

Influence of Density of States and Charge Carrier Mobility on the Performance of CdTe Thin-Film Solar Cells: A SCAPS-1D Study

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Abstract

The performance of cadmium telluride (CdTe) thin-film solar cells is strongly influenced by intrinsic semiconductor properties such as carrier mobility and the effective density of states (DOS) in the conduction and valence bands. In this work, numerical simulations using the Solar Cell Capacitance Simulator in One Dimension (SCAPS-1D) were carried out to investigate the impact of electron and hole mobility (μ_e , μ_h) and effective density of states (N_c , N_v) on the photovoltaic performance of a standard CdTe/CdS heterojunction solar cell. Simulations were performed under standard test conditions (AM 1.5G spectrum, 1000 W m^{-2} , 300 K), with one parameter varied at a time while others remained fixed. Key output parameters analysed were open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (η). Results show that increasing the conduction- or valence-band density of states leads to a significant reduction in V_{oc} , accompanied by a moderate increase in FF and nearly unchanged J_{sc} , resulting in a slight decline in overall efficiency. Increasing electron mobility enhances J_{sc} and FF due to improved carrier transport but slightly reduces V_{oc} , producing minimal net efficiency change. In contrast, higher hole mobility improves V_{oc} and overall efficiency with negligible impact on J_{sc} . Across all cases, V_{oc} was identified as the dominant parameter governing efficiency variations. The findings highlight the complex trade-off between carrier transport enhancement and recombination losses in polycrystalline CdTe absorbers and provide guidance for optimizing material properties to achieve higher-efficiency CdTe thin-film solar cells.

Keywords: Cadmium telluride (CdTe); Thin-film solar cells; SCAPS-1D simulation; Carrier mobility; Effective density of states; Heterojunction

1.0 Introduction

The rapid increase in global energy demand, driven by population growth, industrialization, and technological advancement, has heightened concerns about energy security and environmental sustainability. Fossil fuels still dominate the global energy mix, but their finite availability and significant greenhouse gas emissions have accelerated the transition toward renewable energy sources [1]. Among these, solar photovoltaics (PV) have emerged as one of the most promising options due to the abundance of solar energy, scalability of PV systems, low operational environmental impact, and steadily declining cost per watt [2]. Advances in materials science, device engineering, and large-scale manufacturing have enabled PV technologies to evolve from niche applications to major contributors to electricity generation worldwide.

Thin-film solar cells represent the second generation of PV technologies and offer advantages such as reduced material usage, lightweight modules, and compatibility with large-area deposition techniques. Among thin-film materials, cadmium telluride (CdTe) has achieved remarkable commercial success and is considered one of the most mature technologies in this class. Laboratory-scale CdTe cells have demonstrated efficiencies exceeding 22%, while commercial modules commonly achieve efficiencies above 18% [2, 3]. This success is largely due to the favourable optoelectronic properties of CdTe for single-junction solar conversion.

CdTe is a direct bandgap semiconductor with an energy gap of approximately 1.45–1.5 eV, close to the optimal value predicted by the Shockley–Queisser limit for maximum efficiency under the terrestrial solar spectrum [4]. It also exhibits a very high optical absorption coefficient ($>10^5 \text{ cm}^{-1}$), enabling nearly complete absorption of visible light within only a few micrometres of material [5]. Consequently, efficient devices can be fabricated using much less material than crystalline silicon technologies. Furthermore, CdTe can be deposited using scalable and cost-effective techniques such as close-spaced sublimation, vapour transport deposition, and electrodeposition, making it well suited for large-scale production.

Despite these advantages, CdTe solar cell performance is limited by recombination losses associated with defects, impurities, grain boundaries, and interface states. Intrinsic point defects including cadmium vacancies, tellurium antisites, and deep-level traps act as recombination centres that reduce minority carrier lifetime and limit the open-circuit voltage (V_{oc}) [6]. Grain boundaries in polycrystalline films can further increase recombination and impede carrier transport, preventing devices from reaching the theoretical efficiency limit.

Charge transport properties are critical determinants of device performance. Carrier mobility influences how effectively photogenerated electrons and holes travel through the absorber before recombining, thereby affecting short-circuit current density (J_{sc}) and fill factor (FF). Similarly, the effective density of states in the conduction band (N_c) and valence band (N_v) governs carrier concentration, Fermi-level position, and recombination statistics [7]. Although these parameters are fundamental semiconductor properties, their combined influence on CdTe device performance has not been extensively studied within realistic ranges for polycrystalline thin films.

