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Simulation of HIT solar cells with various emitter layers using AFORS-HET

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Abstract
The present work analyzes the important function of the emitter layer in heterojunction with intrinsic thin layer solar cells, highlighting its involvement in electric field generation and the separation and transport of charge carriers. The AFORS-HET modeling tool is employed to analyze various materials, including amorphous silicon (a-Si:H), nanocrystalline silicon (nc-Si:H), microcrystalline silicon (μc-Si:H), and amorphous silicon carbide (a-SiC:H), with the aim of optimizing their thickness, doping concentration, bandgap, and electrical properties to improve solar cell performance. The simulations indicate that the open circuit voltage (V_{oc}) and short circuit current density (J_{sc}) are enhanced by various emitter layers, with nc-Si:H exhibiting the most substantial improvements owing to its wide bandgap, diminished contact resistivity at the nc-Si:H-Transparent Conducting Oxide (TCO) interface, lower defect density, improved passivation, and superior carrier collection. The research indicates that the fill factor (FF) and efficiency of solar cells improve when the emitter layer shifts from a-Si:H to a-SiC:H, μc-Si:H, and nc-Si:H, with efficiencies increasing from 19.46% to 22.2%. The results emphasize the necessity of choosing suitable emitter materials to attain maximum solar cell efficiency, showcasing the benefits of a-SiC:H, μc-Si:H, and nc-Si:H for conductivity, light transmission, and charge carrier mobility. The study indicates that to achieve optimal efficiency in heterojunction solar cells, emitter layers must have a broad bandgap, high conductivity, and minimal defect density.

Keywords: HIT solar cell, emitter layers, amorphous silicon carbide (a-SiC:H), microcrystalline silicon (μc-Si:H), nanocrystalline silicon (nc-Si:H)

Introduction

Initially, Sanyo designed a novel heterojunction with intrinsic thin layer (HIT) solar cell, with a remarkable efficiency of ~18% [1]. Subsequent, Sanyo (in 2014) achieved an efficiency of ~25% [2]. Presently, the maximum experimentally achieved efficiency is 26.7% [3]. With the enhancement in solar cell efficiency, several researchers have focused on simulating solar cells as the outcomes have been executed to enhance performance of solar cell efficiency. Numerous groups have developed distinct structures of HIT solar cells and investigated the effects of modifying layer thickness, bandgap, doping concentration, interface defect states, and electrical properties [4]. Yao *et al*. achieved a simulated efficiency of 25.75% using gradient doping of the emitter layer, as opposed to uniform doping [5]. Aliani *et al*. demonstrate the impact of the front work function by varying the doping of the emitter layer on solar cell performance [6]. Our previous publication reported an efficiency of 24.14% attained by employing a μc-Si:H layer as both the emitter and back surface field (BSF) layer [7]. By altering multiple layers of variable thicknesses and band gaps of different HIT structures, Dwivedi *et al*. achieved a 27.02% simulated efficiency [8]. Through modification of the densities of interface defect states and interface fixed charges, which further affect the band bending, Oppong *et al*. achieved a simulated efficiency of ~29% [9]. M. Kumar *et al*. attained a simulated efficiency of 24.13% for the TiO2/i-a-Si:H/p-c-Si heterojunction solar cell by the optimization of various parameters [10]. Numerous organizations have integrated experimental results with simulations to improve the efficiency of diverse types of HIT solar cells [11, 12]. Experimental results closely align with simulated outcomes for solar cells.

The emitter layer is essential in HIT solar cells, since it transmits light to the c-Si absorber layer, which produces free electron-hole charge carriers. Furthermore, a suitable emitter layer produces the necessary band bending and sufficient electric field to efficiently separate and transmit charge carriers to the TCO and metal contacts.

