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Optimizing carrier transport properties in the intrinsic layer of a-Si single and double junction solar cells through numerical design

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ABSTRACT

This research aims to improve the performance of a-Si: H solar cells, particularly in terms of carrier transport properties, through a numerical design approach utilizing AFORS-HET simulation software. By performing a series of rigorous computer simulations, we explore the potential regulation of the intrinsic layer thickness, carrier mobility, loading factor, and density of states (DoS) distribution in the solar cell's intrinsic layer. Recombination losses are reduced, and light absorption efficiency is significantly increased when the intrinsic layer thickness is adjusted, as shown by simulation findings. Moreover, reduction of transit times and enhancement of the total efficiency of the solar cells depend on increased carrier mobility. Parameters can be adjusted to attain optimal performance under various operating situations by adjusting the DoS and load factors. Furthermore, the simulations provide insightful information about the interactions between the junctions in solar cells with double junctions. Our results of this research provide an important contribution to efforts to develop more efficient and sustainable a-Si: H solar cells and emphasize the importance of numerical design approaches in photovoltaic technology.

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1. INTRODUCTION

Solar energy is a potentially limitless resource, and solar cells are a key technology in harnessing it into electricity [1]. As energy needs continue to increase and concerns about the impacts of climate change, the development of more efficient and economical solar cells is becoming a global priority [2]. Amorphous solar cells (a-Si: H) are one of the promising photovoltaic technologies [3], especially in thin solar cell applications, such as thin film solar cells [4], which enables more flexible integration and lower production costs [5]. The a-Si: H solar cells have been the subject of intensive research over the past decades [6]. Its popularity is due to several advantages, including the ability to produce thin solar cells [7], flexible [8], and integrated with other applications [9]. However, despite significant progress in the development of a-Si: H solar cells [10], energy conversion efficiency and resistance to degradation of solar cells are still challenges that need to be overcome [11].

The development of a-Si: H solar cells involves a deep understanding of the electronic and optical properties of the material [12]. A key factor in the performance of a-Si: H solar cells is how electrons and

holes (carriers) move through this material [13], which is determined by the transport properties of the carriers [14]. In this context, numerical design has become an invaluable tool for understanding and optimizing carrier transport properties in a-Si: H solar cells [15]. Numerical design allows us to perform sophisticated computer simulations [16], which provide deep insight into the various parameters that influence solar cell performance [17]. In recent years, numerical design has emerged as a very useful tool in the modeling and optimization of the intrinsic layers of a-Si: H solar cells [18]. Numerical design allows engineers and researchers to examine various design scenarios and intrinsic layer parameters without having to create a physical prototype [19]. This saves time and resources and allows in-depth exploration of potential solar cell performance improvements [20].

This research aims to explore the potential of numerical design in improving carrier transport properties in a-Si: H solar cells. The main focus is on the intrinsic layer of the solar cell, which is the a-Si: H layer that is most important in the process of converting solar energy into electricity. The intrinsic layer plays a role in absorbing sunlight and producing electron-hole pairs that will move through the solar cell. One of the critical aspects influencing the performance of a-Si: H solar cells is carrier transport in the intrinsic layer [21]. This involves the mobility of electrons and holes, the recombination rate, and the energy distribution of electrons and holes in the layer [22]. These properties greatly influence the energy conversion efficiency of solar cells [23]. Therefore, understanding and controlling the nature of carrier transportation becomes very important. The main findings of this study highlight the critical role of optimizing carrier transport properties in enhancing the efficiency of a-Si solar cells. By refining the intrinsic layer thickness, carrier mobility, and other key parameters through numerical design, we observed substantial improvements in light absorption efficiency and reductions in recombination losses [24]. These optimizations lead to shorter transit times and better overall performance of both single and double-junction solar cells. The study underscores the importance of precise parameter adjustments and numerical simulations in developing more efficient and sustainable a-Si solar cells, offering valuable insights for future advancements in photovoltaic technology.