Experimental investigation of mobility and density of states is challenging because modifying one property often alters others simultaneously. Numerical simulation therefore provides a powerful alternative for isolating individual effects and understanding underlying physical mechanisms. The Solar Cell Capacitance Simulator in one dimension (SCAPS-1D), developed at the University of Gent is widely used for modelling thin-film solar cells. It solves the coupled Poisson and continuity equations under illumination, enabling detailed analysis of carrier transport, recombination processes, defect states, and interface properties [8] [9].

In this work, SCAPS-1D is employed to investigate the influence of electron and hole mobility (μ_e , μ_h) and effective density of states (N_c , N_v) on the performance of a standard CdTe/CdS heterojunction solar cell. The analysis focuses on key photovoltaic parameters; V_{oc} , J_{sc} , FF, and power conversion efficiency (η) with the aim of identifying optimal parameter ranges that can guide material optimisation and device design for improved CdTe solar cell performance.

2.0 Structure and Operation of CdTe Thin-Film Solar Cells

2.1 Structure

Cadmium Telluride (CdTe) thin-film solar cells are commonly fabricated in a planar heterojunction configuration optimized for strong optical absorption and efficient charge collection. This architecture has become the industry standard for high-efficiency CdTe devices because it is simple, scalable, and compatible with low-cost deposition techniques[3, 6]. The conventional device stack consists of: *Glass / Transparent Conducting Oxide (TCO) / CdS window layer / CdTe absorber layer / Back contact*

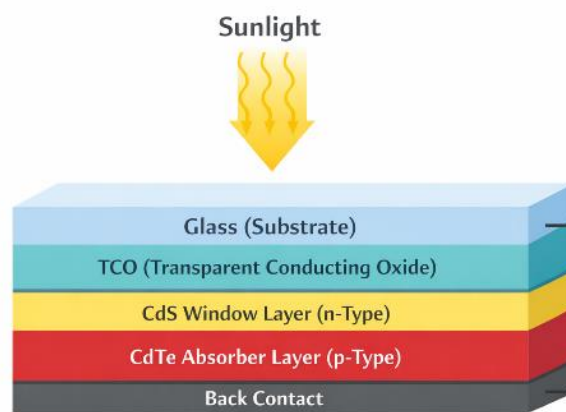


Figure 1 Schematic cross-sectional illustration of a CdTe thin-film solar cell

The **glass substrate** provides mechanical support and high transparency across the solar spectrum. Soda-lime glass is widely used due to its low cost, chemical stability, and ability to withstand high processing temperatures, allowing sunlight to reach the active semiconductor layers with minimal optical loss [5].

The **transparent conducting oxide (TCO)** serves as the front electrode, combining high electrical conductivity with high optical transmittance. Common materials include fluorine-doped tin oxide (FTO) and indium tin oxide (ITO), which allow efficient extraction of photogenerated electrons while permitting most incident light to reach the absorber layer. TCO surface morphology and resistivity influence light trapping, series resistance, and fill factor [10].

The **CdS window layer** is a thin n-type semiconductor with a wide bandgap (~ 2.4 eV). Its main functions are forming a heterojunction with the p-type CdTe, reducing interface recombination, acting as an electron-selective layer, and preventing electrical shunting between the absorber and front contact. CdS primarily absorbs ultraviolet photons, allowing most visible light to reach the CdTe absorber. Excessive thickness can lead to parasitic absorption losses [6].

The **CdTe absorber layer** is a p-type semiconductor with a direct bandgap of 1.45–1.5 eV, near the optimum for single-junction solar energy conversion [4]. CdTe has a very high absorption coefficient ($>10^5$ cm⁻¹), allowing nearly complete light absorption in 2–5 μm of material [5]. The absorber layer is responsible for absorbing incoming photons, generating electron–hole pairs, and transporting these carriers to the junction for collection. Because polycrystalline CdTe films contain numerous grain boundaries and structural defects, these imperfections introduce deep energy levels within the band gap that act as recombination centres for charge carriers, reducing carrier mobility and lifetime. Consequently, careful control of doping and material processing; such as passivation of grain boundaries and optimization of growth conditions is critical for minimizing recombination losses and achieving high photovoltaic efficiency [11].

The **back contact** collects holes from the CdTe layer. Metals such as gold or copper-doped compounds are used to form low-resistance ohmic contacts despite CdTe's high electron affinity and low p-type doping. Proper contact engineering is crucial to minimize series resistance and maximize charge collection [3].