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It is necessary to study and optimize the thickness, bandgap, doping concentration, defect states, and electrical properties of the emitter layers to improve the performance of HIT solar cells. Simulation tools can provide enhanced insights into the influence of materials properties on solar cell performance, hence reducing costs. AFORS-HET (Automat FOR Simulation of Heterostructures) is a simulation program designed for the analysis of heterojunction solar cells [13]. A diverse array of materials has been employed as the emitter layer in solar cells, including amorphous silicon (a-Si:H), amorphous silicon carbide (a-SiC:H), hydrogenated amorphous silicon germanium (a-SiGe:H), microcrystalline silicon oxide (μc-SiO:H), microcrystalline silicon (μc-Si:H) and nanocrystalline silicon (nc-Si:H) [7, 14, 15, 16, 17]. Nevertheless, a limited group of researchers has examined the comparative use of a-Si:H, nc-Si:H, μc-Si:H, and a-SiC:H emitter layers in solar cells.

This study investigates the performance of heterojunction solar cells utilizing various emitter layers composed of a-Si:H, nc-Si:H, μc-Si:H and a-SiC:H employing the AFORS-HET modeling tool. The bandgap, dielectric constant, doping concentration and other electric parameters of each emitter layer on fixed thickness is adjusted to analyze and enhance the performance of the heterojunction solar cells.

Simulation

AFORS-HET is a numerical simulation tool utilized for simulating both homo- and heterojunction devices. It resolves one-dimensional semiconductor equations via Shockley-Read-Hall recombination statistics [11]. A range of boundary conditions may be selected, facilitated by an intuitive interface that enables parameter adjustments for the visualization and comparison of simulations. It employs an optical model based on the Lambert-Beer equation to estimate the optical properties. The solar AM 1.5 radiation was used as the illumination source with a power density of 100 mW/cm². In the simulations, all parameters were utilized as shown in Table 1. The Zinc oxide (ZnO) front contact and the Ag back contact were optically simulated using the default material absorption coefficients and refractive index values provided in the AFORS-HET program. Fig. 1 depicts a schematic representation of the HIT solar cell structure, incorporating various emitter layers, specifically a-Si:H(n), nc-Si:H(n), μc-Si:H(n), and a-SiC:H(n). The characteristics of the various emitter layers, as outlined in Table 1, are analyzed to assess their impact on the performance of the solar cell.

Results and Discussion

The emitter layer thickness was kept at 3 nm. In the simulations, the bandgaps of the a-Si:H(n), nc-Si:H(n), μc-Si:H(n), and a-SiC:H(n) layers were maintained at 1.8 eV, 2.0 eV, 1.6 eV, and 2.2 eV, respectively. These values are almost identical to those of films that were deposited experimentally. The bandgap of the a-Si:H(i) and a-Si:H(p+) layers has been chosen to be 1.75 eV. All of these properties are taken from existing sources [7,14,15]. Fig. 2 presents a schematic band offset diagram of HIT solar cells several emitter layers (specifically a-Si:H, a-SiC:H, nc-Si:H, and μc-Si:H) with a passivation layer (i-a-Si:H).

Variation of open circuit voltage (V_{oc}), short circuit current density (J_{sc}), fill factor (FF) and efficiency (η) as the function of emitter layers for simple HIT solar cell was depicted in Fig. 3.

1. Variation in Open Circuit Voltage with different emitter layers

V_{oc} rises from 707.5 mV to 708.4 mV with the varying emitter layer from a-Si:H, a-SiC:H, μc-Si:H, and nc-Si:H, as shown in Fig. 3(a). Hydrogenated amorphous silicon carbide (a-SiC:H) serves as an effective window layer for solar cells. The a-SiC:H layer is created by incorporating carbon atoms into the a-Si:H matrix. The bandgap of a-SiC:H is wider than that of a-Si:H, resulting in a reduced refractive index, which minimizes reflection losses in the solar cell. Additionally, it demonstrates a lower absorption coefficient across the 300-700 nm wavelength range, signifying improved transparency in this spectrum, thereby allowing the maximum influx of photons to the c-Si wafer for the generation of free electron-hole pairs. Moreover, the mobility and electrical conductivity is high in contrast with a-Si: H. The extensive bandgap of the a-SiC:H layer additionally modifies the band discontinuities between the valence band and conduction band [13]. Also, the a-SiC:H layer resolves the lattice mismatch between the TCO and the intrinsic a-Si:H layer [14]. V_{oc} is increased by about 0.9 mV when utilizing a-SiC:H in comparison to a-Si:H, attributable to the lower recombination density in the a-SiC:H layer.

