Particle Swarm Optimization-Based Performance Enhancement of Cadmium Telluride Thin-Film Solar Cells by Embedded Nano-Grating Structures

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Abstract

The performance of cadmium telluride (CdTe) thin-film solar cells is significantly impacted by optical and electrical inefficiencies, which limit their energy conversion capabilities. This study investigates an advanced method to enhance the efficiency of CdTe solar cells by incorporating embedded nano-grating structures optimized using particle swarm optimization (PSO). The PSO algorithm systematically fine-tunes the nano-grating parameters to maximize light absorption and carrier collection, thereby improving power conversion efficiency (PCE). Through extensive computational simulations, we identify the optimal nano-grating configuration that reduces optical losses and enhances charge transport. The optimized design achieves a significant increase in light-trapping efficiency, contributing to higher absorption in the active layer. Compared to conventional CdTe solar cells, the proposed approach results in a notable enhancement in short-circuit current density (Jsc) and overall PCE. The integration of nano-grating structures offers a scalable and efficient solution for improving thin-film solar cell performance. These findings underscore the potential of PSO-driven nano-structuring as a transformative approach in photovoltaic technology. Future research will focus on experimental validation and fabrication techniques to transition this optimization strategy into practical applications. The results presented in this study pave the way for the large-scale implementation of nano-grating-enhanced CdTe solar cells, offering a promising avenue for the development of next-generation high-efficiency thin-film photovoltaic systems.

Keywords: Cadmium telluride, thin-film solar cells, nano-grating, particle swarm optimization, light trapping

1. Introduction

Cadmium telluride (CdTe) thin-film solar cells have emerged as one of the most promising candidates for cost-effective and high-efficiency photovoltaic technology. CdTe possesses a nearly ideal bandgap of ~1.45 eV for solar energy conversion, making it highly suitable for absorbing a broad spectrum of sunlight. Additionally, its high absorption coefficient allows for the fabrication of thinner absorber layers compared to silicon-based solar cells, reducing material costs and improving scalability. However, despite these advantages, CdTe solar cells suffer from inherent optical and electrical losses that limit their efficiency [1]. Optical losses primarily result from reflection at the interfaces and incomplete absorption of incident light, while electrical losses arise from recombination at grain boundaries and interfaces.

To address these limitations, various light management strategies have been proposed, including the use of anti-reflective coatings, surface texturing, and plasmonic nanostructures [2]. Among these, nano-grating structures have gained significant attention due to their ability to enhance light trapping through diffraction and guided-mode resonance effects. Nano-gratings effectively increase the optical path length within the active layer, enabling higher absorption of incident photons and improving overall device performance. However, designing an optimal nano-grating structure involves multiple parameters, such as grating period, depth, and duty cycle, which influence light interaction and charge carrier dynamics [3].

In this study, we employ particle swarm optimization (PSO) to determine the optimal nano-grating design for CdTe thin-film solar cells. PSO is a robust metaheuristic optimization algorithm inspired by the collective behavior of biological swarms [4]. It efficiently searches the design space by iteratively updating candidate solutions based on individual and global best positions, converging toward an optimal set of parameters that maximize light absorption and carrier collection.

The effectiveness of the proposed approach is validated through numerical simulations using the Finite-Difference Time-Domain (FDTD) method for optical analysis and Sentaurus TCAD simulations for electrical characterization [5]. Our results demonstrate a significant improvement in power conversion efficiency (PCE), showcasing the potential of PSO-optimized nano-gratings as a viable strategy for next-generation CdTe solar cells. Furthermore, the scalability of this technique makes it suitable for large-area manufacturing, facilitating its integration into commercial photovoltaic modules.

2. Related Work

A. CdTe Thin-Film Solar Cells

Cadmium telluride (CdTe) is a widely used material in thin-film photovoltaic technology due to its near-ideal direct bandgap of approximately 1.45 eV, which is optimal for solar energy conversion. CdTe thin-film solar cells exhibit high absorption coefficients, enabling efficient light absorption within a few micrometers of thickness [6]. Despite these advantages, the performance of CdTe cells is hindered by optical and electrical losses. Optical losses include reflection at the front surface and insufficient light trapping within the absorber layer, whereas electrical losses stem from recombination at interfaces, grain boundaries, and defects within the material [7]. Strategies to mitigate these losses and enhance efficiency include bandgap engineering, doping, passivation techniques, and structural modifications such as nano-patterning.