2. METHOD

This research uses a numerical design approach and computer simulation using AFORS-HET software. AFORS-HET is a specialized simulation software developed to model thin film-based photovoltaic devices, including a-Si: H solar cells. The research methodology includes the following steps: preliminary preparation, the first step involves collecting the necessary initial data and information, including relevant a-Si: H material parameters such as electron and hole mobility, effective mass, and density of state (DoS) [25]. This data is necessary to include accurate material parameters in the simulation. Intrinsic layer modeling, we build intrinsic layer models on a-Si: H solar cells for both single-junction and double-junction solar cells. This includes determining layer thickness, mobility, and other relevant parameters that affect carrier transportation. We use AFORS-HET software to perform carrier transport simulations in the intrinsic layers of a-Si: H solar cells. AFORS-HET allows us to input predefined design parameters and model the movement of electrons and holes within the layer. Parameter variation, we performed various simulations with variations in intrinsic layer parameters, including thickness, electron, hole mobility, and contact structure [26]. This allows us to understand how changes in these parameters affect solar cell performance. AFORS-HET has been proven effective in this study to evaluate the impact of various parameters on solar cell performance. Within the framework of this software, the 1-D Poisson equation and the electron and hole continuity equations are solved, and the recombination uses shockley-read-hall (SRH) statistics. Additionally, the formation of electron-hole pairs in the absorbing layer is predicted using the Beer-Lambert equation for the optical model in AFORS-HET. The parameters for modeling using AFORS-HET can be seen in Table 1.

The p-layer is a p-type layer that acts as a carrier for holes in solar cells. This layer is usually made from p-doped a-Si: H material. The i-layer (Intrinsic) is the central part of the solar cell where the process of converting solar energy into electricity occurs. This layer does not have doping, so the main component is pure amorphous material, and the n-layer is an n-type layer that acts as an electron carrier in solar cells. Figure 1 shows the structure of the p-i-n and p-i_1-i_2-n solar cell layers. This layer is usually made from n-doped a-Si: H material. In a p-i-n single junction intrinsic layer solar cell, there is only one junction between the p-layer and the n-layer as seen in Figure 1(a). The intrinsic layer (i) is in between the two. Meanwhile, in the p-i_1-i_2-n double-layer intrinsic layer solar cell, there are two junctions as seen in Figure 1(b). The first junction (i_1) is located between the p-layer and the i_1 layer, while the second junction (i_2) is located between the i_1 layer and the n-layer. This allows the absorption of light of different energies by each junction, increasing the overall efficiency of the solar cell. This schematic drawing provides a visual view of the structure of an a-Si: H solar cell and how the intrinsic layer (i layer) acts as a solar energy conversion center. These solar cells work by generating electron-hole pairs when sunlight is absorbed and then directing these

pairs through an intrinsic layer to generate electricity. The single and dual configurations demonstrate diverse approaches in a-Si: H solar cell technology to optimize performance and energy conversion efficiency [27].

Table 1. Input parameters for modeling using AFORS-HET

Parameters	(p) a-Si:H	(i_1) a-Si:H	(i_2) a-Si:H	(n) a-Si:H
Thickness (nm	15	300	300	25
Dielectric constant	11.9	11.9	11.9	11.9
Elecron affinity (eV)	3.80	3.80	3.80	3.80
Band gap (eV)	2.00	1.70	1.85	2.20
Effective cond. band density (cm^{-3})	2.5×10^{20}	2.5×10^{20}	2.5×10^{20}	2.5×10^{20}
Effective val. band density (cm^{-3})	2.5×10^{20}	2.5×10^{20}	2.5×10^{20}	2.5×10^{20}
Acceptor concentration, Na (cm^{-3})	3.0×10^{18}	0	0	0
Donor concentration, Nd (cm^{-3})	0	0	0	1.0×10^{19}
Electron mobility ($cm^2V^{-1}s^{-1}$)	10	20	20	10
Hole mobility ($cm^2V^{-1}s^{-1}$)	1	2	2	1
Thermal velocity of electron (cms^{-1})	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}
Thermal velocity of hole (cms^{-1})	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}
Defect density at conduction (valence) band edge ($cm^{-3}eV^{-1}$)	6.67×10^{20} (6.67×10^{20})	2.33×10^{21} (2.33×10^{21})	2.0×10^{21} (2.0×10^{21})	2.0×10^{21} (2.0×10^{21})
Urbach energy for conduction (valence) band tail (eV)	0.03 (0.06)	0.03 (0.06)	0.03 (0.06)	0.03 (0.06)
Capture cross- section σ_e (σ_h) for conduction band tail (cm_2)	1.0×10^{-17} (1.0×10^{-15})	1.0×10^{-17} (1.0×10^{-15})	1.0×10^{-17} (1.0×10^{-15})	1.0×10^{-17} (1.0×10^{-15})
Capture cross- section σ_e (σ_h) for valence band tail (cm^2)	1.0×10^{-17} (1.0×10^{-15})	1.0×10^{-17} (1.0×10^{-15})	1.0×10^{-17} (1.0×10^{-15})	1.0×10^{-17} (1.0×10^{-15})
Gaussian density of states (cm^{-3})	8.0×10^{17}	8.0×10^{15}	8.0×10^{15}	8.0×10^{17}
Gaussian peak energy for donor (acceptor) (eV)	1.22(0.70)	1.22(0.70)	1.22(0.70)	1.22(0.70)
Standard deviation of Gaussian for donor (acceptor) (eV)	0.23(0.23)	0.23(0.23)	0.23(0.23)	0.23(0.23)
Capture cross- section σe (σh) for donor-like Gaussian states (cm^2)	1.0×10^{-14} (1.0×10^{-15})	1.0×10^{-14} (1.0×10^{-15})	1.0×10^{-14} (1.0×10^{-15})	1.0×10^{-14} (1.0×10^{-15})
Capture cross- section σ_e (σ_h) for acceptor-like Gaussian states (cm^2)	1.0×10^{-14} (1.0×10^{-15})	1.0×10^{-14} (1.0×10^{-15})	1.0×10^{-14} (1.0×10^{-15})	1.0×10^{-14} (1.0×10^{-15})

