal was selected as the primary absorber layer. The graphene layer, serving as a transparent electrode, allows more light to penetrate into the GaAs crystal, thereby increasing the generation of photocarriers.

To investigate the effect of GaAs substrate thickness on cell performance, the current–voltage (I–V) characteristics were simulated and are shown in Figure 2. The highest density of photogenerated carriers occurs near the graphene/GaAs interface at the top region of the substrate. The results indicate that for thicknesses below 4 μm, increasing the substrate thickness enhances light absorption and improves efficiency. However, in the range of 5–10 μm, the efficiency decreases unexpectedly. Consequently, the photocurrent exhibits an optimal value at a specific substrate thickness, with the maximum power conversion efficiency (PCE) reaching approximately 1.189%.

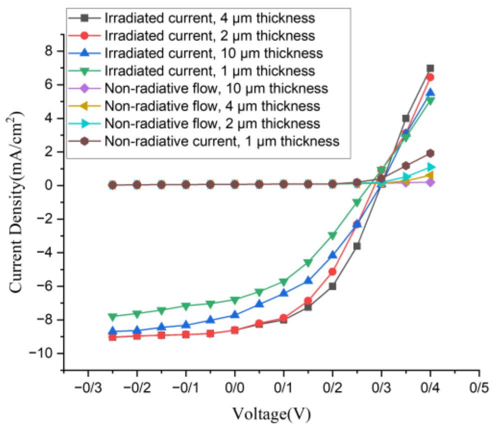
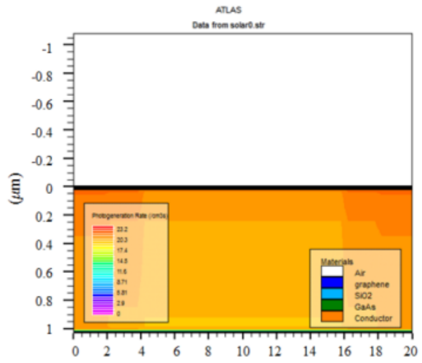


Fig. 2. Comparison of the current–voltage (I–V) characteristics of the graphene/GaAs solar cell for different GaAs substrate thicknesses.

Fig. 3 (a–d) represents the carrier generation rate in the graphene/GaAs solar cell under AM1.5 illumination for different absorber thicknesses. As observed, the most effective absorption region is located near the junction, extending to a depth of approximately 0.1 μm. Furthermore, Figure 3(c) demonstrates that a thickness of 4 μm is sufficient for complete spectral absorption, since the number of photogenerated carriers decreases significantly in the deeper regions of the GaAs substrate.



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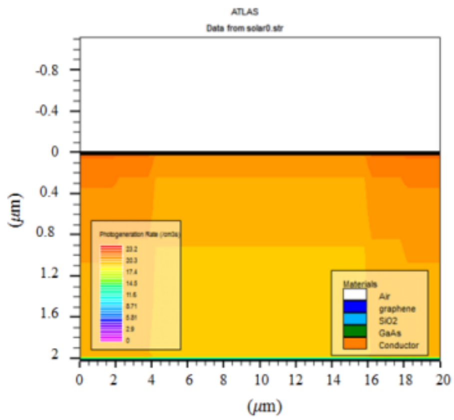

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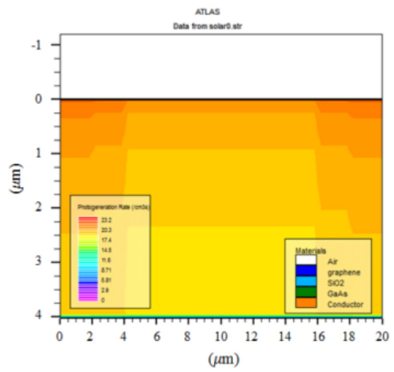

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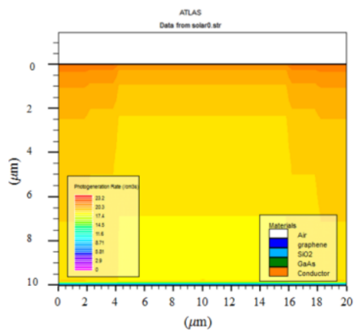


(d)

Fig. 3. Carrier generation rate in the graphene/GaAs solar cell under AM1.5 illumination standard for different substrate thicknesses: (a) 1 μm, (b) 2 μm, (c) 4 μm, and (d) 10 μm.

