

Analysis of the p^+/p window layer of thin film solar cells by simulation*

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Abstract: The application of a p^+/p configuration in the window layer of hydrogenated amorphous silicon thin film solar cells is simulated and analyzed utilizing an AMPS-1D program. The differences between $p^+-p-i-n$ configuration solar cells and $p-i-n$ configuration solar cells are pointed out. The effects of dopant concentration, thickness of p^+ -layer, contact barrier height and defect density on solar cells are analyzed. Our results indicate that solar cells with a $p^+-p-i-n$ configuration have a better performance. The open circuit voltage and short circuit current were improved by increasing the dopant concentration of the p^+ layer and lowering the front contact barrier height. The defect density at the p/i interface which exceeds two orders of magnitude in the intrinsic layer will deteriorate the cell property.

Key words: p^+/p configuration; thin film solar cells; hydrogenated amorphous silicon solar cells; window layer

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1. Introduction

It is well known that the window layer sandwiched between transparent conductor oxides (TCOs) and the intrinsic layer plays a vital role not only in the initial efficiency of solar cells but also in their stability. The performance of solar cells is primarily determined by the materials they are made up from. The hydrogenated amorphous silicon as an emitter adding carbon atoms can increase the optical band gap and improve the efficiency of solar cells^[1]. Series resistance can be decreased by using a heavily doped emitter, which can improve the open circuit voltage (V_{oc}). However, V_{oc} is restricted by the recombination of the emitter, and series resistance affects the fill factor (FF) of solar cells. To improve the performance of solar cells, the influences of thickness, dopant concentration, optical band gap and the material^[2] of the p -type layer are studied. Photoelectric characteristics of amorphous silicon are closely related to the $p-i$ interface because of the high recombination. There are usually two kinds of basic thoughts to reduce recombination^[3]. One of the ways is changing the materials of the emitter layer and the intrinsic layer. $A-SiC:H$, $\mu c-Si:H$ and $nc-SiC:H$ are widely used as p -type window layers. The other way is inserting a wide band gap, high conductivity film as a buffer layer into the $p-i$ interface. The advantages of a buffer layer are as follows: (1) it adjusts the band offset of the $p-i$ heterojunction, (2) it enhances the electric field in this area, (3) it prevents electrons diffusing into the p -layer, (4) it reduces the recombination of the $p-i$ interface. A large amount of research has focused on the $p-i$ interface and $i-n$ interface^[4-6], fewer studies have concentrated on the influence of a window layer configuration. The heavily-lightly doped (p^+-p) junction is commonly used in the back surface field (BSF) of bulk silicon solar cells^[7],

but used less in the window layer of thin film solar cells. It is a deterrent to the movement of photogenerated minority carriers in the base region, and is capable of reducing surface recombination, and improves the short circuit current (J_{sc}) and V_{oc} . Ma *et al.*^[8] inserted p -type $\mu c-Si:H$ into TCO/ p - $a-SiC$ as an interface layer to investigate the influence of the thickness of p -type $\mu c-Si:H$ on the performance of solar cells with a TCO/ p - $a-SiC/i$ - $a-Si/n$ - $\mu c-Si/ITO/Ag$ structure. However, the influences of dopant concentration and optical band gap were not taken into consideration. Letha *et al.*^[9] designed the window layer of the device with a three layered structure of graded doping for a higher device performance without studying dopant concentration and thickness of the material.

In this paper, the influences of the p^+-p junction as a window layer on solar cells are investigated by simulation. The window layer demands high conductivity, high optical transparency and wide optical band gap, so we choose $a-SiC$ as the window layer material. The device employed in this work consists of TCO/ $p^+-a-SiC/p$ - $a-SiC/i$ - $a-Si/n$ - $a-Si/ITO/Ag$. The front contact barrier height, density of interface, the dopant concentration and thickness of the p^+-p junction are taken into consideration to investigate how they influence the device performance.

