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Light Trapping Performance of Amorphous Silicon Thin-Film-based Photovoltaic Devices: Modelling and Simulation

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Abstract

A fundamental understanding of the optical and electrical characteristics of thin-film-based photovoltaic devices is essential for their rapid prototyping. Mathematical modeling and computer simulations play a crucial role in this process, particularly for the inherently complex semiconductor nanomaterial-based solar cells. This study employs Silvaco Atlas, a commercial computer-aided design software, to model plasmonic gold nanoparticle-doped amorphous silicon thin-film photovoltaic devices. The incorporation of gold nanoparticles was found to enhance light trapping, resulting in improved optical and electrical performance. Specifically, the enhancement in current-voltage characteristics and external quantum efficiency under illumination was attributed to photon scattering mediated by gold nanoparticles. Furthermore, localized surface plasmon resonance interactions reduced carrier recombination rates in the photoactive layer, thereby enhancing photovoltaic performance. The achieved fill factor of 83.33% surpasses the reported state-of-the-art simulation value of 77.79%. Future research should explore the integration of other plasmonic materials and optimization of nanoparticle distribution for further improvements in device efficiency.

Keywords: *Plasmonic Au nanoparticles, light trapping, modelling and simulation, amorphous Si thin-film, photovoltaic devices.*

INTRODUCTION

Solar radiation trapping by various plasmonic metal nanoparticles became a promising route to improve the performance of semiconductors thin-films-based photovoltaic (PV) devices made of GaAs, polysilicon, and organic materials (Zemi et al., 2021). Metal nanoparticles embedded in PV architectures can induce plasmons in the form of surface oscillations of conduction electrons in metal nanoparticles, enabling the trapping of light by the excitation of localized surface plasmon resonance (LSPR). For deeper understanding of the plasmonic effects of metal nanoparticles on the overall performance of thin-film PV devices various advanced optoelectronic modelling tools have been developed. These tools can be used to simulate the optical and electrical characteristics of these PV devices simultaneously, providing some basic insight into the solar cells' efficiency enhancement. It is known that the engineering of plasmonic PV devices requires the unification of optical (light scattering) and electrical effects to optimize their performance (Arefinia, 2020). The knowledge regarding such combined effects and their relationship can be advantageous for the design of plasmonic PV devices.

The optical and electrical modelling for light trapping in thin film amorphous silicon photovoltaic devices play a decisive role to optimize the device architecture by simultaneously optimizing the optical and electrical properties(Zemi et al., 2021)1. This may lead to a detailed understanding of the plasmonic PV cells wherein advanced tools can be beneficial for rapid prototyping. The influence of light for the combination of different window layers on the CdTe thin film solar cells performance was fully evaluated(Yadav et al., 2020). Matching the n-type partner with the CdTe absorber layer has been very effective for increasing the efficiency of the thin-film solar cell (Hossen et al., 2026). Also, the minority carrier generation, carrier collection, and recombination rate at the p-n junction are directly affected by the composition of the window layer. Various advanced models have been implemented to simulate the light trapping phenomenon of plasmonic metal nanoparticle structures for PV applications(Doroody et al., 2022).

Over the years, various computer-aided design (TCAD) software packages have been developed to simulate the working of PV devices, leading to the solar cells' parameters optimization(Thirunavukkarasu et al., 2021). Several challenges exist in the design of complex plasmonic devices and/or calculations of optoelectronic interactions of the plasmonic structures when coupled with the device science. Shameli and Yousefi demonstrated the impact of plasmonic nanoparticles incorporation into amorphous silicon (a-SiH) thin-film (n-i-p)-based PV devices wherein the device performance was evaluated in the superstrate configuration(Shameli et al., 2021). It has been realized that for rapid prototyping of PV devices with improved efficiency, accurate models are essential to simulate the optoelectronic characteristics. Meanwhile, it has been acknowledged that the design and simulation time complexity of the novel PV devices increases with the inclusion of plasmonic metal nanostructures into their. Despite various model-based simulation studies, a comprehensive knowledge regarding the optimization of the electrical and optical characteristics of the plasmonic nanostructures-doped solar cells remain deficient (Alam et al., 2025).

In this perception, a commercial computer-aided design (TCAD) software called Silvaco Atlas was used to design and model the plasmonic gold nanoparticles-doped amorphous silicon thin-film PV cells. The main aim is the develop a relationship between the optical and electrical characteristics of the proposed PV device, unravelling the role of gold nanoparticles towards the improvement of cell performance (Mohd Pauzi & Shahadat Hossen, 2025). After lighting the PV device, the optical and electrical properties were simulated simultaneously to determine the current–voltage (J–V) relationship and external quantum efficiency of the cell. The simulation results indicated that light trapping due to scattering and localized surface plasmon resonance interactions by nanoparticles has led to the optical and electrical properties enhancement, thus improving the cell performance. Essentially, the carriers' recombination rates in the photoactive layer were reduced due to the presence of gold nanoparticles in the amorphous silicon thin films. In brief, the developed model provided a route to optimize the device architecture by simultaneously optimizing the optical and electrical properties, leading to an in-depth understanding of the plasmonic PV cells design and rapid prototyping using advanced tools (Alam et al., 2025).