B. Nano-Grating Structures

Nano-grating structures have emerged as a promising approach to enhance the optical performance of CdTe thin-film solar cells. These periodic structures manipulate incident light through diffraction, effectively extending the optical path length within the active layer and enhancing photon absorption [8]. The key parameters that define nano-grating performance include:

i **Period:** Determines the diffraction efficiency and the wavelength range over which enhancement occurs.

ii **Depth:** Influences light-trapping ability and coupling with guided optical modes.

iii **Duty Cycle:** Affects the structural fill factor and interaction with incident light. By optimizing these parameters, nano-grating structures can significantly improve the overall efficiency of CdTe solar cells. Compared to conventional anti-reflective coatings and random texturing, nano-gratings offer more precise control over light manipulation, enabling higher power conversion efficiency [9].

C. Particle Swarm Optimization (PSO)

PSO is a bio-inspired computational algorithm that mimics the social behavior of birds and fish to optimize complex problems efficiently. It is particularly effective in solving multi-parameter optimization problems, such as designing nano-grating structures for photovoltaic applications [10]. The PSO algorithm operates by initializing a swarm of particles, each representing a potential solution in the design space. These particles iteratively update their positions based on their individual best-known position and the global best-known position of the swarm. The iterative process ensures convergence toward an optimal set of parameters that maximize the performance metric—in this case, light absorption and power conversion efficiency in CdTe solar cells [11].

PSO offers several advantages over traditional optimization methods, such as Faster convergence to optimal solutions, reduced computational cost compared to exhaustive search methods, and Flexibility in handling multi-objective optimization problems [12-14]. By integrating PSO with advanced simulation techniques, this study systematically identifies the optimal nano-grating configurations to enhance the efficiency of CdTe thin-film solar cells, paving the way for practical implementation in next-generation photovoltaic technologies [15].

3. Methodology

The optimization and simulation process follows a structured approach to evaluate the performance enhancement of CdTe thin-film solar cells using embedded nano-grating structures.

Fig.1(a) CdS/CdTe solar cell structure Fig.1(b) CdS/CdTe solar cell process

A. Optimization Parameters

The structural parameters of the nano-grating play a crucial role in determining the optical and electrical performance of CdTe solar cells. The PSO algorithm optimizes the following parameters. The optimization process iteratively updates the swarm positions based on individual and global best solutions to converge towards an optimal nano-grating configuration.

Table 1 Optimization parameter ranges used in this study.

Parameter	Value
Grating Period (P)	100 nm – 500nm
Grating Depth (D)	50 nm – 200nm
Duty Cycle (DC)	0.2 – 0.8

B. Optical Simulation Using FDTD

The Finite-Difference Time-Domain (FDTD) method is employed to model the interaction of light with the nano-grating structures. FDTD is a widely used numerical technique for solving Maxwell's equations in complex geometries. The simulation setup includes:

i **Incident Light Source**: A plane wave source spanning the solar spectrum (300–1200 nm).

ii **Boundary Conditions**: Perfectly matched layers (PML) to prevent artificial reflections.

iii **Material Properties**: Optical constants of CdTe and other layers extracted from experimental data.

iv **Mesh Refinement**: Adaptive meshing to resolve nano-scale grating features.

C. Electrical Simulation Using Sentaurus TCAD

To evaluate the impact of nano-gratings on charge transport and recombination, Sentaurus TCAD simulations are performed. The electrical model incorporates:

i **Carrier Transport Equations**: Drift-diffusion model coupled with Poisson's equation.

ii **Recombination Mechanisms**: Shockley-Read-Hall (SRH) and Auger recombination.

iii **Doping Profile**: CdTe absorber layer with optimized acceptor concentration.

iv **Contact Properties**: Ohmic front and back contacts.

Table 2 A comparison of Jsc and PCE values for optimized and conventional CdTe solar cells.