2.2 Operating Principle

CdTe solar cells operate via the photovoltaic effect at a p–n heterojunction. Photons with energy \geq bandgap generate electron–hole pairs in the CdTe layer. The depletion region at the CdS/CdTe interface creates a built-in electric field that separates carriers: electrons move toward the n-type CdS and front contact, while holes move toward the p-type CdTe and back contact [7]. After separation, carriers are transported by drift and diffusion. Efficient collection requires minimal recombination and low contact resistance. When connected to an external load, electron flow produces photocurrent, which combined with the junction photovoltage yields usable electrical power. Overall efficiency depends on recombination, carrier mobility, defect density, band alignment, and interface quality, all of which must be optimized for high-performance CdTe devices [5, 6].

3.0 Methodology

3.1 Simulation Tool: SCAPS-1D

This study employs the Solar Cell Capacitance Simulator in One Dimension (SCAPS-1D), a well-established numerical modelling software specifically developed for the analysis of thin-film photovoltaic devices. SCAPS-1D enables detailed investigation of semiconductor device physics by solving the fundamental transport equations governing charge carriers under steady-state conditions. The program incorporates optical generation, bulk and interface recombination, drift–diffusion transport, and boundary conditions at electrical contacts [12].

To determine the internal electrical behaviour of the solar cell, SCAPS-1D simultaneously solves the following coupled semiconductor equations:

Poisson's Equation (Electrostatic Potential)

Poisson's equation relates the electrostatic potential to the spatial distribution of charge within the device:

$$\frac{d}{dx} \left(\varepsilon \frac{d\psi}{dx} \right) = -q(p - n + N_D^+ + N_A^-) \quad (1)$$

Where: ε = permittivity of the semiconductor

ψ = electrostatic potential

q = elementary charge

n, p = electron and hole concentrations

N_D^+, N_A^- = ionized donor and acceptor densities

Electron and Hole Continuity Equations

The electron continuity equation expresses conservation of electrons, accounting for generation, recombination, and current transport:

$$\frac{dn}{dt} = \frac{1}{q} \frac{dJ_n}{dx} + G - R \quad (2)$$

Similarly, the hole continuity equation ensures conservation of holes:

$$\frac{dp}{dt} = -\frac{1}{q} \frac{dJ_p}{dx} + G - R \quad (3)$$

Where J_n and J_p are the electron and hole current densities, G is the generation rate, and R represents recombination processes [9]. Together, these nonlinear coupled equations describe the electrostatic potential distribution, carrier transport by drift and diffusion, and recombination–generation processes within the solar cell. SCAPS-1D solves them numerically across the device structure using appropriate boundary conditions at interfaces and contacts, enabling accurate prediction of current–voltage characteristics, quantum efficiency, capacitance, and other performance parameters of thin-film solar cells[8, 12, 13].

SCAPS-1D is particularly suitable for CdTe solar cells because it allows:

- Multilayer device modelling
- Inclusion of defect states and recombination mechanisms
- Simulation under realistic illumination spectra
- Extraction of current–voltage (I–V) characteristics

- Determination of key performance parameters

All simulations were performed under standard test conditions:

- Temperature: 300 K
- Illumination: AM 1.5G solar spectrum
- Incident power density: 1000 W/m²

3.2 Baseline Material Parameters

To isolate the effects of transport and electronic properties, a standard CdTe/CdS device structure was defined using material parameters consistent with experimentally reported values for high-efficiency CdTe solar cells.

The parameters of the TCO and CdS layers were kept constant throughout the simulations, while selected properties of the CdTe absorber layer were systematically varied.

Key baseline properties of the CdTe absorber include:

- Bandgap: 1.5 eV
- Thickness: 4.0 μm
- Relative dielectric constant: ~9.4
- Electron affinity: 3.9 eV
- Electron thermal velocity: 1×10^7 cm/s
- Hole thermal velocity: 1×10^7 cm/s

The primary variables investigated in this study were:

Effective Density of States

- Conduction band density of states (N_c): $6.8 \times 10^{17} - 9.2 \times 10^{17}$
- Valence band density of states (N_v): $6.0 \times 10^{18} - 3.0 \times 10^{19}$

These parameters influence carrier concentration, Fermi level position, and recombination statistics.

Charge Carrier Mobility

- Electron mobility (μ_e): $2.6 \times 10^2 - 3.8 \times 10^2$ cm²/Vs
- Hole mobility (μ_h): $3.4 \times 10^1 - 4.6 \times 10^1$ cm²/Vs

Carrier mobility determines how efficiently photogenerated carriers move through the absorber layer before recombining.

During simulations, only one parameter was varied at a time while all others remained fixed. This approach allows a clear assessment of the individual influence of each parameter on device performance.