Methodology

Simulation Framework

The modeling and simulation of plasmonic gold nanoparticles-doped amorphous silicon thin-film photovoltaic (PV) devices were conducted using Silvaco Atlas, a robust technology computer-aided design (TCAD) software. This software enables the concurrent simulation of optical and electrical properties, which is crucial for optimizing complex photovoltaic architectures. The focus was to explore how localized surface plasmon resonance (LSPR) effects induced by gold nanoparticles (AuNPs) influence the performance of thin-film-based PV cells.

Device Structure and Material Parameters

The proposed PV device model comprised a photoactive amorphous silicon (a-Si:H) layer doped with uniformly distributed AuNPs. The incorporation of AuNPs was hypothesized to enhance photon trapping through plasmonic scattering and resonance effects. The structural and material parameters for the device were selected based on reported experimental studies to ensure accurate and reliable simulations. Parameters such as layer thickness, refractive index, absorption coefficient, and doping concentration were defined in alignment with standard practices (Hossen et al., 2023)**.**

Optical Simulation

The optical characteristics of the device were evaluated using the ray tracing and finite-difference time-domain (FDTD) methods integrated within the Silvaco Atlas framework. These methods enabled the assessment of light absorption, scattering, and trapping facilitated by the LSPR effects of AuNPs. Key metrics such as the absorption profile and photogeneration rate were extracted to analyze the light-trapping efficacy.

Electrical Simulation

The electrical characteristics of the device, including current-voltage (I-V) behavior, fill factor (FF), and external quantum efficiency (EQE), were simulated under standard AM1.5G solar illumination. The simulations accounted for the role of AuNPs in reducing carrier recombination and improving charge transport in the photoactive layer. Drift-diffusion equations were solved to model charge carrier dynamics, including generation, recombination, and transport processes (Rashed et al., 2025).

Validation and Optimization

The developed model was validated against existing literature data to ensure its accuracy and reliability. Comparative analyses were performed to benchmark the simulated results, particularly the achieved fill factor (83.33%) and EQE improvements, against reported state-of-the-art devices. Furthermore, iterative optimizations were carried out to refine the device architecture, ensuring simultaneous enhancements in both optical and electrical performance.

Data Analysis

The simulated data were systematically analyzed to derive insights into the effects of plasmonic doping on device performance. Key performance indicators (KPIs) such as short-circuit current density (Jsc), open-circuit voltage (Voc), and FF were evaluated to determine the efficacy of the proposed design. Discussions were aligned with theoretical predictions and experimental observations in the literature.

Results and Discussion

Figure 1 displays the plasmonic gold nanoparticles-doped PV cell structure used in the studied model. An advanced optoelectronic device simulation method was used to simultaneously optimize the electrical and optical properties of the plasmonic PV device. Improvements in the PV device performance was aided by increasing the localized light generation rate in the vicinity of nanoparticles and light scattering from LSP excited in the nanoparticles.

Silvaco Atlas TCAD software provided a comprehensive analysis of the underlying mechanism at the nanoscale, facilitating for the design and optimization of the plasmon-mediated PV device. In addition, this advanced tool enabled to virtually design and prototyping the optimized PV device, demonstrating the advantages of plasmonic operation in two different modes and affirming a relative improvement in a-SiH plasmonic PV power conversion efficiency (Rahman et al., 2025).

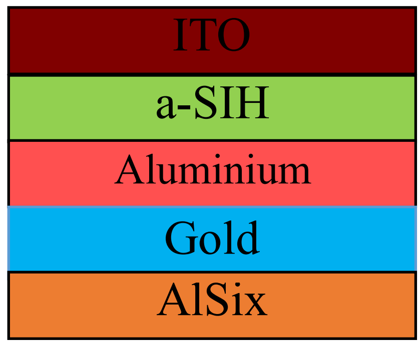

Figure 1: Plasmonic gold nanoparticles-doped amorphous Si thin-film-based PV cell structure.

The simulation tool was used to simultaneously model the optical and electrical effects of plasmonic nanoparticles, generating the equivalent J-V curves (Figure 2). The total grated recombination rate was calculated from the dark J-V curves, thus estimating the recombination current contribution to the leakage current of the reverse biased diode.

