Simulation of High Efficiency Heterojunction Solar Cells with AFORS-HET

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Abstract: In this paper, the high efficiency TCO/a-Si:H (n)/a-Si:H(i)/c-Si(p)/uc-Si(p+)/Al HIT (heterojunction with intrinsic thin-layer) solar cells was analyzed and designed by AFORS-HET software. The influences of emitter, intrinsic layer and back surface field (BSF) on the photovoltaic characteristics of solar cell were discussed. The simulation results show that the key role of the intrinsic layer inserted between the a-Si:H and crystalline silicon substrate is to decrease the interface states density. If the interface states density is lower than $10^{10} \text{cm}^{-2} \text{V}^{-1}$, thinner intrinsic layer is better than thicker one. The increase of the thickness of the emitter will decrease the short-current density and affect the conversion efficiency. Microcrystalline BSF can increase conversion efficiency more than 2 percentage points compared with HIT solar cell with no BSF. But this BSF requires the doping concentration must exceed $10^{20} \text{cm}^{-3}$. Considered the band mismatch between crystalline silicon and microcrystalline silicon, the optimal band gap of microcrystalline silicon BSF is about 1.4-1.6eV.

1. Introduction
Silicon HIT solar cell is now attracting much interest, because very high efficiencies (above 22%) have been demonstrated [1]. This technology is based on Sanyo’s successful technologies for fabricating high-quality a-Si film and solar cells with low plasma damage processes. It combines many advantages, such as (1) it simultaneously enables an excellent surface passivation and p-n junction, resulting in high efficiency, (2) its low-temperature processed (<200°C) can prevent any degradation of bulk quality that happen with high-temperature cycling processes in low-quality silicon materials such as solar grade Czochralski (CZ) Si, and (3) compared with conventional diffused cells, a much

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better temperature coefficient can be obtained with high $V_{oc}$ cells [2]. Though SANYO’s original design used an n-type substrate as the absorber for the HIT solar cell, current researches concentrate on developing the HIT solar cell on a p-type substrate, because of its popularity in the photovoltaic industry [3]. However, inferior performance was observed for devices fabricated on c-Si(p) as compared with those on c-Si(n) except SANYO, which suggests that a further investigation is necessary to fully understand the factors that affect the performance of the HIT solar cells.

Owing to the large numbers of processing variables, such as the thickness of the emitter, the interface states density, the band gap of the back surface field, etc, it is a formidable task to scrutinize the effect of each variable on the performance of the solar cell experimentally. Fortunately, numerical simulation software AFORS-HET provides a convenient way to evaluate the role of the various parameters present in the fabrication processing of HIT solar cells, and its reliability is proved by many references [3-4]. In this paper, the HIT solar cell TCO/a-Si:H (n)/a-Si:H(i)/c-Si(p)/uc-Si(p+)/Al is designed and optimized by AFORS-HET.

2. Simulation

![Figure 1 The gap state distribution in n-type a-Si:H layer.](image)

AFORS-HET is a very general computer simulation code for analyzing and designing the HIT solar cells, device operation may be in dark or under light illumination. In our simulation process, the solar AM1.5 radiation was adopted as the illumination source with a power density of 100mW/cm$^2$. The front and back contacts are assumed as flat band ones to neglect the contact potential influence. The surface recombination velocities of both electrons and holes are set as $10^7$cm/s. For the density of localized states in the band gap of amorphous silicon it has been assumed that there are both acceptor-like states and donor-like states modeled by exponential band tails (Urbach tails) and Gaussian mid-gap states (associated to silicon dangling bonds) [5]. The detailed localized states distributions are shown in figure 1. Other parameters used in the simulation are given in Table 1. During the simulations, all the parameters were adopted as the above setting values except for the specific declared one.
Table 1 The parameters used for HIT solar cell simulation