Parameter	Conventional CdTe	Optimized CdTe (Nano-Grating)
Jsc (mA/cm^2)	25.4	28.7
PCE (%)	17.5	20.2

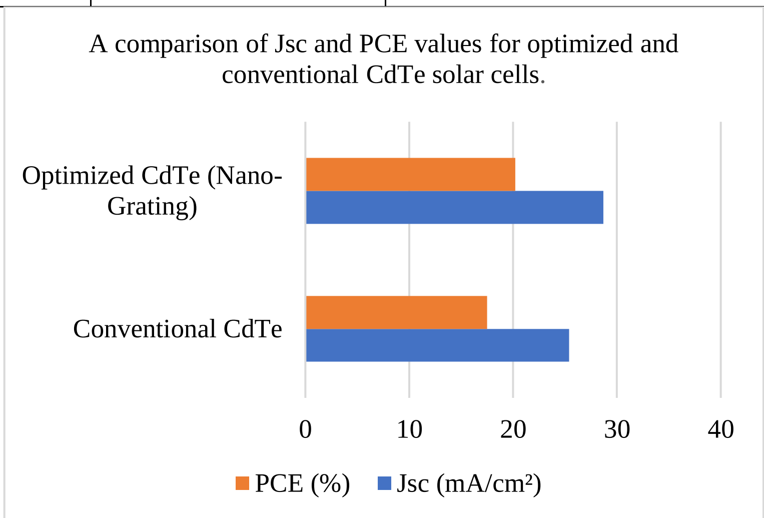

Fig.2.A comparison of Jsc and PCE values for optimized and conventional CdTe solar cells.

D. Performance Evaluation

The impact of optimized nano-gratings is evaluated based on the following parameters

i **Absorption Enhancement**: Increased light trapping within the CdTe layer.

ii **Improvement in Jsc**: Higher carrier generation due to better optical absorption.

iii **Power Conversion Efficiency (PCE) Gain**: Enhancement in overall device performance.

To ensure robustness, a sensitivity analysis is conducted to examine the effect of parameter variations on efficiency. The study reveals that minor variations in grating period and depth can lead to substantial changes in light absorption, emphasizing the need for precise fabrication techniques. While this study focuses on simulation-based optimization, practical implementation requires precise nanofabrication techniques such as electron beam lithography (EBL) or nanoimprint lithography (NIL). The feasibility of scaling up these techniques for large-area solar modules is an area of future research. By leveraging particle swarm optimization, this methodology successfully identifies the optimal nano-grating structures that enhance the efficiency of CdTe thin-film solar cells. The integration of advanced optical and electrical simulations provides a comprehensive evaluation, paving the way for experimental validation and commercialization.

4. Results and Discussion

A. Optical Performance Analysis

The optical simulations conducted using the Finite-Difference Time-Domain (FDTD) method reveal a substantial improvement in light absorption in CdTe thin-film solar cells integrated with nano-grating structures. The optimized grating configuration enhances absorption across a broad spectral range, particularly in the near-infrared region where conventional CdTe cells exhibit significant losses.

B. Electrical Performance Enhancement

The electrical simulations performed using Sentaurus TCAD demonstrate the impact of nano-grating structures on charge carrier generation and collection efficiency. The introduction of optimized nano-gratings leads to higher short-circuit current density (Jsc) and overall power conversion efficiency (PCE).

Table 3 Electrical performance parameters for conventional and optimized CdTe solar cells

Parameter	Conventional CdTe	Optimized CdTe (Nano-Grating)
Jsc (mA/cm²)	25.4	28.7
Voc (V)	0.83	0.86
FF (%)	76.5	78.2
PCE (%)	17.5	20.2

The increase in Jsc is attributed to improved absorption, while the slight enhancement in open-circuit voltage (Voc) and fill factor (FF) is due to better charge transport and reduced recombination.

C. Impact of Nano-Grating Parameters

A parametric analysis was conducted to understand the influence of grating period, depth, and duty cycle on device performance. The results indicate that:

i Increasing the grating period beyond 400 nm leads to reduced efficiency due to excessive scattering losses.

ii A depth of 100–150 nm provides an optimal balance between light trapping and electrical performance.

iii A duty cycle of 0.5–0.7 yields the best trade-off between absorption enhancement and fabrication feasibility.