Further, open circuit voltage has been increased by about 1.2 mV and 0.3 mV when using μc-Si:H instead of a-Si:H and a-SiC:H, respectively. μc-Si:H is a structure in which crystalline structures (~ > 10 nm) are embedded in an amorphous matrix. μc-Si:H is a significant material for the emitter layer of HIT solar cells due to its exceptional properties such as decreased defect density, appropriate bandgap, high conductivity, high carrier mobility and diffusion length [7]. The V_{oc} of microcrystalline silicon has been raised relative to amorphous silicon through enhanced light absorption, particularly in the near-infrared spectrum, and perhaps enhanced carrier transport attributed to crystalline structures within the amorphous network. Though, open circuit voltage of a-SiC:H and μc-Si:H is nearly same.

Hydrogenated nanocrystalline silicon (nc-Si:H) possesses a substantial bandgap, reduced defect density, and enhanced conductivity relative to a-Si:H films, these characteristics of nc-Si:H enable it an appropriate material for the emitter layer in solar cells. These films include silicon nanocrystallites, measuring a few nanometers, incorporated inside an amorphous silicon structure. There is a rise in the open circuit voltage of about 2.3 mV, 1.4 mV, and 1.1 mV when utilizing nc-Si:H in place of a-Si:H, a-SiC:H, and μc-Si:H, respectively. The increased bandgap and reduced defect density in the bulk and interface of the nc-Si:H of nc-Si:H emitter layer enhances the open-circuit voltage in contrast with a-Si:H, a-SiC:H, and μc-Si: H. The extensive bandgap of nc-Si:H enhances the absorption of high-energy photons in c-Si, thereby producing a substantial quantity of electron-hole pairs, and its electrical conductivity is higher than that of the other layers.

2. Variation in Short Circuit current density with different emitter layers

From Fig. 3(b) it is evident that J_{SC} increases from 33.66 mA/cm^2 to 37.58 mA/cm^2 with the varying emitter layer from a-Si:H, a-SiC:H, μc-Si:H and nc-Si:H. The short circuit current increases by approximately 1.3 mA/cm² due to the a-SiC:H layer improving light transmission to the c-Si absorber layer, attributed to its broader bandgap and reduced absorption coefficient. The enhanced transparency of the a-SiC:H layer allows the c-Si substrate to absorb an increased number of photons, thus enhancing the photocurrent and consequently elevating the short circuit current density relative to a-Si:H. Furthermore, employing the µ-Si:H emitter layer in place of a-Si:H and a-SiC:H has increased the short circuit current density by approximately 2.82 mA/cm² and 1.5 mA/cm², respectively. The primary reason for the elevated short-circuit current density was enhanced light absorption and efficient carrier transport inside the µc-Si:H layer. µc-Si:H has a higher optical absorption coefficient relative to a-Si:H and a-SiC:H, leading to an increased generation of electron-hole pairs inside the layer. The crystalline structure of µc-Si:H promotes enhanced charge carrier mobility and diffusion lengths compared to the disordered structures of a-Si:H and a-SiC:H. This facilitates the effective separation and transit of charge carriers across the heterojunction, hence enhancing the photocurrent. µc-Si:H exhibits better contact with the c-Si absorber, leading to reduced recombination and improved current collection efficiency.