In addition, to evaluate the performance of this solar cell, its key parameters were simulated under 1.5 AM illumination for absorber layer thicknesses ranging from 1 to 10 μm. The obtained results are presented in Figures 4 to 7.

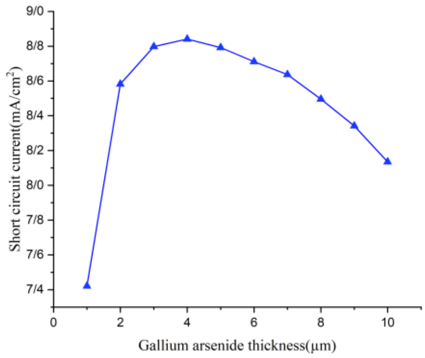


Fig. 4. Variation of short-circuit current density with GaAs substrate thickness.

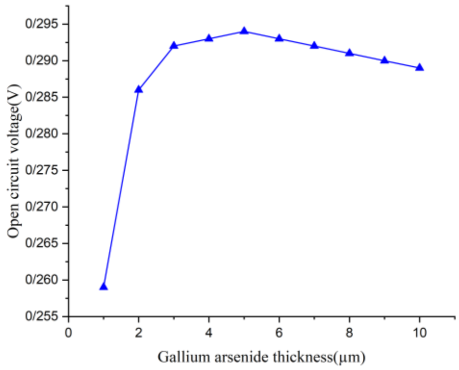


Fig. 5. Variation of open-circuit voltage with GaAs substrate thickness.

As observed in the simulation results, increasing the GaAs absorber layer thickness beyond 4 μm leads to a significant reduction in the short-circuit current density (Jsc), open-circuit voltage (Voc), fill factor (FF), and overall power conversion efficiency (PCE) of the solar cell. This performance degradation is primarily attributed to enhanced carrier recombination processes, which are strongly dependent on the depletion width and substrate thickness. In this simulation, while the Schottky barrier height was kept constant, increasing the absorber thickness forced the photogenerated electrons and holes to travel longer distances before reaching the electrodes. This extended path length increases the probability of recombination within the bulk material, thereby reducing the number of carriers that contribute to useful photocurrent.

Therefore, although thicker layers can provide higher optical absorption, excessive thickness (greater than ~4 μm) decreases carrier collection efficiency and ultimately reduces both the electrical performance and the overall efficiency of the solar cell.

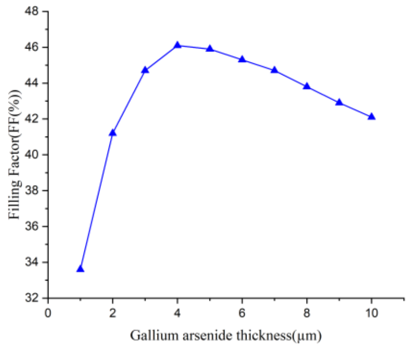


Fig. 6. Variation of fill factor with GaAs substrate thickness.

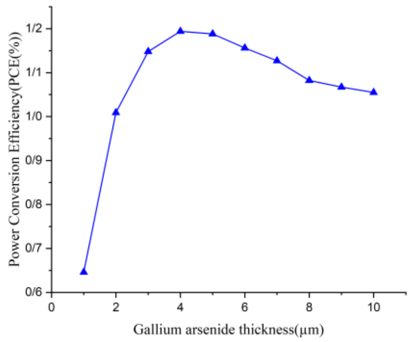


Fig. 7. Power conversion efficiency variation with GaAs substrate thickness.

According to the findings reported in Ref. [23], the effect of GaAs substrate thickness on the performance of graphene/GaAs-based solar cells was investigated using advanced numerical simulations at four different thickness levels. The results, summarized in Table 2, indicate that increasing the substrate thickness up to approximately 5 μm leads to a considerable enhancement in key performance parameters, including Jsc, Voc, FF, and PCE. This improvement is mainly attributed to enhanced light absorption and more efficient charge carrier generation and collection within the moderately thicker substrate.

However, further increasing the substrate thickness beyond this value results in a pronounced decline in cell efficiency. The primary reason for this degradation is the intensification of carrier recombination in thicker layers, as photogenerated electrons and holes are required to travel longer distances to reach the electrodes, thereby increasing the probability of non-radiative recombination.

This behavior reflects a trade-off between two competing effects: on one hand, a thicker substrate improves light absorption and enhances carrier generation; on the other hand, excessive thickness reduces carrier collection efficiency and increases recombination losses. Therefore, determining the optimal substrate thickness plays a crucial role in improving the overall photovoltaic performance of the device.