2. Simulation and calculation

To study the effects of a p^+-p junction on solar cells, an AMPS-1D program, which was developed by the University of Pennsylvania is applied^[10]. It uses the first-principles continuity and Poisson's equations approach to analyze the transport behavior of semiconductor electronic and optoelectronic device structures. These device structures can be composed of

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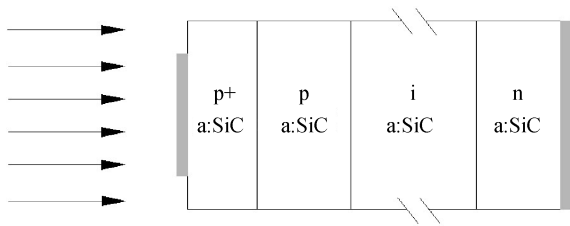


Fig. 1. Structure of a p⁺-p-i-n solar cell.

crystalline, polycrystalline, or amorphous materials or combinations thereof. The three governing semiconductor device equations (the Poisson's equation, the electron and hole continuity equations) are numerically solved by AMPS-1D. The configuration of TCO/p⁺-a-SiC/p-a-SiC/i-a-Si/n-a-Si/ITO/Ag is adopted, in which the parameters used in this calculation are general parameters based on Ref. [11]. Figure 1 shows the structure of solar cells. In this reference, the parameters of a-Si and a-SiC have been ascertained from the authors' efforts to match computer simulations of Schottky diode behavior and single heterojunction a-SiC/a-Si p-i-n cell behavior to experimentally measured characteristics. The absorption coefficient of a-Si and a-SiC are absent from the official website of AMPS-1D. To simplify this calculation, we assumed that the working temperature is 300 K, there is no light trapping and the surface recombination velocity is 10⁷ cm/s.

3. Results and discussion

P-type a-SiC thin film is usually utilized as the window layer of amorphous silicon solar cells because of the wide optical band gap and high conductivity characteristics. A wide optical band gap can enhance optical transmissivity, promote the collecting efficiency of short waves and improve J_{sc} and V_{oc} . However, a wide optical band gap and a dark current are inter-constraint. Owing to the fact that a p⁺-p junction is an obstruction to minority carriers in the base region, surface recombination and dark current can be efficiently reduced by adopting this structure. Figure 2 draws the comparisons between a p-i-n configuration and p⁺-p-i-n configuration with the same parameters, which are from Ref. [11]. It is clearly observed that a solar cell with a p⁺-p junction shows a better performance than the conventional device, and the conversion efficiency (E_{ff}) improves by 6%.

3.1. Influence of the dopant concentration of a p⁺-p junction

A method utilizing the junction composed two thin films with the same doping type but different doping concentrations to increase E_{ff} has been reported^[12]. The most common application is the BSF, which means depositing a p-p⁺ junction on the back contact surface. The theory of a p⁺-p junction is similar to that of a p-p⁺ junction, which is expounded and proved by Chen Jinting when he studied the BSF of bulk silicon solar cells^[13]. As we all know, the theoretical maximum photovoltage is the built-in potential V_d , which is indicated by following equation:

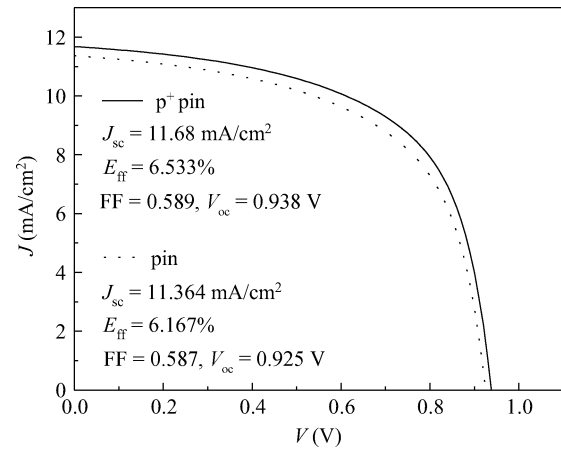


Fig. 2. J - V curves of the two solar cells.