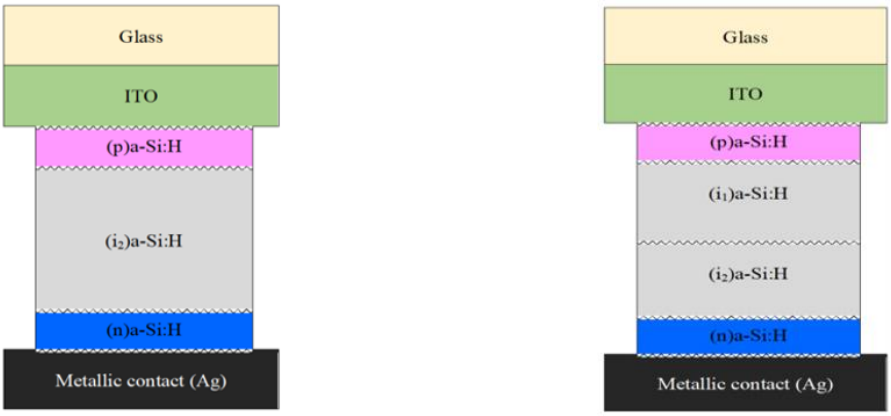
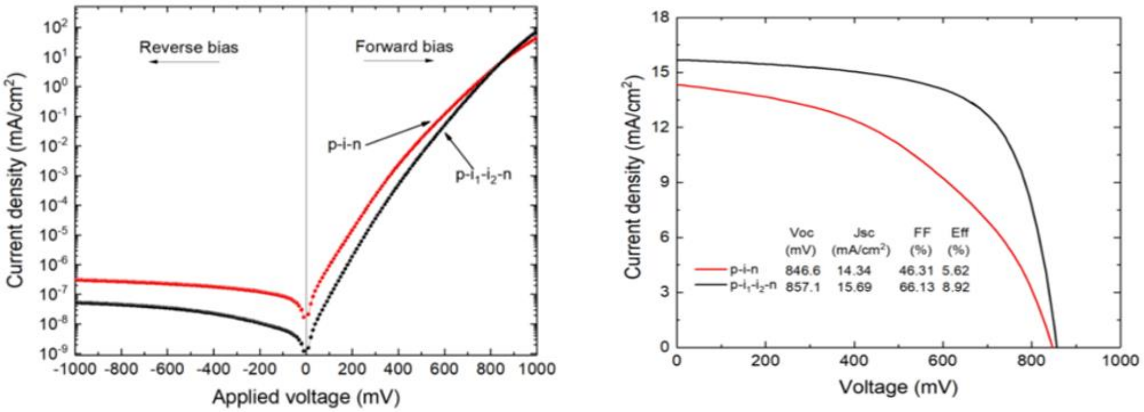


