Role of Interfacial Oxide Layer in MoO$_x$/n-Si Heterojunction Solar Cells

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Interfacial oxide layer plays a crucial role in a MoO$_x$/n-Si heterojunction (MSHJ) solar cell; however, the nature of this interfacial layer is not yet clarified. In this study, based on the experimental results, we theoretically analyzed the role of the interfacial oxide layer in the charge carrier transport of the MSHJ device. The interfacial oxide layer is regarded as two layers: a quasi-$p$-type semiconductor interfacial oxide layer (SiO$_2$(Mo)$_{1}$) in which numerous negatively charged centers existed due to oxygen vacancies and molybdenum-ion-correlated ternary hybrids and a buffer layer (SiO$_2$(Mo)$_{2}$) in which the quantity of Si-O bonds was dominated by relatively good passivation. The thickness of (SiO$_2$(Mo)$_{1}$) and the thickness of (SiO$_2$(Mo)$_{2}$) were about 2.0 nm and 1.5 nm, respectively. The simulation results revealed that the quasi-$p$-type layer behaved as a semiconductor material with a wide band gap of 2.30 eV, facilitating the transport of holes for negatively charged centers. Additionally, the buffer layer with an optical band gap of 1.90 eV played a crucial role in passivation in the MoO$_x$/n-Si devices. Furthermore, the negative charge centers in the interfacial layer had dual functions in both the field passivation and the tunneling processes. Combined with the experimental results, our model clarifies the interfacial physics and the mechanism of carrier transport for an MSHJ solar cell and provides an effective way to the high efficiency of MSHJ solar cells.

1. Introduction

As a novel structure for a silicon-based solar cell, selective passivated contact has attracted much attention in recent years due to its successful transport of majority charge carriers and the reduction of the recombination rate of minority charge carriers [1–7]. Among the transition metal oxide thin films, substoichiometric molybdenum oxide (MoO$_x$, $0 < x < 3$) has previously been reported as an effective hole-collecting material for solar cells [4, 7–11]. MoO$_x$ thin films were recently directly integrated into silicon-based heterojunction (SHJ) devices, and a photovoltaic (PV) feature was successfully obtained due to the appropriate band gap of $\sim$3.00 eV and the higher work function [6, 12]. Furthermore, the SHJ device showed an excellent photovoltaic (PV) performance [3, 4, 13].

MoO$_x$ combines a wide bandgap with a high work function, which makes it possible to provide an excellent hole-selective function. It has been reported that a 7 nm-thick MoO$_x$ film has been used to replace the a-Si:H$(p)$ layers in SHJ devices, resulting in a conversion efficiency of 22.5% [13]. We demonstrated a different MoO$_x$/n-Si SHJ solar cell with an efficient hole collection and simple fabrication process by evaporating MoO$_3$ powder onto an $n$-type silicon. A 3.5 nm-thick amorphous interfacial layer formed naturally was observed between the MoO$_x$ film and the $n$-Si substrate via high-resolution transmission electron microscopy (HRTEM). Although the high work function of the MoO$_x$ layer induced an interfacial inversion layer in the surface of the $n$-Si substrate, forming the build-in-potential, it was not negligible that the 3.5 nm interfacial oxide layer also played a significant role in the transport of carriers.

In this research, we achieved an $\eta$ of 13.94% for an MSHJ solar cell by employing this simple process, as well as a $V_{oc}$ of 569.96 mV, an $J_{sc}$ of 32.10 mA cm$^{-2}$, and a fill factor (FF) of 76.21%. To determine the optoelectrical properties of the
interfacial layer, we used AFORS-HET v2.5 to model and implement the reconstruction of the interfacial layer [14]. This interfacial layer was regarded as two layers, including a quasi $p$-type semiconductor interfacial oxide layer ($\text{SiO}_x(\text{Mo})_1$) and a buffer layer ($\text{SiO}_x(\text{Mo})_2$). In detail, the quasi $p$-type layer was a semiconductor material that facilitated the transport of holes. At the same time, the buffer layer played the role of chemical passivation for the MoO$_x$/n-Si devices. Importantly, the negative charge centers in the interfacial layer had dual functions in both the field-effect passivation and the tunneling processes. Finally, we numerically achieve an $\eta$ of 16.91% for an MSHJ combined with advanced light trapping textures and rear surface passivation. The simulation results help us achieve an effective way to the high efficiency from the clarification of the interfacial physics in the MSHJ solar cells.