Applying the emitter layer nc-Si:H in place of a-Si:H, a-SiC:H, and µc-Si:H yields an enhancement in short current density of around 3.92 mA/cm², 2.61 mA/cm², and 1.11 mA/cm², respectively. nc-Si:H provides an expanded bandgap, reduced defect density, and increased conductivity, which together allow improved light absorption and carrier transport. The increased bandgap of nc-Si:H facilitates the transmission of a broader spectrum of photons through the emitter layer, which are then absorbed by the underlying c-Si substrate. This leads to an increased generation of electron-hole pairs, hence enhancing the J_{sc}. The extensive bandgap of the nc-Si:H layer reduces the lattice mismatch with the transparent conducting oxide (TCO), leading to reduced contact resistivity at the nc-Si:H-TCO interface [18, 19]. Furthermore, the nc-Si:H-TCO interface demonstrates a decreased electron transport barrier relative to other silicon thin films, hence enhancing the carrier transport mechanism at the TCO-n-layer interface. The nc-Si:H layer has significantly higher dark conductivity than a-Si:H, a-SiC:H, and µc-Si:H, due to the prevalence of crystallites that substantially reduce resistive losses inside the layer. The nc-Si:H layer exhibits a reduced activation energy and an elevated work function, resulting in advantageous band bending at the c-Si surface area [19]. Consequently, the n-nc-Si:H exhibits a significantly greater disparity between hole and electron concentrations, hence enhancing electrical passivation. The aggregation of electrons via tunneling is enhanced by the reduced and more pronounced energy barrier resulting from the optimized band bending at the n layer-i layer-p-Si stack. The improved conductivity of nc-Si:H promotes the effective collection and transport of charge carriers, hence providing a greater flow of generated current through the solar cell.

3. Variation in Fill Factor with different emitter layers

Fig. 3 (c) shows that the Fill Factor ranges between 82.65% and 83.18% across various emitter layers. A high fill factor has been observed in the nc-Si:H emitter layer due to enhanced passivation and carrier collection, as the nc-Si:H layer establishes an effective interface between the c-Si and the i-a-Si:H passivation layer. Moreover, nc-Si:H may effectively passivate the c-Si surface, reducing the number of dangling bonds that might trap charge carriers, hence enhancing carrier collection efficiency. Additionally, by enhancing the interface between the nc-Si:H emitter layer and the TCO, the nc-Si:H layer can raise the fill factor (FF).

4. Variation in Efficiency with different emitter layers

Fig. 3(d) indicates that efficiency increases from 19.46% to 22.2% as the emitter layer transitions from a-Si:H to a-SiC:H, µc-Si:H, and nc-Si:H, respectively, this indicate that employing nc-Si:H(n), µc-Si:H(n), and a-SiC:H(n) emitter layers improve the efficiency of HIT cells compared to a-Si:H(n). The efficiency of solar cells of a-Si:H was negatively impacted by the higher defect density, higher absorption coefficient and low conductivity. The open circuit voltage and short-circuit current density are improved by the low absorption coefficient and wider bandgap of the a-SiC:H layer, as these properties facilitate greater light penetration into the c-Si(p), leading to enhanced generation of free charge carriers and diminished recombination losses. Furthermore, the µc-Si:H layer demonstrates improved charge carrier mobility, diffusion lengths, high conductivity, reduced defect density due to its crystalline structure, and, hence enhancing its efficiency compared to disordered structures (a-Si:H and a-SiC:H). The improved microstructure, defined by a crystallite arrangement, increased bandgap, high conductivity, diminished coordination defects, and advantageous band bending at the c-Si surface due to the lowered activation energy of the nc-Si:H layer and reduced contact resistivity at the nc-Si:H-TCO interface, is attributed to the decreased lattice mismatch with the transparent conducting oxide, thereby enhancing its efficiency.