| Parameter and units | a-Si(n) | a-Si(i) | c-Si(p) | uc-Si(p+) |
|---------------------|---------|---------|---------|-----------|
| Thickness(nm)       | variable| variable| 30000   | variable  |
| Dielectric constant | 11.9    | 11.9    | 11.9    | 11.9      |
| Electron affinity (eV) | 3.9 | 4       | 4.05    | 4         |
| Bandgap(eV)         | 1.72    | 1.72    | 1.12    | variable  |
| Effective conduction band density (cm$^{-3}$) | $10^{20}$ | $10^{20}$ | $2.8 \cdot 10^{19}$ | $10^{20}$ |
| Effective valence band density (cm$^{-3}$) | $10^{20}$ | $10^{20}$ | $1.04 \cdot 10^{19}$ | $10^{20}$ |
| Electron mobility (cm$^{2}$V$^{-1}$s$^{-1}$) | 5       | 5       | 1041    | 10        |
| Hole mobility (cm$^{2}$V$^{-1}$s$^{-1}$) | 1       | 1       | 412     | 3         |
| Acceptor concentration (cm$^{-3}$) | 0       | 0       | 1.5$\cdot 10^{16}$ | variable |
| Donor concentration (cm$^{-3}$) | 2.49$\cdot 10^{19}$ | 100     | 0       | 0         |
| Thermal velocity of electrons(cm.s$^{-1}$) | $10^{7}$ | $10^{7}$ | $10^{7}$ | $10^{7}$ |
| Thermal velocity of holes(cm.s$^{-1}$) | $10^{7}$ | $10^{7}$ | $10^{7}$ | $10^{7}$ |
| Layer density (g.cm$^{-3}$) | 2.328   | 2.328   | 2.328   | 2.328     |
| Auger recombination coefficient for electron(cm$^6$.s$^{-1}$) | 0       | 0       | 2.2$\cdot 10^{31}$ | 0         |
| Auger recombination coefficient for hole(cm$^6$.s$^{-1}$) | 0       | 0       | 9.9$\cdot 10^{32}$ | 0         |
| Direct band-to-band recombination coefficient (cm$^3$.s$^{-1}$) | 0       | 0       | 0       | 0         |

3. Results and Discussion

Firstly, the HIT solar cell with structure TCO/a-Si:H(n)/c-Si(p)/Al is considered. The emitter thickness is 5nm and the related J-V curve is shown in figure 2. The detailed photovoltaic properties are $V_{oc}=646.1$mV, $J_{sc}=35.32$mA/cm$^2$, FF=82.68% and $E_{ff}=18.87%$.

3.1. Optimization of the intrinsic layer

While SANYO develops HIT solar cells with a very thin intrinsic a-Si:H(i) layer inserted between different type a-Si:H and c-Si, it should be noted that there is a controversy on the need of such a layer.
Some authors claim that it is beneficial, while others get good results without it and do not see significant improvements if they introduce it. One reasonable explanation for the benefit of this undoped buffer layer is that the density of states in undoped a-Si:H is weaker than in doped a-Si:H, so we can expect to have less interface defects when the heterointerface is formed with undoped rather than doped a-Si:H.

3.1.1. The influence of the intrinsic layer thickness. Figure 3 shows the photovoltaic characteristics of HIT solar cell varies with the thickness of the intrinsic layer. As can be seen from figure 3, the conversion efficiency of HIT is up to 19.27% with 1nm intrinsic layer is inserted, which is 0.4% higher compared with no intrinsic layer solar cell. But as I layer thickness increases, the conversion efficiency decreases. When the thickness of intrinsic layer reaches 5nm, the conversion efficiency of HIT solar cell with intrinsic layer is equivalent to solar cell with no intrinsic layer. Compromising the production processes and the conversion efficiency, the optimal intrinsic layer thickness should be set at 3nm. In addition, in figure 3, we can see that with the increase of intrinsic layer thickness, the open circuit voltage keeps almost unchanged, while the short circuit density decreases. This is because, as I layer thickness increases, the electric field strength of space charge region decreases and the short-spectrum absorption of amorphous silicon increases. The corresponding light-induced carriers cannot be effectively collected, resulting in the decrease of short circuit current density.