$$\begin{aligned}
 V_d(p^+-p-n) &= [V_{oc}(p^+-p-n)]_{\max} \\
 &= [V_{oc}(p^+-p)]_{\max} + [V_{oc}(p-n)]_{\max} \\
 &= \frac{1}{q} [(E_{Fp^+} - E_{Fp}) + (E_{Fp} - E_{Fn})] \\
 &= \frac{kT}{q} \left[\ln \frac{N_A^+}{N_A} + \ln \frac{N_D N_A}{n_i^2} \right] \\
 &= \frac{kT}{q} \ln \frac{N_A^+ N_D}{n_i^2}, \tag{1}
 \end{aligned}$$

where p⁺, p, n, q, k, T, E_{Fp^+} , E_{Fp} , N_A^+ , N_A , N_D and n_i respectively represent heavy doping p-type layer, light heavy doping p-type layer, n-type layer, a unit charge, the Boltzmann constant, temperature, the quasifermi level in the p⁺-layer, the quasifermi level in the p-layer, doping concentration in p⁺-layer, doping concentration in p-layer, doping concentration in n-layer and intrinsic carrier concentration.

As shown in Eq. (1), V_{oc} has a lot to do with the dopant concentration of the p⁺-layer. With an increase in the dopant concentration, it is enhanced. Considering the point of front contact interface characteristic, the TCO/p interface is improved by the p-type heavily doped layer. Ma *et al.*^[8] have proved that the interface characteristics of the front and back contact region, among various factors which are closely related with the photovoltaic performances, play a vital role in the determination of photovoltaic characteristics. Inserting a high conductivity thin film into a TCO/p interface can widen the band gap and thus enhance the built-in potential.

Figure 3 shows the changes of solar cells with various dopant concentrations of p⁺ layer. We can see that V_{oc} increases as the dopant concentration increases, following the same trend as in our previous investigation. Not only that, J_{sc} , FF, E_{ff} are in accord with the change of V_{oc} .

It is demonstrated that the Fermi level position, the type of conduction and density of state (DOS) will be changed when the materials are doped. In addition, the solar cells' band diagram can be drawn by plotting the Fermi level position, the type of conduction, the DOS, electron affinity and band gap. Figure 4 describes how the band programs vary with dopant concentration of the p⁺ layer. It can be seen from the graph that

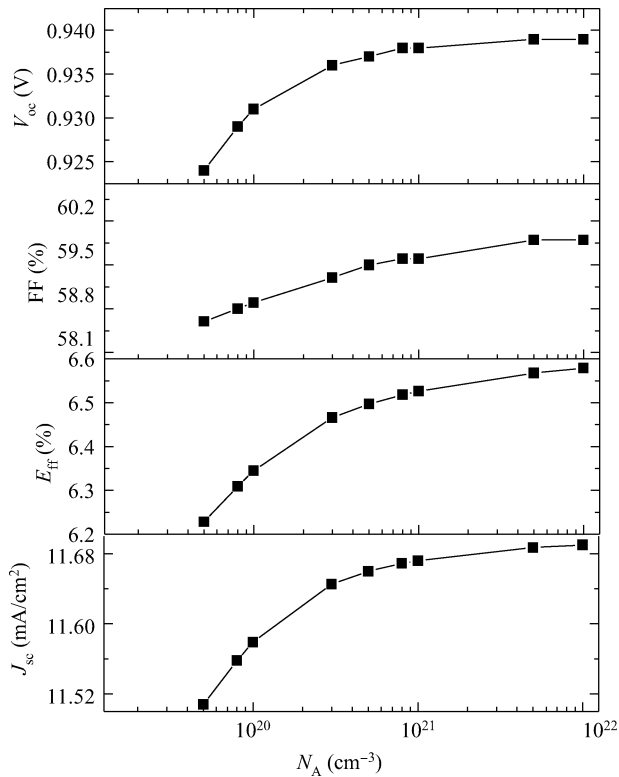


Fig. 3. Solar cell performance dependent on various dopant concentrations of the p^+ layer.