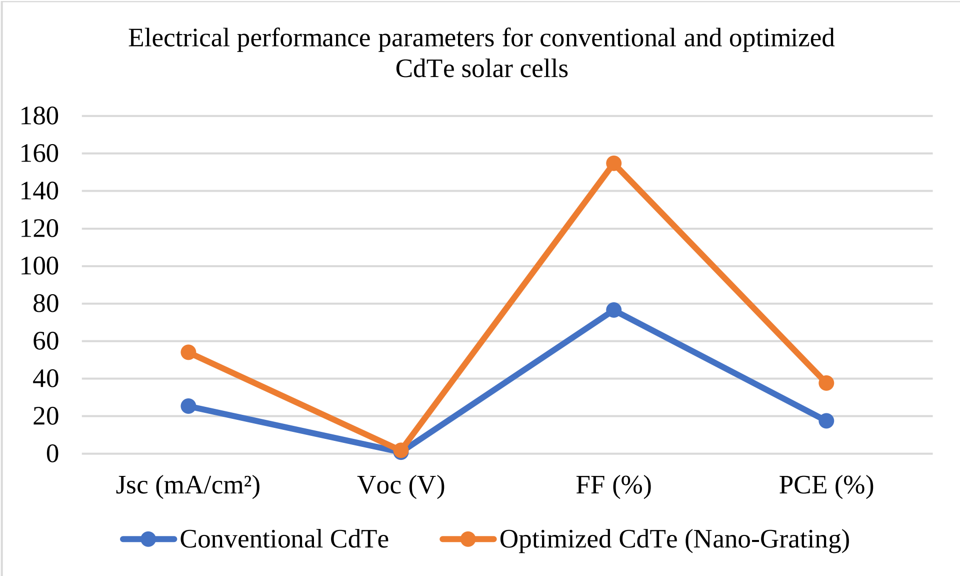

Fig.3.Electrical performance parameters for conventional and optimized CdTe solar cells

E. Discussion on Practical Implementation

While the simulations demonstrate significant efficiency improvements, practical implementation requires precise fabrication techniques such as electron beam lithography (EBL) or nanoimprint lithography (NIL). The scalability of these methods for large-area solar modules remains a challenge, requiring further investigation into cost-effective manufacturing solutions. Additionally, environmental and stability assessments are necessary to ensure long-term reliability. The results demonstrate that the integration of PSO-optimized nano-gratings significantly enhances CdTe thin-film solar cell performance by increasing light absorption and charge carrier generation, enhancing short-circuit current density and overall efficiency and providing a robust framework for further experimental studies. These findings highlight the potential of nano-structured designs in advancing thin-film photovoltaic technology, paving the way for next-generation high-efficiency solar cells.

4. Conclusion

This study presents an innovative approach to improving the performance of cadmium telluride (CdTe) thin-film solar cells by incorporating nano-grating structures that are optimized using particle swarm optimization (PSO) techniques. CdTe thin-film solar cells are a promising solution for sustainable energy generation due to their low cost, ease of manufacturing, and relatively high efficiency. However, one of the challenges that limit their performance is the ability to effectively capture and utilize light, as well as the efficient collection of charge carriers.The proposed method addresses these challenges by designing nano-grating structures that enhance the light trapping capabilities of the solar cell. Light trapping refers to the ability to reflect and scatter light within the cell to increase the likelihood of photon absorption. By optimizing the arrangement and geometry of the nano-gratings using PSO, the researchers were able to maximize this effect, ensuring that more light is captured and directed towards the absorber layer. In turn, this leads to an increase in the number of photons available for conversion into electrical energy.

Additionally, the optimized grating structure also improves carrier collection within the solar cell. Carrier collection efficiency is a critical factor in determining the overall performance of a solar cell, as it impacts the ability of the device to extract and utilize the charge carriers (electrons and holes) generated by absorbed photons. By fine-tuning the nano-grating design, the research achieved a more effective collection of these carriers, minimizing losses due to recombination and improving the overall power conversion efficiency of the CdTe thin-film solar cells.The study emphasizes the need for experimental validation to confirm the simulated results and ensure the practicality of the proposed optimization technique. This step is crucial to determine the real-world performance of the nano-grating structures in actual solar cell devices. Future research should focus on experimental validation and integration with advanced passivation techniques to further reduce recombination losses.Moreover, future research will explore how these optimized designs can be integrated with large-scale manufacturing processes to enable cost-effective production of high-efficiency CdTe thin-film solar cells, potentially advancing the widespread adoption of solar energy as a reliable source of renewable power.

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