![Figure 3](image-url)
3.1.2. The influence of the interface states density. In the actual solar cell production processes, the impact of interface states density can not be ignored. In this paper, the interface defect states is assumed to insert between the I-type a-Si:H layer and the p-type crystalline silicon substrate layer. The interface states is assumed as continuous donor-like states and acceptor-like states with average distribution in the band gap, with the capture cross sections of electron and hole both are $10^{-14}$ cm$^2$. The interface state density of a-Si:H/c-Si interface varies from $10^{9}$ cm$^{-2}$.eV$^{-1}$ to $10^{13}$ cm$^{-2}$.eV$^{-1}$, and its effects on the photovoltaic performances of the solar cell are shown in figure 4.

As shown in figure 4, when the interface state density $D_n$ is lower than $10^{10}$ cm$^{-2}$.V$^{-1}$, the solar cell performance is almost unaffected by the interface states. Under this condition, the efficiency is still maintained at 18.97 %, which is very close to the one without interface states. But when the interface state density $D_n$ is higher than $10^{10}$ cm$^{-2}$.V$^{-1}$, the open circuit voltage decreased rapidly, while short-circuit current remained almost unchanged, even increased slightly. When the interface state density varies from $10^{10}$ cm$^{-2}$.V$^{-1}$ to $10^{12}$ cm$^{-2}$.V$^{-1}$, the open circuit voltage decrease from 644.5mV down to 549.2mV and the short-circuit current density increased from 35.52mA/cm$^2$ to 35.56mA/cm$^2$. The open circuit voltage reduction results from the increase of p-n junction reverse saturation current. As the interface defect density increases, the carrier recombination probability at interface increases, leading to the increase in reverse saturation current and reducing the open circuit voltage and fill factor. In order to obtain high-efficiency HIT solar cells, surface passivation methods is essential, such as plasma-assisted H passivation, in order to control interface state defect density as down to $10^{10}$ cm$^{-2}$.V$^{-1}$ as possible.

3.2. Optimization of the emitter
Because of the structural disorder and high doping concentration, the diffusion length of carriers in amorphous emitter is shorter. And there is only drift current and no diffusion current in emitter. Furthermore, since the amorphous silicon layer is a higher-doping layer, the space charge region of p-n junction has fallen mainly on crystalline silicon side, and even there is no electric field in amorphous silicon area. Therefore, emitter should be prepared as thin as possible with higher-doping. Figure 5 shows the influence of emitter thickness on the photovoltaic properties of solar cell.

![Graphs showing the influence of emitter thickness on photovoltaic properties](image)

**Figure 5** The impact of emitter thickness on the photovoltaic properties of HIT solar cell.

As can be seen from figure 5, with the emitter thickness increases, the open circuit voltage changed little, while the short circuit current is dramatically reduced. This is because with the emitter thickness increases, the absorption of the photon in emitter has increased. Considering the large amounts of recombination centers and the feature of no electric field in emitter, the photo-induced carriers are impossible to reach the edge of space charge region and contribute to light current. On the contrary, they will be recombined in the region and disappeared, resulting in the reduced short-spectrum response and short-circuit current. Fill factor also decreases with the n region thickness increases, for as the n layer thickness increases, series resistance will increases, which will reduce the fill factor [6]. Taking into account the technical production and conversion efficiency, the emitter thickness should be chosen about 5nm.

### 3.3. Optimization of the back surface field

The back surface field refers to a region which will be a barrier of minority carrier, thereby reducing the recombination rates of photo-induced carriers in the back surface. This barrier can not only enhance the photocurrent, but also increase photo-voltage to some extent [7]. Similar with the crystalline silicon solar cells, the back surface field can be achieved by a layer doped with the same type, but with higher doping concentration. Considering the microcrystalline silicon is a coexistence
mixed phase of nano-crystalline silicon, amorphous silicon and grain boundaries, and its band gap can be adjusted by crystallization phase, so microcrystalline silicon was used to simulate the back-field structure [8], and the corresponding parameters were listed in Table 1.