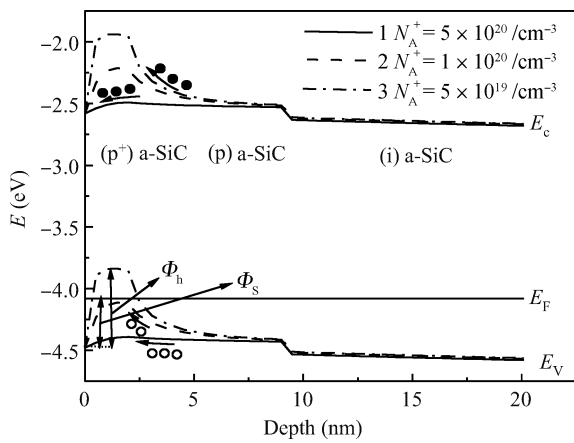


Fig. 4. Band diagram of a solar cell with a $p^+-p-i-n$ configuration.

the potential difference between the p^+ layer and the p layer increases with increasing the dopant concentration. In addition, with a change of the dopant concentration, the band program bends in the p^+-p interface. This is because the dopant causes the Fermi level position to move down, detach from the center of the band gap and approach the valence band maximum. The upward band bending forms a potential, which hinders minority carrier (electron) transportation and promotes majority carrier transmission, thus front surface recombination is reduced and dark current decreases. This directly causes J_{sc} to be enhanced. Different dopant concentrations change the contact barrier height. In this picture, high dopant concentration increases the contact barrier height, which is beneficial to solar cells, therefore, the dopant concentration of p^+ should be

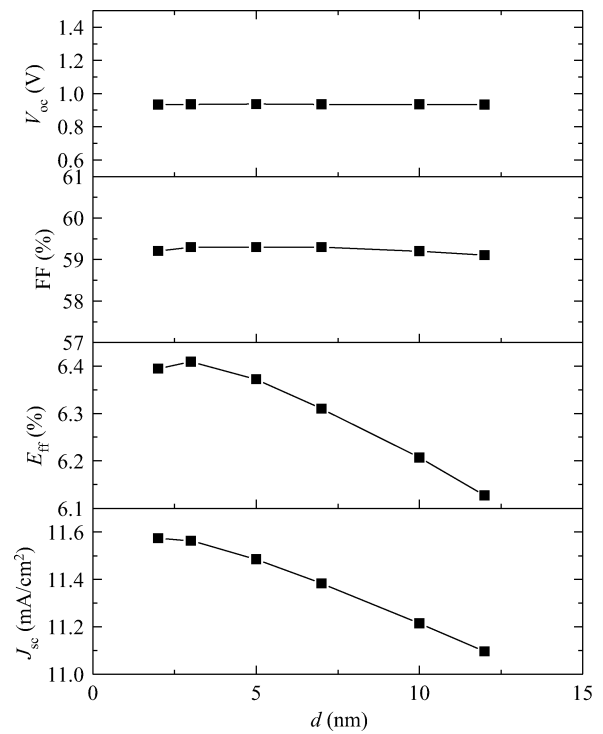


Fig. 5. Dependence of the device photovoltaic characteristics on the thickness of the p^+ -layer.

high.

The quantity Φ_h in Fig. 4 denotes the degree of band bending at thermodynamic equilibrium in the p^+ -a-SiC material. It depends on the front contact barrier height, the p^+ -layer dopant concentration and DOS, and the thickness of the p^+ -layer. In this paper, we assumed that all parameters are constant except for the dopant concentration of the p^+ -layer. The value of Φ_h will increase when the p^+ -layer is highly doped. Majority carriers (hole) are collected at the front contact. However, we can see from the graph that the band bending Φ_h presents a barrier to photogenerated holes trying to exit the cell. But the simulation result of J_{sc} is evidently enhanced, we believe that it is because a tunneling effect presents at the front contact^[14]. Photogenerated holes tunnel over Φ_h at a certain probability, causing a tunneling current. In fact, tunneling current plays a significant role, and even a dominant part, in a heavily doped semiconductor or working at low temperature^[15].