Table 2. Effect of GaAs substrate thickness on the performance characteristics of the solar cell.

Cell	GaAs Thickness (μm)	J_{sc} (mA/cm²)	V_{oc} (V)	FF	η(%)
Present Work	1	7.421	0.259	0.336	0.646
	2	8.582	0.286	0.412	1.009
	5	8.792	0.294	0.459	1.188
	10	8.135	0.289	0.421	1.055
Ref. [23]	1	7.082	0.255	0.344	0.772
	2	8.483	0.268	0.406	1.174
	5	8.261	0.281	0.473	1.392
	10	7.519	0.289	0.433	1.196

The effect of graphene's work function and its optical properties on the performance of the graphene/gallium arsenide (GaAs) solar cell has been evaluated. Figure 8 illustrates the current–voltage (I–V) characteristics of three different structures where graphene with varying numbers of layers and work functions (4.4, 4.55, and 4.8 eV) was employed as a transparent electrode.

An increase in the graphene work function leads to a higher Schottky barrier height at the graphene/GaAs interface. For instance, with a work function of 4.4 eV, the open-circuit voltage (Voc) is 0.246 V, whereas increasing the work function to 4.55 eV and 4.8 eV raises Voc to 0.287 V and 0.285 V, respectively. This improvement in Voc can be attributed to the larger difference between the graphene work function and the electron affinity of GaAs, which results in a higher potential barrier and reduced carrier recombination rate at the interface.

Despite the increase in Voc, the variations in Jsc exhibit a more complex behavior. Specifically, for graphene with a 4.4 eV work function, Jsc is 8.947 mA/cm^2; this value slightly decreases to 8.912 mA/cm^2 when the work function increases to 4.55 eV. The reduction becomes more significant at 4.8 eV, where Jsc drops to 8.037 mA/cm^2. This decline can be explained by the reduced optical transparency of multilayer graphene, as each additional graphene layer absorbs approximately 2.3% of the incident light, thereby lowering the light intensity reaching the absorber substrate.

The fill factor (FF) also improves with increasing graphene work function. For graphene with a work function of 4.4 eV, FF is 0.412, which increases to 0.462 and 0.476 for work functions of 4.55 eV and 4.8 eV, respectively. This improvement can be attributed to the reduction in of series resistance with the addition of graphene layers and the enhancement of electrical contact quality.

The power conversion efficiency (η) of the investigated solar cells exhibits a similar increasing trend with the graphene work function, rising from 0.906% for 4.4 eV to 1.181% for 4.55 eV and 1.090% for 4.8 eV. It is noteworthy that the highest efficiency is achieved at a graphene work function of 4.55 eV, which provides a favorable balance among open-circuit voltage (Voc), Jsc, and FF.

Although the 4.8 eV graphene electrode yields the highest Voc and FF, the pronounced reduction in Jsc results in a lower overall efficiency compared to the 4.55 eV case.

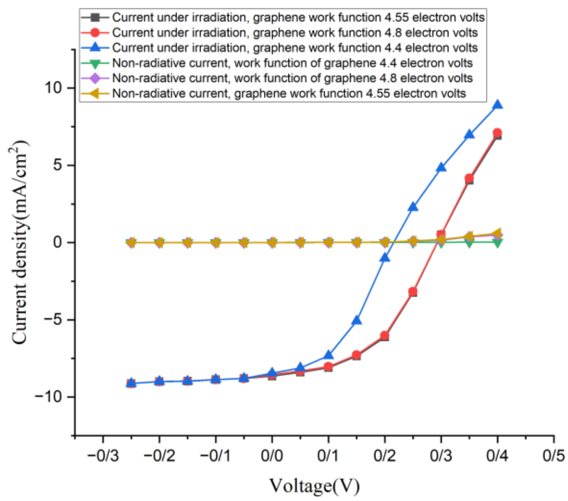
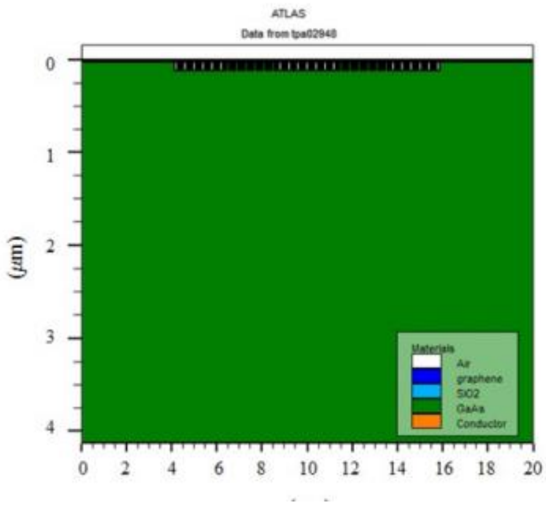


Fig. 8. Current–voltage (I–V) characteristics of the graphene/gallium arsenide solar cell considering three different graphene work function values.