Figure 1. Schematic of (a) single (p-i-n) and (b) double (p-i_1-i_2-n) junction intrinsic layer a-Si: H solar cells

3. RESULTS AND DISCUSSION

Figure 2 shows the J-V (current-voltage) characteristics of a-Si: H intrinsic layer solar cells. The J-V characteristics in dark conditions between single-junction (p-i-n) and double-junction (p-i_1-i_2-n) a-Si: H intrinsic layer solar cells as seen in Figure 2(a). Here you can see the differences in structure and performance of each. each type of solar cell. In p-i-n solar cells, which are single junctions, the J-V characteristic reflects the overall performance of the solar cell. Zero current potential (V_{oc}) reflects the open voltage in dark conditions, while short current (I_{sc}) is the maximum current generated in darkness when the voltage is zero. Peak power (P_{max}) is the maximum power that can be produced in dark conditions. On the other hand, the p-i_1-i_2-n solar cell is a double junction which has two junctions, namely i_1 and i_2. Each junction has its own J-V characteristics, which leads to fundamental differences [28]. The zero current

potential (V_{oc}) in the p-i_1-i_2-n solar cell has two values, namely V_{oc1} and V_{oc2}, which reflect the open potential at each junction. Similarly, there are two short current values (I_{sc1} and I_{sc2}) that reflect the maximum current produced by each junction when the voltage is zero. This difference also affects the peak power (P_{max}) of the p-i_1-i_2-n solar cell, which will be influenced by contributions from both junctions. In addition, the efficiency under illumination conditions can also be different due to the ability of p-i_1-i_2-n solar cells to absorb light with different energies at each junction as seen in Figure 2(b). Thus, differences in J-V characteristics in dark conditions and conditions in the illumination between these two types of solar cells are related to their structure and ability to optimize performance in dark conditions [29]. P-i_1-i_2-n solar cells have the potential for higher efficiency in dark conditions due to the presence of two junctions that can absorb light of different energies, but this also requires more careful management of the interactions between the two junctions to achieve optimal performance [30].



(a) (b)

Figure 2. J-V characteristics (a) in dark conditions and (b) in illumination conditions

Figure 3 shows the schematic band diagram and electric field distribution of a-Si: H intrinsic layer solar cells. The schematic ribbon diagram depicts three main layers p-type layer (p), the intrinsic layer (i), and the n-type layer (n) seen in Figure 3(a). In the band diagram, the intrinsic layer is a layer with an energy bandwidth that corresponds to electron conduction. This means that the intrinsic layer acts as a layer where free carriers (electrons and holes) are generated when sunlight is absorbed. However, in the p-i-n configuration, there is only one junction, namely between the p-layer and n-layer. On the other hand, in a p-i_1-i_2-n solar cell, the schematic ribbon diagram will show the presence of two junctions: the first junction between the p-layer and the i_1 layer, and the second junction between the i_1 layer and layer n. In this band diagram, the difference in energy bandwidth between layer i_1 and layer i_2 reflects the difference in energy required to generate electron-hole pairs at the respective junctions [31]. Therefore, this allows p-i_1-i_2-n solar cells to absorb light with different energies at each junction. The differences in these schematic band diagrams reflect the ability of p-i_1-i_2-n solar cells to maximize absorption of sunlight of different energies and increase overall efficiency [32]. In the context of solar energy, the p-i_1-i_2-n configuration offers the potential to improve the overall performance of a solar cell in a way that cannot be achieved in a single p-i-n solar cell.

Increasing the efficiency and mobility of carrier transport in a-Si solar cells requires a nuanced approach to optimizing carrier recombination within the intrinsic layer. Our study demonstrates that fine-tuning the intrinsic layer thickness, carrier mobility, and DoS distribution can significantly impact solar cell performance. Optimizing the intrinsic layer thickness improves light absorption and reduces recombination losses, while enhanced carrier mobility shortens transit times, thus improving overall efficiency. However, balancing these parameters is crucial, as excessive thickness can lead to increased recombination, while overly high mobility might not always translate to better performance due to potential trade-offs with recombination dynamics. Additionally, varying load factors and DoS settings provide a pathway to achieve optimal performance across different conditions but require careful calibration to avoid unintended effects. This discussion highlights the importance of precise numerical design in addressing these challenges, offering a pathway to more efficient and reliable a-Si solar cells. Our comparative analysis between single and double-junction solar cells highlights that double-junction cells when optimized, achieve higher efficiency than single-junction cells [33]. However, our study provides a more refined optimization