4. Results and Discussion

This study investigates how variations in **conduction band (CB) and valence band (VB) effective density of states** as well as **electron and hole mobilities** affect key photovoltaic parameters; open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF), and power conversion efficiency (η).

4.1 Influence of Conduction Band Effective Density of States

As shown in Table I, increasing the CB effective density of states from 6.8×10^{17} – 9.2×10^{17} results in a monotonic **decrease in Voc** from 1.0185 V to 0.9811 V, while **Jsc remains almost constant** (~ 24.18 mA/cm²). This trend aligns with established understanding that the density of states distribution plays a crucial role in determining Voc because trap states and recombination centres associated with a larger DOS can increase non-radiative recombination, leading to reduced quasi-Fermi level splitting and lower Voc values. This effect has been demonstrated experimentally in organic solar cells, where changes in the density of states significantly affected Voc through variations in recombination dynamics [14, 15]. The fill factor increases from 65.45 % to 67.27 % as the conduction-band density of states increases, indicating improved carrier transport and charge extraction efficiency. Enhanced density of states near the band edge can facilitate carrier conduction and reduce transport limitations, leading to modest improvements in FF. Such behaviour is consistent with semiconductor device theory and numerical simulation studies, which show that improved carrier mobility and reduced resistive losses can enhance FF even when Voc declines due to increased recombination or altered band-structure properties [7, 8, 16]. The overall efficiency decreases slightly from 16.12 % to 15.96 %, primarily due to the dominant impact of the reduced Voc. According to fundamental solar-cell theory, Voc is strongly influenced by recombination processes and the dark saturation current, and a decrease in Voc directly lowers the maximum achievable power output when other parameters remain nearly constant [4]. This demonstrates that maintaining high Voc is critical for achieving optimal device efficiency.

Table I. CB effective density of states and I-V characteristic parameters

CB effective density of states (cm^{-3})	Voc (V)	Jsc (mA/cm ²)	FF(%)	The electrical power conversion efficiency (%)
6.800E+17	1.0185	24.184657	65.45	16.12
7.200E+17	1.0111	24.184629	65.80	16.09
7.600E+17	1.0043	24.184602	66.14	16.06
8.000E+17	0.9979	24.184575	66.45	16.04
8.400E+17	0.9919	24.184548	66.74	16.01
8.800E+17	0.9864	24.184522	67.01	15.99
9.200E+17	0.9811	24.184495	67.27	15.96

4.2 Effect of Valence Band Effective Density of States

Similarly, increasing VB effective density of states from 6.0×10^{18} to 3.0×10^{19} cm⁻³ (Table II) leads to a significant decrease in Voc from 1.0868 V to 0.9535 V, while **Jsc remains nearly unchanged**. This observation is consistent with theoretical work showing that both the conduction and valence band DOS influence Voc because lower effective DOS values are

associated with reduced recombination losses and improved voltage output. For perovskite and other compound semiconductor cells, lower densities of band states have been identified as a factor contributing to higher Voc and enhanced efficiency [17]. The increase in fill factor (FF) from 62.00 % to 68.82 % indicates improved charge transport and carrier extraction within the device. However, the overall power conversion efficiency decreases slightly from 16.28 % to 15.87 %, suggesting that the reduction in open-circuit voltage (Voc) outweighs the benefits of the FF improvement. Since solar-cell efficiency depends directly on the product of Voc, short-circuit current density (Jsc), and FF, even a modest decline in Voc can significantly reduce device performance [13]. This result therefore highlights Voc as the primary performance parameter sensitive to changes in electronic properties such as density of states and recombination mechanisms [4].

Table II. VB effective density of states and I-V characteristic parameters

VB effective density of states (cm^{-3})	Voc (V)	Jsc (mA/cm²)	FF(%)	The electrical power conversion efficiency (%)
6.000E+18	1.0868	24.159551	62.00	16.28
1.000E+19	1.0480	24.172569	63.88	16.18
1.400E+19	1.0197	24.179891	65.31	16.10
1.800E+19	0.9979	24.184575	66.45	16.04
2.200E+19	0.9803	24.184463	67.38	15.97
2.600E+19	0.9658	24.184368	68.15	15.92
3.000E+19	0.9535	24.184285	68.82	15.87

4.3 Effect of Electron Mobility

In Table III, electron mobility was varied between 260 and 380 cm²/V·s. As mobility increases, **Voc slightly decreases**, while **Jsc and FF increase**, indicating improved charge transport and reduced series resistance. These trends are consistent with simulation studies on perovskite solar cells, which show that while higher carrier mobility can reduce recombination losses and improve current and FF, there is often an optimal mobility result beyond which efficiency gains diminish or plateau [18]. Despite the improvements in Jsc and FF, the overall efficiency η remains relatively stable (from 16.10 to 15.98 %) because the decreased Voc offsets the gains in transport parameters.