The effect of the number of graphene layers on solar cell performance was further simulated using Silvaco software, and the results are presented in Table 3. The analysis indicates that the simulation results for six-layer graphene differ from the data reported in–Ref. [23], but they are consistent with the experimental results reported in Ref. [24]. According to [24], increasing the number of graphene layers up to three enhances the device efficiency, whereas further increases in layer count leads to performance degradation.

Table 3. Comparative analysis of the effect of graphene layer number on solar cell performance parameters.

Cell	Graphene Work Function [eV]	J_{sc}(mA/cm^2)	V_{oc}(V)	FF	η(%)
Present Work	4.4	8.947	0.246	0.412	0.906
	4.55	8.912	0.287	0.462	1.181
	4.8	8.037	0.285	0.476	1.090
Ref. [23]	4.4	8.613	0.263	0.451	1.298
	4.55	8.261	0.281	0.473	1.392
	4.8	7.951	0.296	0.496	1.481



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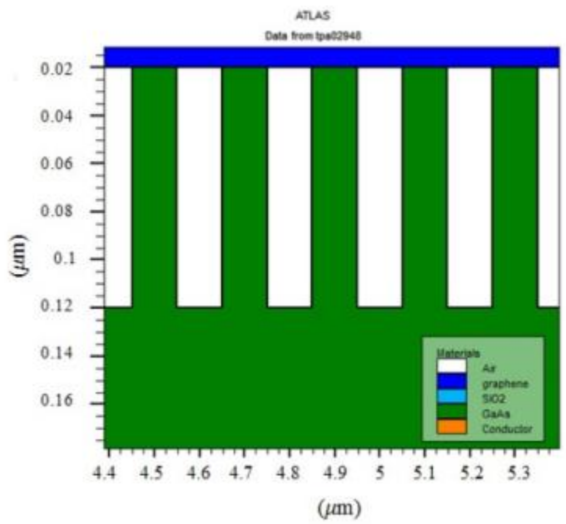

(b)

Fig. 9. (a) Schematic diagram of the rectangular nanograting structure on the graphene/GaAs solar cell. (b) Two-dimensional simulation model of the nanograting structure.

To enhance light absorption and improve the performance of the graphene/gallium arsenide (GaAs) solar cell, rectangular nanograting structures were introduced at the metal/semiconductor interface (Fig. 9). In this study, the drift–diffusion physical model under AM1.5 illumination was employed to evaluate the device performance for gratings with different periodicities. The initial design incorporated a nanograting with a fixed height of 100 nm and a period of 100 nm implemented on the GaAs substrate. The grating period was then gradually increased up to 800 nm, and the corresponding performance parameters—including efficiency and fill factor—were simulated.

The simulation results, presented in Figures 10 and 11, indicate that the cell performance exhibits a distinctly nonlinear dependence on the grating period. As shown in Figure 10, the maximum power conversion efficiency was achieved at a grating period of 200 nm, reaching approximately 2.005%, which represents a significant improvement compared to the device without gratings. Beyond this point, the efficiency decreased with further increase in period and eventually reached a nearly saturated state at larger values.

Fig. 11 shows the variation in the FF for different grating periods. The maximum FF was observed at a period of 100 nm; however, at 200 nm—where the efficiency reached its peak—the FF decreased to about 66.82%. This finding suggests that the improvement in device performance primarily originates from enhanced optical absorption and photocurrent generation rather than electrical parameters such as the fill factor.

Overall, it can be concluded that the rectangular nanograting structure with a period of 200 nm and a height of 100 nm effectively behaving like a square grating provides the best performance response. These results are consistent with previous studies, such as Ref. [25], and highlight the importance of optimizing nanograting dimensions in the design of high-efficiency solar cells. Specifically, the enhanced light trapping induced by the grating structure plays a critical role in improving power conversion efficiency, underscoring the potential of precise geometric engineering in the development of next-generation graphene-based solar cells.