framework by incorporating additional design parameters that further enhance performance. Additionally, our work extends the models developed by integrating a broader set of variables and considerations, leading to more precise optimization outcomes [8]. This advancement addresses limitations in previous models and offers a more comprehensive approach to optimizing carrier transport properties, underscoring the value of detailed numerical design in achieving superior solar cell performance.

Figure 3(b) shows the electric field distribution between p-i-n solar cells and p-i_1-i_2-n a-Si: H solar cells reflect the differences in the structure and flow pattern of the electric field inside them. In p-i-n solar cells, the electric field is usually concentrated at a single junction located between the p-layer and the n-layer. This is the place where a strong electric field helps separate the electron-hole pairs produced when sunlight is absorbed by the intrinsic layer (i). This electric field plays a role in directing the pair to the appropriate electrode, producing an electric current [34]. On the other hand, in p-i_1-i_2-n solar cells, there are two junctions, as a result, the electric field distribution in this solar cell is more complex. The electric field at junction i1 will play a role in separating the electron-hole pairs produced in the i1 layer, while the electric field at junction i_2 will play a role in processing the electron-hole pairs that are not separated at junction i_1.

These results demonstrate the ability of p-i_1-i_2-n solar cells to absorb light with different energies at each junction, which allows more efficient use of the sunlight spectrum as shown in Table 2. In addition, this double junction structure makes it possible to manage imperfect electron-hole pair reactions that may occur at the first junction, thus maximizing the use of sunlight energy [35]. In other words, the electric field distribution reflects how the structure of the solar cell influences the way the cell optimizes the absorption of sunlight and directs electron-hole pairs to produce an electric current [36]. This is an important factor in increasing the overall efficiency of solar cells and maximizing the conversion of solar energy into electricity.

Table 2. Results of characterization p-i-n and p-i_1-i_2-n

Structures	d buffer (nm)	V_{oc} (mV)	J_{sc} (mA/cm^2)	FF	Eff (%)
p-i-n	Experiments	720.0	15.7	0.550	5.61
	AFORS-HET simulation	846.6	14.34	0.463	5.62
p-i_1-i_2-n	Experiments	790.0	17.20	0.620	8.86
	AFORS-HET simulation	857.1	15.69	0.661	8.92

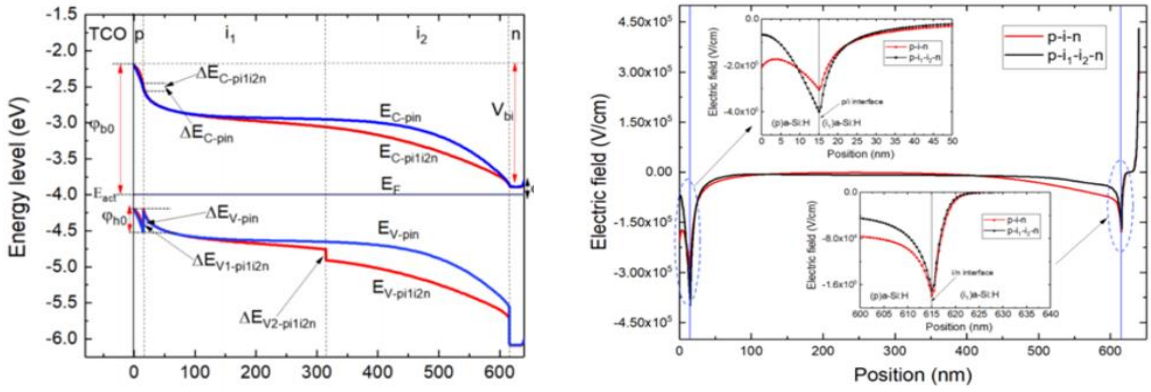
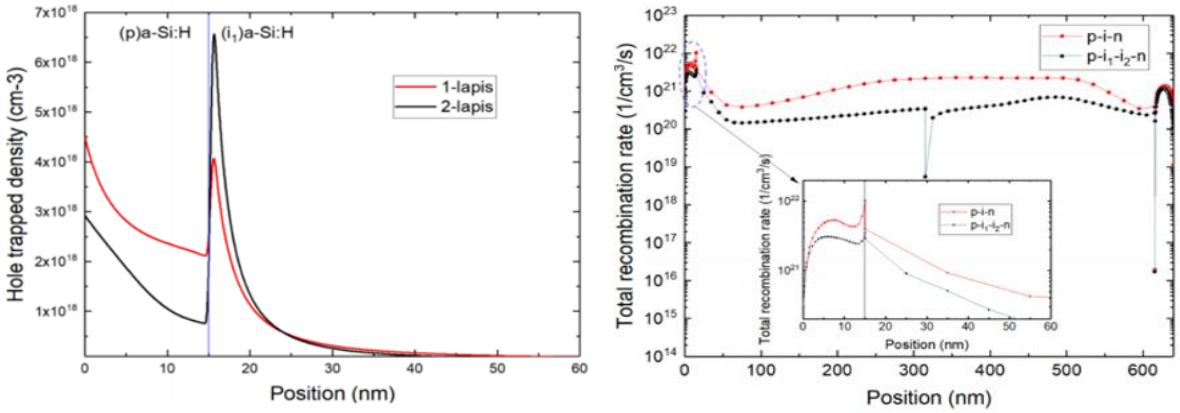