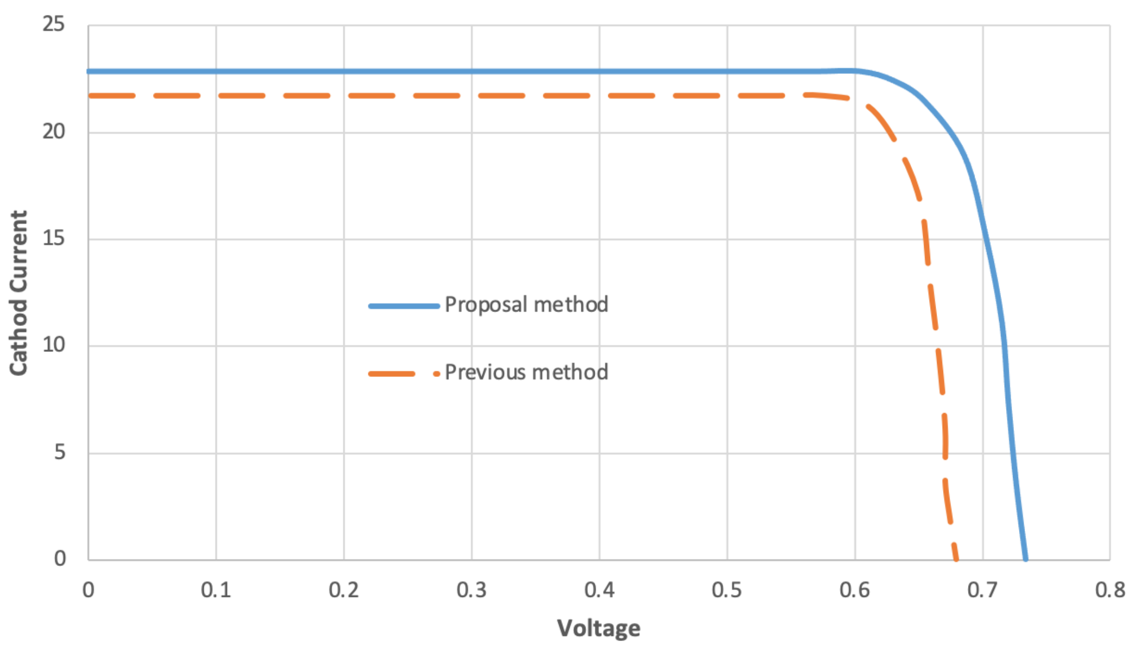

Figure 2: Comparison of the current-voltage response of the proposed structure with previous work.

The substrate of the PV cell was modelled based on a silicon dioxide (SiO_2)/indium tin oxide (ITO)/a-SiH/aluminium (Al) structure with 24.6 µm thick SiO_2 buffer layer. In this novel design, the thickness of the ITO layer was 100 nm that acted as the front transparent conductive electrode, the n-i-p a-SiH active layer thickness was 200 nm and Al back electrode thickness was 100 nm with a total cell thickness of 25 µm. The proposed PV cell designed in the substrate configuration was exposed to sunlight. Light was absorbed by the stratified layers made of transparent substrate glass (SiO_2) and transparent conductive oxide (ITO) layer, and partially absorbed by the amorphous silicon layer (Hossen & Pauzi, 2025). The unabsorbed light is reflected. The plasmonic gold nanoparticles of diameter range 10 to 30 nm were embedded between the ITO and SiO_2 substrate and between ITO and a-SiH active layer as shown in Figures 3 and 4.

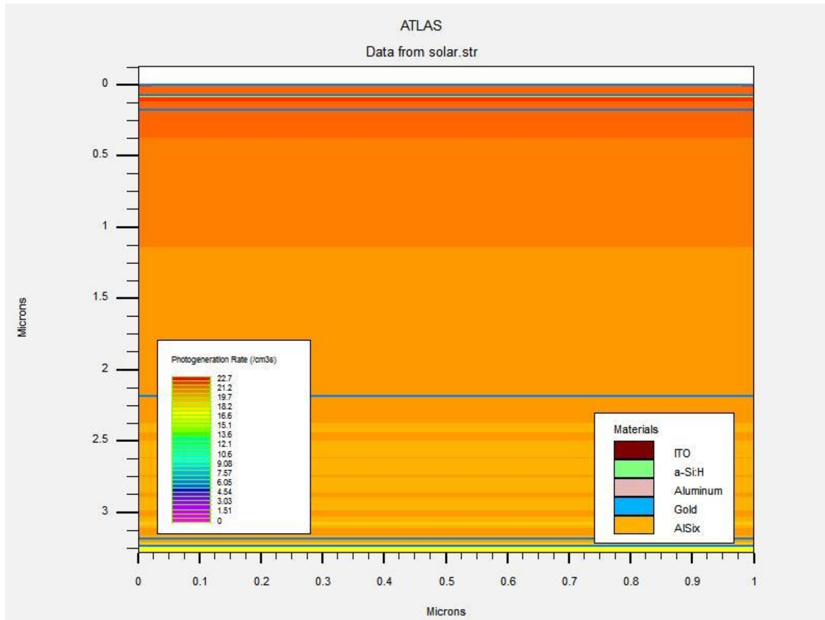

Figure 3: The doping structure of the PV device.