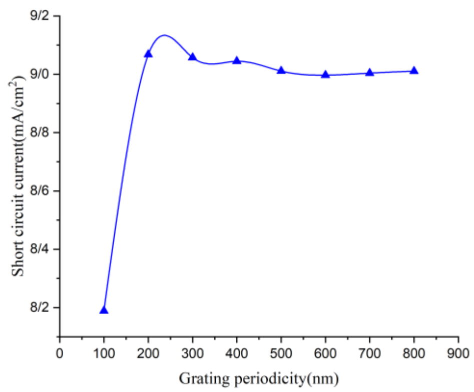

Fig. 10. Variation of short-circuit current with the periodicity of the rectangular nanograting.

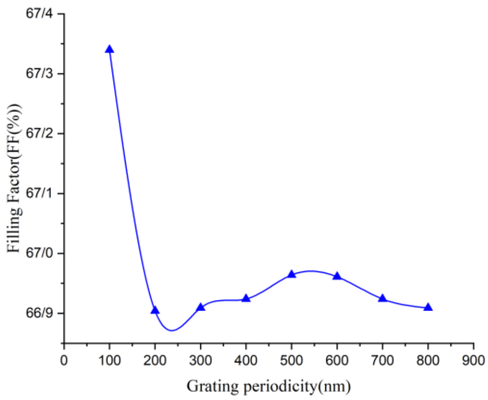

Fig. 11. Variation of fill factor with the periodicity of the rectangular nanograting.

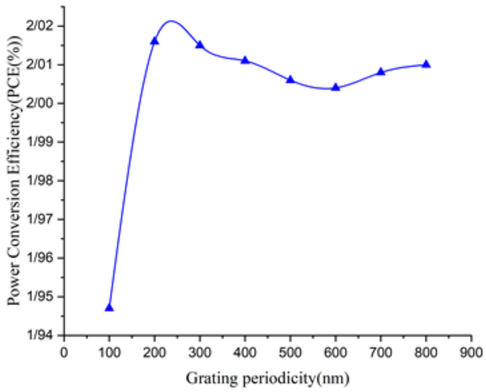

Fig. 12. Variation of power conversion efficiency with the periodicity of the rectangular nanograting.

Next, the simulation of the rectangular–rectangular nanograting structure, which includes both top and bottom gratings, is presented. The top grating directs more light into the solar cell through diffraction effects, leading to enhanced light absorption and improved overall cell efficiency. At the bottom surface, the reflective grating is designed so that the transmitted light, which is not absorbed by the cell on the first pass, is reflected back, providing another opportunity for absorption. This process increases energy-conversion efficiency to 2.01%. It should be noted, however, that this efficiency improvement is smaller compared to that of the top-surface nanograting, and the enhancement effect in this structure is relatively limited.

3. Conclusions

In this study, numerical simulations using Silvaco software were conducted to improve the performance of graphene/gallium arsenide (GaAs)-based Schottky solar cells. The main objective was to analyze the impact of structural parameters—including substrate thickness, number of graphene layers, graphene work function, and nanograting designs—on key performance indicators such as open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and power conversion efficiency (PCE).

The results demonstrated that employing three layers of graphene with a work function of approximately 4.55 eV, combined with a GaAs substrate thickness of 4 μm, yielded the most optimal optoelectronic performance. While increasing the substrate thickness can enhance light absorption, excessive thickness leads to elevated carrier recombination, thus underscoring the importance of identifying an optimal thickness for effective charge collection. Additionally, increasing the graphene work function enhanced the Schottky barrier height and reduced carrier recombination at the interface, as reflected by improvements in V_{oc} and FF. However, multilayer graphene reduced optical transparency, leading to a drop in J_{sc}. This highlights the need to balance the number of layers with against electrical and optical properties to achieve maximum efficiency. Moreover, introducing rectangular nanograting structures—particularly with a 200 nm period and 100 nm height—resulted in a significant efficiency increase up to approximately 2.05%. The use of combined top and bottom grating layers further improved light trapping and raised efficiency to around 2.01%. These findings emphasize the critical role of geometric optimization in nanostructures to enhance light absorption and overall device performance.

In conclusion, this research demonstrates that the integration of advanced materials like graphene with optimized geometrical design and engineered physical parameters can pave the way for developing a new generation of solar cells that are both highly efficient and structurally simple.

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Conflicts of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Authors Contribution Statement

Yaser Shamsi: Data analysis and experimentation, Manuscript writing and editing, Data analysis and

interpretation. **Abdolrahim Baharvand and Amin Salehi**: Conceptualization and study design, Manuscript writing and editing, Data analysis and interpretation, Supervision and project administration.

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