Figure 3. Schematic of (a) the band diagram p-i-n and p-i_1-i_2-n and (b) the electric field distribution p-i-n and p-i_1-i_2-n

Figure 4 shows the electronic results of structures containing Hole trapped density p-i-n and p-i_1-i_2-n, and total recombination rate p-i-n and p-i_1-i_2-n. The density of trapped holes in p-i-n solar cells often occurs at the interface or interface between different layers in the solar cell structure as seen in Figure 4(a). This is caused by differences in band energy, electric field, and material properties between these layers. p-i interfaces, at the interface between the p-layer (positive) and the intrinsic layer (i), there is a significant band energy difference. When sunlight is absorbed by the intrinsic layer, electron-hole pairs are formed. The strong electric field present around the p-i junction helps separate the electron-hole pairs [37]. Electrons will move toward the n-layer, while holes, which have a positive charge, will move toward the p-layer. Some of the holes reaching the p-layer may experience trapping around this region, mainly due to the higher hole in the p-layer. As for the i-n interface, there is a significant difference in band energy between the two. Holes

that reach this interface may have quite high energy. Holes that cannot be immediately extracted to layer n may experience trapping along their journey toward layer n. This often occurs near i-n junctions, where strong electric fields play a role in separating electron-hole pairs [38]. Hole trapping at the interface between these layers is a phenomenon that needs to be managed wisely in solar cell development. Too many trapped holes can reduce the efficiency of converting solar energy into electricity [39]. Therefore, research continues to reduce hole trapping at the interface between these layers and maximize the overall performance of p-i-n solar cells. Figure 4(b) shows the total recombination rate in a-Si:H p-i-n and p-i_1-i_2-n solar cells which depends on the efficiency and ability of the solar cells to extract energy from sunlight. P-i-n solar cells have lower efficiency in converting sunlight energy into electricity compared to p-i_1-i_2-n solar cells as can also be seen in quantum efficiency in Figure 5. This is caused by the loss of potential energy due to higher recombination. In other words, p-i_1-i_2-n solar cells can produce more electricity than p-i-n because they can extract energy from different wavelengths of sunlight [40]. This makes them more efficient, especially in applications where high efficiency is a key factor, such as commercial solar cells and large photovoltaic applications.