3.2. Influence of thickness of a p^+-p junction

To study the role of thickness of a p^+-p junction, the value of the p -layer, i -layer and n -layer is respectively fixed at 7 nm, 300 nm and 10 nm, while the values of the p^+ -layer varies at 2, 3, 5, 7, 10 and 12 nm. The dependence of the device photovoltaic characteristics on the thickness of the p^+ a-SiC layer is shown in Fig. 5. From the chart, we can see that J_{sc} and E_{ff} decrease with increasing thickness d , while V_{oc} and FF are almost constant. The maximum value of E_{ff} is achieved when d is 3 nm. Along with the change in the p^+ -layer, the E_{ff} of the cell diminishes, which is in agreement with the experiment result in Ref. [8]. There are two ways of interpreting the reduction of J_{sc} . On one hand, due to the change of thickness, optical absorption increases in the p^+ -layer. However, the light

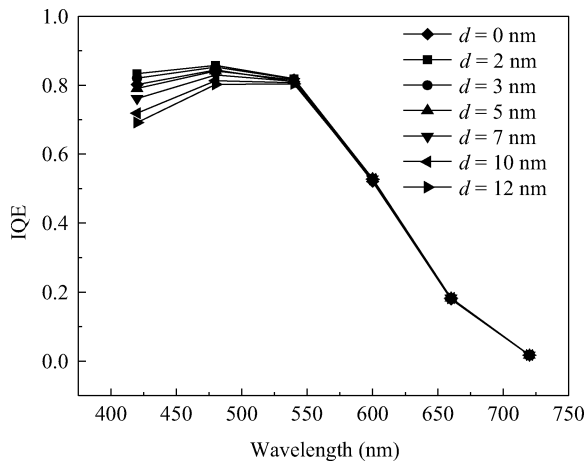


Fig. 6. Quantum efficiency varies with the thickness of the p⁺-layer.

in this layer has no contribution to current. On the other hand, because the amount of light passing through the active layer is reduced, the photogenerated current decreases, causing the current through the whole device to decrease.

Figure 6 displays what happens to quantum efficiency when the thickness of the p⁺-layer is changed. We discover that a solar cell with the right thickness p⁺-layer can catch more waves than one without a p⁺-layer. It's obvious that the appearance of a p⁺ layer improves the absorption of short waves. When the thickness of the p⁺ layer exceeds 3 nm, quantum efficiency decreases, which maybe due to the change in carrier recombination in the excessively thick p⁺ layer. Clearly seen is that quantum efficiency in the short wavelength region becomes weaker along with increasing thickness, thus photogenerated current decreases. The reason why V_{oc} doesn't change is probably because a 2 nm p⁺-layer is thick enough to create an electric field to collect photogenerated carriers in the active layer. Greater thickness will not further strengthen the built-in potential.

3.3. Influence of the front contact barrier height

Hu *et al.*^[16] have found that, because the work functions of TCO and amorphous silicon exit from a certain gap, at TCO/p⁺ and the n/metal interface, there are large numbers of interface states which can lead to the Fermi level pinning effect and the formation of a Schottky barrier and which exert considerable effects on amorphous silicon solar cells. The TCO/p⁺ interface plays a more vital role because of the nonequivalence between photogenerated holes and photogenerated electrons. In this paper we only take the front contact barrier height Φ_s into consideration, while the barrier height at the n/metal interface is assumed to be constant, where Φ_s is shown in Fig. 4.

The front contact barrier height Φ_s depends on dopant concentration, electron affinity and the work function of the materials. The $J-V$ curves are drawn in Fig. 7 varying with the front contact barrier height Φ_s . When Φ_s decreases, the band bending Φ_h will also decrease, thus the probability of tunneling will become greater, causing an improvement in current. A high doping concentration in the p⁺-layer can enhance the performance of the device, but at the same time, it makes Φ_h increase. So there is a value of Φ_s that causes the best cell per-

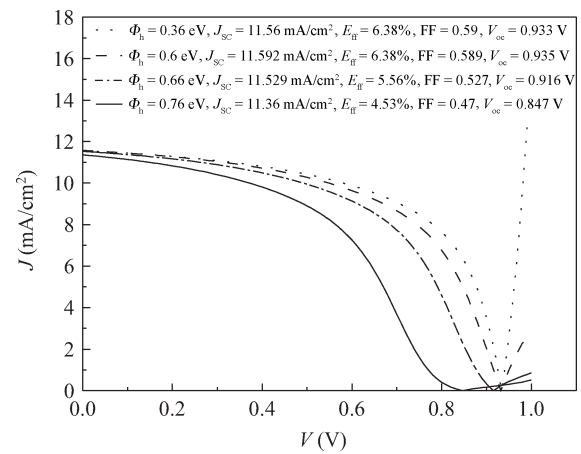


Fig. 7. The dependence of $J-V$ curves vary with Φ_s .