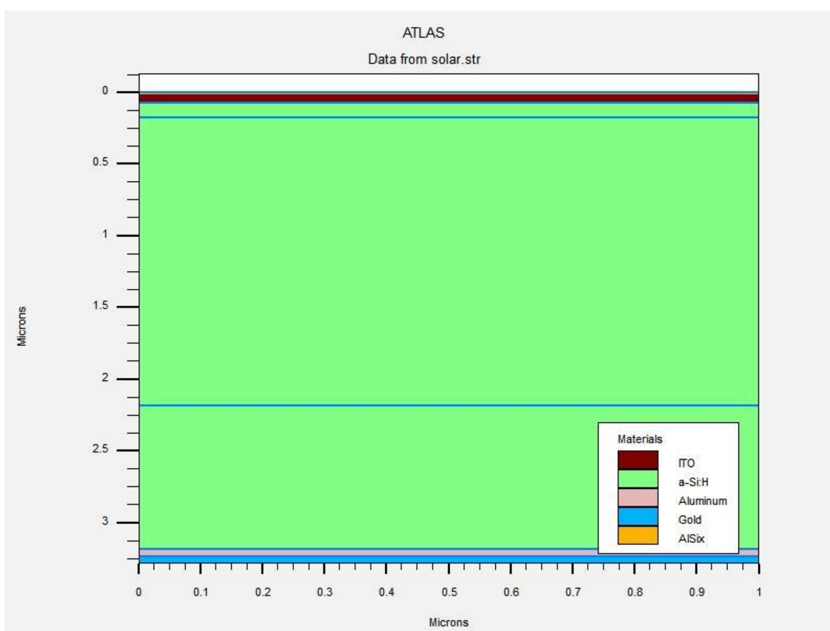

Figure 4: Simulated structure of the plasmonic au nanoparticles-doped PV device.

Table 1 compares the results of the proposed work with the previous work reported in the recent literature.

	Proposed Work	Previous Work
jsc	23.2	22.1
Voc	0.72	0.69
FF	83.33	82.78
EFF	15.38	14.76

It was observed that advanced optoelectronic device simulation method for the simultaneous optimization of the electrical and optical properties of plasmonic nanoparticles-incorporated PV devices can be more efficient than the one without nanoparticles doping. The obtained improvements in the PV devices performance can be mainly attributed to the increasing the rate of localized light generation in the vicinity of the nanoparticles and light scattering from the LSP excited in the nanoparticles. It was asserted that Silvaco Atlas TCAD software can provide a comprehensive understanding of the physical phenomena at the nanoscale, indicating a feasibility to design and optimize plasmon nanoparticles activated PV devices. In addition, device performance of modelled a-SiH PV cells was significantly affected by the presence of plasmonic nanoparticles, wherein the position and morphology of gold nanoparticles played a vital role. The achieved improvement in the optical properties or both optical and electrical characteristics was mainly due to LSPR-mediated strong local electromagnetic effects. The studied model provided a route to optimize the device architecture by simultaneously optimizing the optical and electrical properties, leading to a detailed understanding of plasmonic PV cells. This observation can be beneficial from the design perspective that may provide an advanced tool for rapid device prototyping and simulation. The obtained fill factor of the designed device was 83.33, which is higher compared to the previous work (77.79). In short, light management being a fundamental aspect to improve the conversion efficiency of solar cells and photovoltaic devices more intensive studies are required in future to determine the spectral responses (reflection and absorption characteristics) of arrays of random silicon nanowires (Si-NWs) with various lengths and doping types.

Conclusion

The photovoltaic performance of some gold nanoparticles-doped amorphous silicon thin-film solar cells were determined using model and simulation. The commercial Silvaco Atlas software was used to model plasmonic amorphous silicon thin-film-based photovoltaic devices. It was shown that the overall performance of the proposed thin-film-based photovoltaic devices can be improved by doping plasmonic gold nanoparticles, affecting the optical and electrical properties of the cells. Gold nanoparticles-mediated localized surface plasmon resonance interactions and scattering made significant contribution to the enhanced trapping of light, leading to the improvement in the current-voltage traits and quantum efficiency of studied PV devices. The presence of gold nanoparticles contributed to the decrease of carrier recombination rates in the photoactive layer, improving the photovoltaic performance (high fill factor of 83.33). It was affirmed that our result is much better than the existing reported values of fill factor 77.79. Present work may be beneficial the development of high-performance solar cells, leading to sustainable growth.

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Data Availability: The author has all the data employed in this research and is open to sharing it upon reasonable request.

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