(a) (b)

Figure 4. Electronic results of structures containing (a) hole trapped density p-i-n and p-i_1-i_2-n, and (b) total recombination rate p-i-n and p-i_1-i_2-n

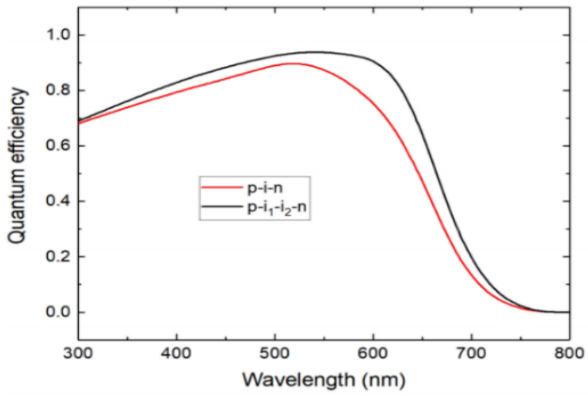


Figure 5. Quantum efficiency p-i-n and p-i_1-i_2-n

Simulation results using AFORS-HET show several important findings in efforts to improve carrier transport properties in single and double junction a-Si: H solar cells. Some of the main results include the optimization of intrinsic layer thickness, simulations reveal that intrinsic layer thickness plays a key role in carrier transportation [41]. Increasing the thickness of the intrinsic layer in a-Si: H single junction solar cells increases light absorption and minimizes recombination, resulting in higher energy conversion efficiency [42]. However, in double-junction solar cells, there is a balance that needs to be considered between the layer thicknesses at both junctions to achieve maximum efficiency.

The influence of electron and hole mobility, mobility of electrons and holes greatly influences the responsiveness of a-Si: H solar cells to sunlight. The increased mobility of electrons and holes in the intrinsic layer leads to shorter transit times and lower recombination rates, which in turn improves solar cell performance. Load factors and DoS, variations in load factors and DoS also influence the carrier's transportation properties [43]. Adjustment of these parameters allows us to achieve a balance between transit time and energy conversion efficiency. The blunter DoS distribution minimizes non-radical recombination and improves solar cell performance. The results of this research illustrate that numerical design and simulation using AFORS-HET is a powerful tool in improving the performance of a-Si: H solar cells. Improving the carrier transport properties in the intrinsic layer is a key step in optimizing solar cell efficiency. Several aspects that need to be considered in this context include the thickness of the intrinsic layer. Setting the thickness of the intrinsic layer is very important to obtain optimal energy conversion efficiency. Using an intrinsic layer that is too thin reduces light absorption, while a layer that is too thick increases the risk of higher recombination. Therefore, the use of numerical design is a very valuable approach to finding the right thickness.

Electron and hole mobility, understanding and improving electron and hole mobility is key. Higher mobility allows operators to move faster through the intrinsic layer, which reduces transit time and improves overall performance. Load factor and DoS, variation of load factor, and DoS distribution provide flexibility in managing the nature of the operator's transportation [44]. By optimizing these parameters, we can achieve better performance in a wide range of sunlight and operating conditions. Double junction solar cells offer the potential for higher performance, but proper design is required to maximize efficiency. The interaction between the two junctions must be carefully considered to achieve optimal synergy [45]. This research provides a strong basis for the development of more efficient single and double junction a-Si: H solar cells. Through numerical design and simulation, we can optimize carrier transport in the intrinsic layer, which is an important step in improving solar cell efficiency. In the context of increasingly urgent renewable energy, this effort has great potential to produce more efficient and sustainable a-Si: H solar cells [46]. These results validate that numerical design and simulation using AFORS-HET is a powerful tool in optimizing carrier transport properties in a-Si: H solar cells. By understanding and managing design parameters, we can achieve higher efficiency in the conversion of solar energy to electricity. In the increasingly important framework of renewable energy, this research contributes to the development of more efficient and sustainable solar cell technology.

4. CONCLUSION

In summary, they demonstrated that optimizing carrier transport properties in the intrinsic layer of a-Si single and double junction solar cells can lead to substantial efficiency improvements. Our numerical design approach, which integrates advanced doping profiles and precise layer thickness adjustments, has shown a significant enhancement in performance, particularly for double junction cells. This work addresses key challenges in solar cell design by providing a comprehensive optimization framework that combines multiple parameters to achieve higher efficiency. The findings suggest that targeted optimization of carrier mobility and recombination rates is crucial for advancing solar cell technology. For the field, our research highlights the potential for substantial efficiency gains through detailed numerical modeling, offering a path for future innovations in photovoltaic design. The implications extend to practical applications, including the development of more efficient and cost-effective solar energy solutions. Future research should focus on experimental validation of our models and exploration of additional parameters, such as material quality and long-term stability. By addressing these areas, we can further enhance the performance of a-Si solar cells and contribute to the broader goal of advancing renewable energy technologies.

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