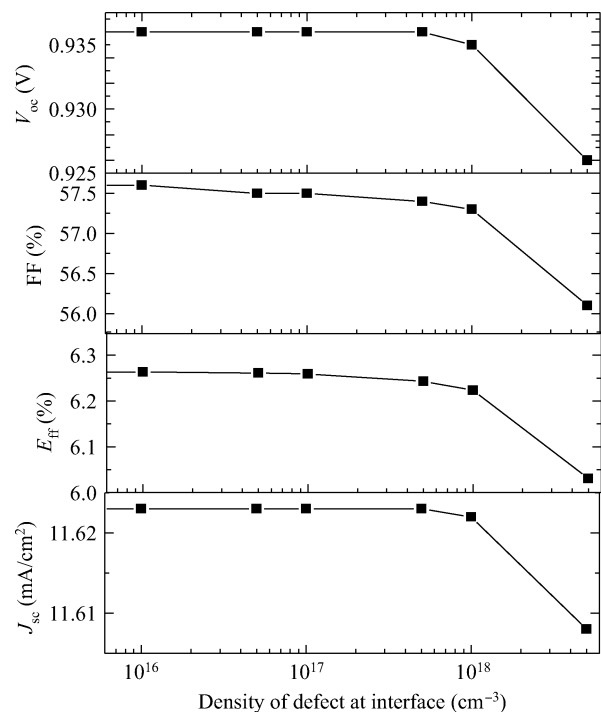


Fig. 8. Influence of defect density at the interface on solar cells.

formance. Experimental results show that the reduction of Φ_s enhances the built-in potential, which is in agreement with our outcomes. The changes in FF should be connected to the enhancement of the built-in potential, a decrease in recombination at the interface and the improvement of ohmic contact.

3.4. Influence of the p/i interface

The effects of defect density at the p/i interface on solar cells are investigated by inserting an interface layer. Defect density in the p⁺-layer, p-layer, i-layer and n-layer are fixed at 1×10^{20} , 7×10^{18} , 1×10^{15} , and 1×10^{15} cm⁻³, respectively, while the value of defect density varies at 5×10^{15} , 1×10^{16} , 5×10^{16} , 1×10^{17} , 5×10^{17} , 1×10^{18} , and 5×10^{18} cm⁻³.

The changes in device performance are displayed in Fig. 8 and vary with the defect densities at the p/i interface. The cell performance begins to change when the defect density is

greater than $1 \times 10^{17} \text{ cm}^{-3}$. When it reaches $1 \times 10^{18} \text{ cm}^{-3}$, E_{ff} decays drastically. However, there is no change to the solar cell performance when defect density is between 5×10^{15} and $1 \times 10^{17} \text{ cm}^{-3}$. According to this phenomenon, we learn that defect density at the p/i interface is unfavorable if it exceeds that of the intrinsic layer by two orders of magnitude. This result is of certain directive significance to our experiments. When an i-layer is deposited on a p-layer by PECVD, we should first reduce the deposition power to reduce defects caused by bombardment. Deposition should occur using low power for about ten minutes then at high power at top speed. In this way, the defect density will decrease. Mai^[17] coped with the interface problem in an unique way. He inserted an intrinsic microcrystalline buffer deposited by HWCVD onto PECVD cells at a p/i interface, successfully enhancing cell performance.

4. Conclusions

In this paper, the effect of p^+/p configuration as window layer of solar cells is investigated by an AMPS-1D program. Our results show that solar cells with a $p^+-p-i-n$ configuration have a better performance and J_{sc} , V_{oc} and E_{ff} are improved. A high doping concentration of the p^+ -layer can improve cell performance. The front contact barrier height Φ_s plays a vital role in amorphous silicon solar cells. When Φ_s decreases, E_{ff} increases. The thickness of the p^+ -layer also plays a crucial role. It should not be too thick, and its best value is 3 nm. J_{sc} and E_{ff} decrease with increasing thickness d , while V_{oc} and FF are almost constant. Defect density at the p/i interface is unfavorable if it exceed that in the intrinsic layer by two orders of magnitude.

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