Table III. Electron Mobility and I-V Characteristic Parameters

Electron Mobility (cm ² /Vs)	The open circuit voltage (Voc)	The short circuit current density (Jsc)	The Fill factor (FF)	The electrical power conversion efficiency (%)
2.600E+2	1.0254	24.159496	64.98	16.10
2.800E+2	1.0154	24.168429	65.51	16.08
3.000E+2	1.0063	24.176758	65.99	16.06
3.200E+2	0.9979	24.184575	66.45	16.04
3.400E+2	0.9900	24.191916	66.87	16.02
3.600E+2	0.9827	24.198851	67.28	16.00
3.800E+2	0.9758	24.205401	67.66	15.98

4.4 Influence of Hole Mobility

Table IV shows that increasing hole mobility from 34 to 46 cm²/V·s leads to a **modest increase in Voc** (0.9875 – 1.0066 V). This suggests that improved hole transport reduces recombination at interfaces and increases quasi-Fermi level splitting, which has been identified as a mechanism for improving Voc in high-performance semiconductor devices. The **Jsc remains nearly constant**, and **FF** decreases slightly, while the overall efficiency improves modestly from 15.92 to 16.13 %. Studies reviewing carrier mobility in high-efficiency photovoltaic materials, including perovskites, highlight that improved mobility contributes significantly to efficient charge extraction and reduced losses, which supports the trend observed here [19].

Table IV. Hole Mobility and I-V Characteristics Parameters

Hole Mobility (cm ² /Vs)	The open circuit voltage (Voc)	The short circuit current density (Jsc)	The Fill factor (FF)	The electrical power conversion efficiency (%)
34	0.9875	24.184250	66.65	15.92
36	0.9912	24.184434	66.58	15.96
38	0.9946	24.184530	66.51	16.00
40	0.9979	24.184575	66.45	16.04
42	1.0009	24.184563	66.38	16.07
44	1.0039	24.184526	66.31	16.10
46	1.0066	24.184450	66.25	16.13

4.5 Summary of Observations

Across all parameter variations, **Jsc** shows **minimal sensitivity** to changes in DOS and carrier mobility, suggesting that photon absorption and charge generation are comparatively stable under the simulated conditions. The primary parameters influencing overall efficiency remain **Voc** and **FF**:

- i. Increasing CB or VB effective densities increases FF but reduces Voc, resulting in a slight drop in η .
- ii. Increasing electron mobility enhances FF and Jsc but leads to a modest decline in Voc, stabilizing η around the same value.
- iii. Increasing hole mobility slightly increases Voc and overall η , with only minor effects on FF and Jsc.

These results are consistent with established photovoltaic device physics and literature showing that careful optimization of carrier transport and density of states is essential to maximizing performance. The trade-off between increased carrier extraction (improving FF/Jsc) and increased recombination (reducing Voc) illustrates the complexity of photovoltaic optimization and supports trends seen in experimental and modelling studies [18].

Conclusion

This study employed SCAPS-1D numerical simulation to systematically examine how variations in carrier mobility and effective density of states influence the performance of a CdTe/CdS thin-film solar cell. The results demonstrate that electronic transport properties and band-edge state densities play a critical role in determining device output parameters.

Increasing the conduction- or valence-band effective density of states leads to a pronounced decrease in open-circuit voltage due to enhanced recombination, while fill factor increases as a result of improved carrier transport and extraction. Because solar-cell efficiency depends strongly on Voc, the net effect is a slight reduction in overall efficiency despite improved FF. Short-circuit current density remains largely unaffected, indicating that optical absorption and photogeneration are stable over the investigated parameter ranges.

Enhancement of electron mobility improves charge transport, leading to increases in Jsc and FF, but simultaneously causes a modest decrease in Voc, resulting in little overall efficiency gain. Conversely, increasing hole mobility improves Voc and efficiency, suggesting that efficient hole transport is particularly important for CdTe absorber performance.

Overall, the study reveals that optimizing CdTe solar cells requires balancing improved carrier extraction against recombination losses associated with higher densities of electronic states. Among the investigated parameters, Voc emerges as the most sensitive and decisive factor controlling efficiency. These findings provide valuable insight into the design and material engineering of high-performance CdTe thin-film solar cells and demonstrate the usefulness of SCAPS-1D as a predictive tool for guiding experimental optimization.

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