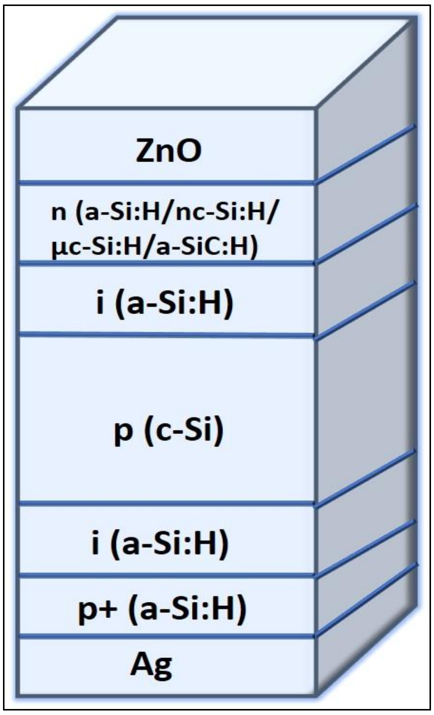

Fig 1: HIT solar cell structure

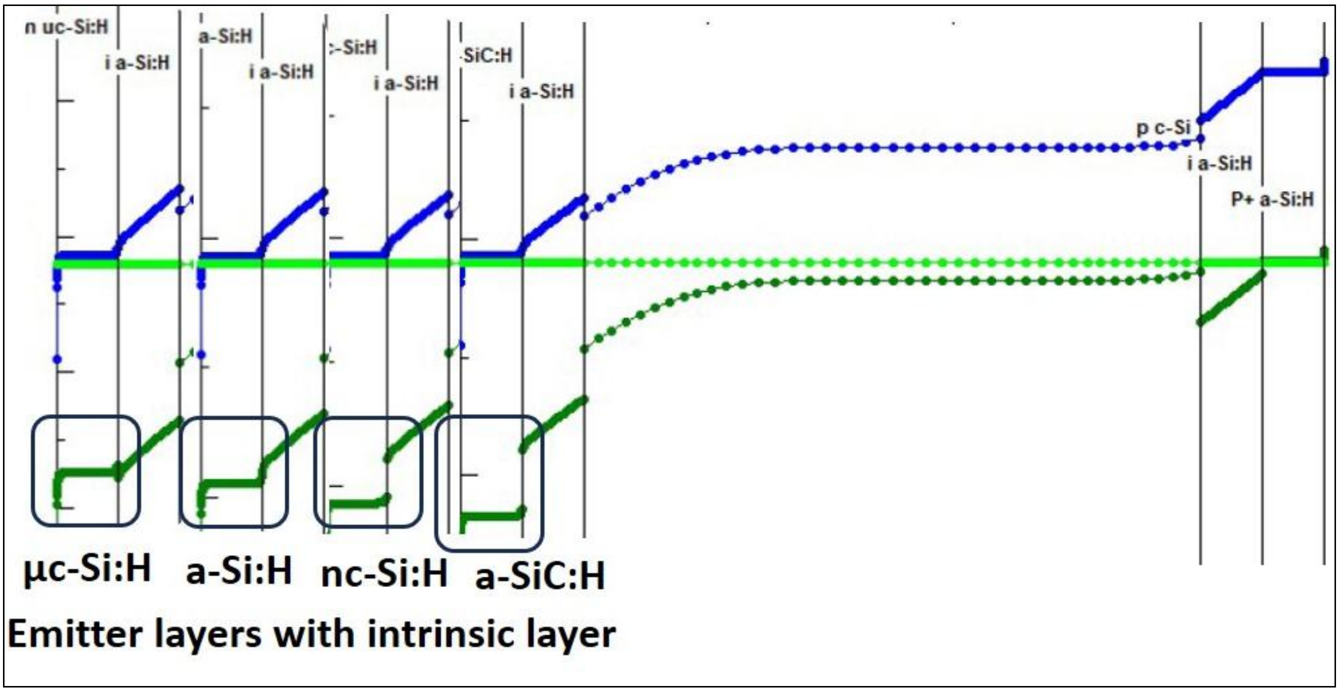

Fig 2: Simulated band diagram with different emitter layer showing band offset with intrinsic layer