2. Simulation Model

A schematic of the MSHJ solar cell is shown in Figure 1(a). An amorphous interfacial layer with a thickness of approximately 3.5 nm, as shown in Figure 1(b), was naturally formed between the MoO$_x$ and the n-Si substrate during the evaporation of the MoO$_x$, as confirmed by cross-sectional HRTEM imaging. X-ray photoelectron spectroscopy (XPS) with depth profiling was used to determine the elemental composition of the interfacial layer, as shown in Figure 1(c). One could find that Si, O, and Mo were the constituents of the interfacial transition. Except for the measured thickness and the elemental composition, there was no other direct observation of the $-\text{SiO}_x(\text{Mo})$ interface because the interface was ultrathin and located inside of the structure. However, the role of a the $a$-$\text{SiO}_x(\text{Mo})$ layer in the MSHJ was not yet clear. To understand the nature of the interfacial layer, we constructed a physical model and simulated the optical and electrical properties of the $a$-$\text{SiO}_x(\text{Mo})$ layer in the AFORS-HET v2.5 software. The intraband and Schottky barrier tunneling through the spikes in the conduction and valence bands that occurred at interfaces were also considered.

In our previous studies [15, 16], we calculated a periodic $a$-$\text{SiO}_x$ structure with Mo doping by using first-principles calculations to explain the mechanism of charge carrier transfer.
of the simulation results was 16.91%, together with a $J_{sc}$ of 35.72 mA·cm$^{-2}$, a $V_{oc}$ of 581.10 mV, and an FF of 81.45%, which represented a better performance than that of the fabricated MSHJ with an $\eta$ of 13.94%, a $J_{sc}$ of 32.10 mA·cm$^{-2}$, a $V_{oc}$ of 569.96 mV, and an FF of 76.21%. Despite the better theoretical performance, the simulated $J$–$V$ curve agreed with the measured curve, which guaranteed that the simulated $J$–$V$ curve reflected the experimental results well.

### 3.2. Optical Band Gap of the a-SiO$_x$(Mo) Interlayer

Figure 3 shows the $J$–$V$ characteristics for the simulated MSHJ solar cells with different energy band gap ($E_g$) values and different electron affinities for the SiO$_x$(Mo)1 and SiO$_x$(Mo)2 compared to the experimental solar cell with AM1.5 illumination. As shown in Figures 3(a) and 3(b), the simulated $J$–$V$ plot of the SiO$_x$(Mo)1 for an optical band gap of $\approx$2.30 eV ($\pm$0.02 eV) and an electron affinity of 3.50 eV ($\pm$0.05 eV) had the good agreement with the experimental data of the MSHJ solar cell according to the shapes of $J$–$V$ curves. Table 2(a) shows photovoltaic characteristics of the MoO$_x$/n-Si solar cells with different band gaps of the SiO$_x$(Mo)1 layer. One can find that $V_{oc}$ and $J_{sc}$ hardly experienced change while band gap of SiO$_x$(Mo)1 varied. By comparison, it had relatively obvious impact on FF (Fill factor). A simulated FF of $\approx$81.45% was close to 76.21% of the PV device for optical band gap of $\approx$2.30 eV ($\pm$0.02 eV) in spite of the idealized approximation on interface states. Meanwhile, a simulated $\eta$ of $\approx$16.91% was near 13.94% of solar cell in practice. Table 2(b) shows photovoltaic characteristics of the MoO$_x$/n-Si solar cells with affinity of the SiO$_x$(Mo)1 layer. The same condition also applied to the affinity of the SiO$_x$(Mo)1 layer. The $J$–$V$ plot with an affinity of $\approx$3.50 eV ($\pm$0.05 eV) similar had the ideal agreement due to FF and $\eta$.