3.3.1. The effect of the BSF thickness. Table 2 lists the effect of the BSF thickness on the J-V characteristics of HIT solar cell. We can see that when the thickness increases, the open circuit voltage and short circuit current are nearly unchanged, and only a slight change in fill factor and cell efficiency. So the efficiency can be considered as independent with the thickness [7], which is very beneficial. In view of technology, the difficulty in fabricating microcrystalline silicon thin films is that its growth rate is very low. If the required thickness is very thin, production time can be dramatically saved. Therefore, the BSF thickness can be set to 5nm.

| thickness/nm | $V_{oc}$/mV | $J_{sc}$/mA.cm$^{-2}$ | FF/% | η/% |
|--------------|-------------|----------------------|------|-----|
| 2            | 646.1       | 35.53                | 82.65| 18.97|
| 5            | 646.1       | 35.53                | 82.67| 18.98|
| 10           | 646.1       | 35.54                | 82.69| 18.98|
| 15           | 646.1       | 35.54                | 82.71| 18.98|
| 20           | 646.1       | 35.55                | 82.73| 19   |

3.3.2. The effect of the BSF doping concentration. Figure 6 shows the influence of BSF doping concentration on the photovoltaic characteristics of solar cell. In figure 6, we can see that the doping concentration must reach a certain value, preferably more than $10^{20}\text{cm}^{-3}$ before the conversion.
efficiency increased by 0.5 percentage points. With the doping concentration increases, the open circuit voltage, short circuit current, fill factor and so on all are increasing. This can attributed to the BSF band structure. When the doping concentration is low, the reflection role of BSF is not clear, and the barrier on the carrier transport can be reduced by increasing the doping concentration, which explains the high doping concentration is guarantee of good BSF. Microcrystalline silicon, due to its special crystallization phase and possibility of high doping, is selected as the BSF here.

3.3.3. The effect of the BSF band gap. With the development of thin film deposition process, silicon films with different band gap can be prepared under different deposition temperature and crystallization phase. In general, the band gap of nano-crystalline silicon is larger, up to 1.8eV and above; followed by amorphous silicon, the band gap of crystalline silicon is smaller. Therefore, we supposed that the band gap of microcrystalline silicon varies between 1.12eV-2eV. Figure 7 shows the parameters of HIT solar cells vary with the band gap of microcrystalline silicon BSF.

![Figure 7](image)

Figure 7 The effect of BSF band-gap.

As can be seen from figure 7, with the band gap increases, the open circuit voltage increased firstly and then saturated; when the band gap is above 1.8eV, the fill factor began to decrease, leading to decreased conversion efficiency. The reason is that with the band gap broader, although the BSF provides barrier for the minority carriers, but also will impede the transport of majority carriers. So an optimum band gap should be selected in the 1.4-1.6 eV.

3.3.4. The comparison between HIT solar cells with and without BSF. Figure 8 shows the efficiency comparison of HIT solar cells before and after the BSF. In figure 8, we can see that with the BSF is added, all parameters of solar cells are improved, indicating a reasonable design of the back field, especially the optimization of doping concentration and the band gap, will increase the conversion efficiency by 2 percentage points. The detailed information also shown in figure.
As shown in figure 8, when a 5nm thick microcrystalline silicon layer with doping \(10^{20} \text{cm}^{-3}\) and band gap 1.5eV is added as BSF, it can improve \(V_{oc}\) 30mV and raise \(J_{sc}\) 1.5mA/cm\(^2\).

4. Conclusion
In this paper, the TCO / a-Si: H (n) / a-Si: H (i) / c-Si (p) / uc-Si (p\(^+\)) / Al HIT solar cell is simulated with AFORS-HET software. It was found that with the increase of the n layer thickness, the short-spectrum response and the short-circuit current density of solar cell will decrease; the introduction of intrinsic amorphous silicon layer is mainly to reduce the interface defect state density. If the interface states density is lower, the better intrinsic thickness is no more than 5nm. The thickness of BSF has little effect on the conversion efficiency, while reasonable doping and band gap design can improve efficiency more than 2 percentage points. At that time, the photovoltaic parameters of HIT solar cells are \(V_{oc}=678.9\text{mV}, J_{sc}=37.35\text{mA/cm}^2, \text{FF}=83.97\%\), \(\square=21.29\%\).

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