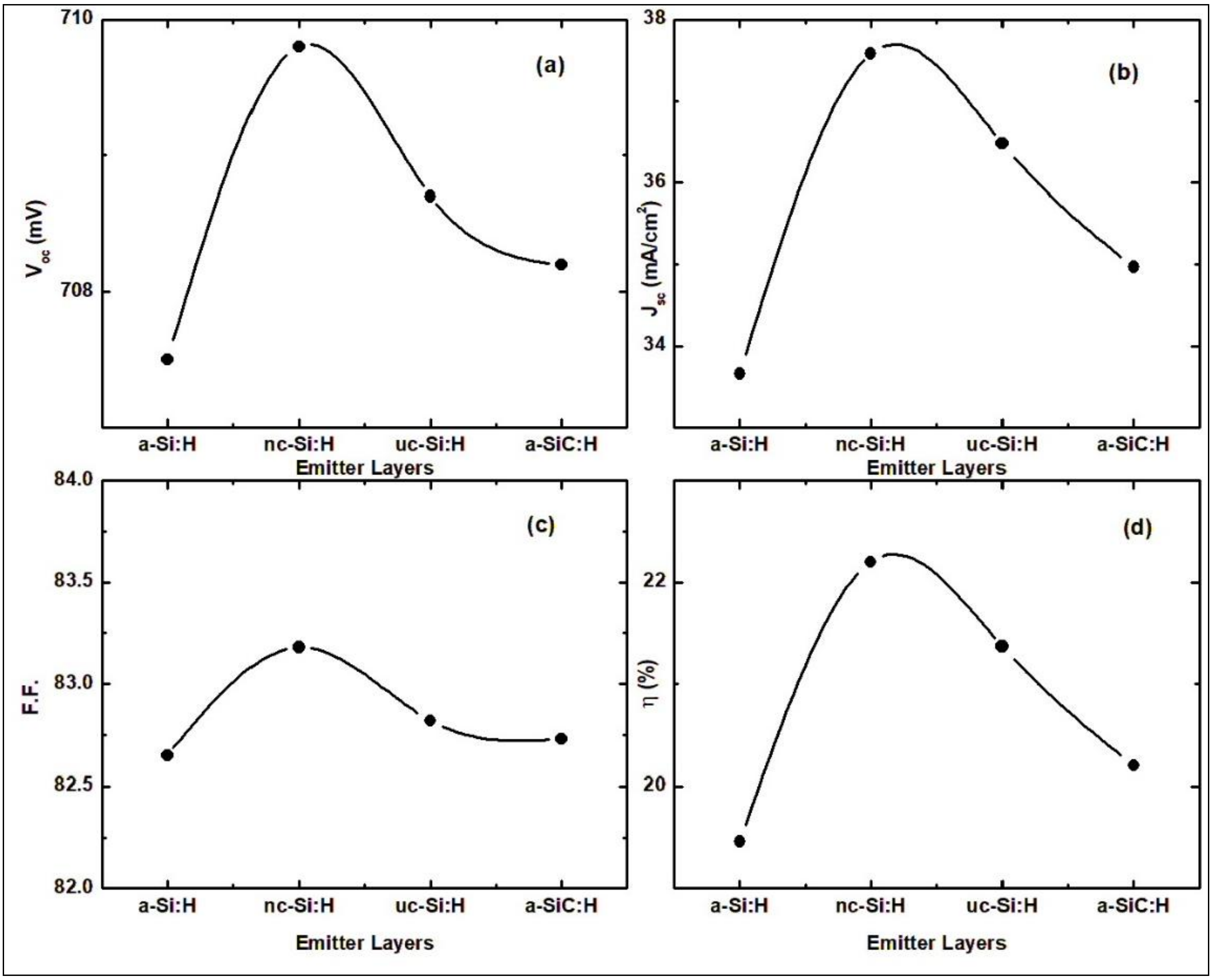

Fig 3: (a)-(d) Variation of Open circuit Voltage (V_{oc}), Short current density (Jsc), Fill factor (FF) and efficiency (η) as a function of different emitter layer.

Table 1: Input parameters used in present simulation

	a-Si:H (n)	aSiC:H (n)	μc-Si:H (n)	nc-Si:H (n)	a-Si:H (i)	c-Si (p)	a-Si:H (p+)
Dielectric Constant	11.1	11.1	11.1	11.1	11.1	11.1	11.1
Electron Affinity (eV)	3.9	3.9	4	4	3.9	4.05	3.9
Thickness (nm)	3	3	3	3	3	300000	50
Band gap (eV)	1.8	2.2	1.6	2.0	1.75	1.12	1.75
Effective valence-band density (cm^{-3})	10^{20}	3×10^{20}	10^{19}	5×10^{19}	10^{20}	2.8×10^{19}	10^{20}
Effective conduction-band density (cm^{-3})	10^{20}	3×10^{20}	10^{19}	5×10^{19}	10^{20}	2.8×10^{19}	10^{20}
Electron mobility ($cm^2V^{-1}s^{-1}$)	7	9	50	60	7	1140	7
Hole mobility ($cm^2V^{-1}s^{-1}$)	1	1	5	6	1	420	1
Acceptor concentration (cm^{-3})	0	0	0	0	0	1.5×10^{16}	5×10^{21}
Donor concentration (cm^{-3})	5×10^{20}	9×10^{20}	2×10^{19}	5×10^{19}	0	0	0
Thermal velocity of electrons ($cm\ s^{-1}$)	10^7	10^7	10^7	10^7	10^7	10^7	10^7
Thermal velocity of holes ($cm\ s^{-1}$)	10^7	10^7	10^7	10^7	10^7	10^7	10^7
Layer density ($g\ cm^{-3}$)	2.328	2.328	2.328	2.328	2.328	2.328	2.328

Conclusions

The emitter layer is essential in heterojunction with intrinsic thin layer (HIT) solar cells, producing an electric field and band bending to facilitate effective charge carrier separation and transport. It transmits light to the c-Si absorber layer, producing free electron-hole charge carriers. Enhancing thickness, doping concentration, bandgap, and electrical properties is crucial for enhancing solar cell performance. This work use the AFORS-HET modeling tool to evaluate and enhance the performance of HIT solar cells utilizing several emitter layers: a-Si:H, nc-Si:H, μc-Si:H, and a-SiC:H. Hydrogenated amorphous silicon carbide (a-SiC:H) serves as an effective window layer for solar cells, enabling the transmission of the maximum number of incoming photons to the c-Si wafer, owing to its wide band gap, elevated mobility, and superior electrical conductivity compared to hydrogenated amorphous silicon (a-Si:H). Hydrogenated microcrystalline silicon (μc-Si:H) is an essential material for the emitter layer of HIT solar cells because to its exceptional properties, including superior conductivity, decreased coordination defect density, and an ideal bandgap. Hydrogenated nanocrystalline silicon (nc-Si:H) possesses a broad bandgap, reduced defect density, enhanced conductivity, and beneficial band bending at the c-Si surface due to the diminished activation energy of the nc-Si:H layer. Additionally, the decreased contact resistivity at the nc-Si:H-TCO interface is ascribed to the lower lattice mismatch with the transparent conducting oxide compared to a-Si:H, a-SiC:H, and μc-Si:H films, making it appropriate for the emitter layer in solar cells. In this investigation, the open circuit voltage rises from 707.5 mV to 708.4 mV due to modifications in the emitter layer. The investigation reveals that the short circuit current density (J_{SC}) increases from 33.66 mA/cm² to 37.58 mA/cm² with different emitter layers, with a-Si:H, a-SiC:H, μc-Si:H, and nc-Si:H demonstrating the highest efficiency. The a-SiC:H layer augments light transmission to the c-Si absorber layer, hence enhancing photocurrent and short-circuit current density. The μc-Si:H layer has an enhanced optical absorption coefficient, promoting greater charge carrier mobility and diffusion lengths. The nc-Si:H layer has significantly enhanced dark conductivity, hence augmenting electrical passivation and electron accumulation by tunneling. The Fill Factor ranges from 82.65% to 83.18% across various emitter layers. The nc-Si:H layer demonstrates a high fill factor due to enhanced passivation and carrier collection, together with increased carrier collection efficiency. The efficiency of heterojunction solar cells increases from 19.46% to 22.2% when the emitter layer transitions from a-Si:H to a-SiC:H, μc-Si:H, and nc-Si:H, respectively. The research indicates that emitter layers have to possess a wide bandgap, elevated conductivity, and reduced defect density for maximal efficiency.

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