Figures 3(c) and 3(d) show the comparison of the different energy band gap values and the different electron affinities of SiO$_x$(Mo)2. The figure also displays the fact that the $V_{oc}$ and $J_{sc}$ hardly experienced changes with the energy band gap and the electron affinity of the SiO$_x$(Mo)2 layer, but FF and $\eta$ varied greatly while the energy band gap and the electron affinity of SiO$_x$(Mo)2 changed. And it could be found

### 3. Results and Discussion

#### 3.1. Comparison of the Fabricated MSHJ Performance and Simulated Results

Figure 2 shows a comparison of the simulated and measured $J$–$V$ curves of the MSHJ solar cell. The $\eta$ of the simulation results was 16.91%, together with a $J_{sc}$ of 35.72 mA·cm$^{-2}$, a $V_{oc}$ of 581.10 mV, and an FF of 81.45%, which represented a better performance than that of the fabricated MSHJ with an $\eta$ of 13.94%, a $J_{sc}$ of 32.10 mA·cm$^{-2}$, a $V_{oc}$ of 569.96 mV, and an FF of 76.21%. Despite the better theoretical performance, the simulated $J$–$V$ curve agreed with the measured curve, which guaranteed that the simulated $J$–$V$ curve reflected the experimental results well.

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**Table 1: Simulation parameters of the interfacial layer in the MSHJ solar cell.**

| Parameter                  | Quasi-$p$-SiO$_x$ (Mo) | Quasi-$i$-SiO$_x$ (Mo) | N-$c$-Si |
|----------------------------|------------------------|------------------------|----------|
| Layer thickness (cm)       | $2.0 \times 10^{-7}$   | $1.5 \times 10^{-7}$   | $1.5 \times 10^{-2}$ |
| Electron affinity (eV)     | 3.50                   | 3.50                   | 4.05     |
| Mobility gap (eV)          | Variable               | Variable               | 1.12     |
| Optical gap (eV)           | Variable               | Variable               | 1.12     |
that the $J$–$V$ curve with the energy band gap of $\sim 1.90$ eV ($\pm 0.10$ eV) and the electron affinity of $\sim 3.60$ eV ($\pm 0.20$ eV) agreed well with the measured $J$–$V$ plot.

The energy barriers for the electrons and holes were determined by the band gap and the electron affinity. As noted in the literature [23], the FF was influenced by the series resistance, which was closely related to the energy gap. A larger gap for the same electron affinity indicated a higher barrier, thereby producing a bigger series resistance that showed a lower FF. It is well known that the optical band gap of the $a$-SiO$_x$ layer, which directly influences the transport of carriers, plays an essential role in the performance of the MoO$_x$/n-Si heterostructure.

Nicolae Tomozeiu also discussed the optical band gap of the SiO$_x$ $(0 \leq x \leq 2)$ in their O’Leary–Johnson–Lim (OJL) model, reporting that the optical band gap of $a$-SiO$_x$ increased from 1.7 eV to 3.1 eV as $x$ increased from 0.35 to 1.43 [24]. Therefore, it was reasonable for the $a$-SiO$_x$(Mo)1 interlayer to have an optical band gap of 2.30 eV. The band gap of the $a$-SiO$_x$(Mo)2 interlayer nearer to the Si substrate, $\sim 1.90$ eV, was slightly lower than that of the $a$-SiO$_x$(Mo)2 interlayer because of the higher Si atom content.

3.3. Role of the Negative Charge Centers. Another crucial problem of the interfacial layer was the concentration of negative charge centers associated with oxide vacancies and Mo–

Figure 3: Comparison between the $J$–$V$ curves of the simulated MSHJ solar cells with (a) different optical $E_g$ of SiO$_x$(Mo)1, (b) different optical $E_g$ of SiO$_x$(Mo)2, (c) different affinities of SiO$_x$(Mo)1, and (d) different affinities of SiO$_x$(Mo)2 and the experimental results.
To achieve high output performances of the device, the negative charge centers remained unchanged for the negative charge center ion-correlated in the a-SiO$_x$(Mo) layer. Table 3 shows the photovoltaic parameters of the MSHJ devices with different negative charge center concentrations in the range of $1 \times 10^{15} - 1 \times 10^{18}$ cm$^{-3}$. Notably, the photovoltaic characteristics remained unchanged for the negative charge center concentrations below $1 \times 10^{16}$ cm$^{-3}$, which directly verified that the built-in field mainly originated from the work function difference between the MoO$_x$ (5.50 eV) and the n-Si (4.31 eV). To achieve high output performances of the device, the negative charge center concentrations should be controlled in the range of $1 \times 10^{16} - 10^{18}$ cm$^{-3}$, meaning a wide adjustable range of fabricating process. These negative charge centers repel electron to the back side of solar cells so as to obtain large $J_{sc}$.

The simulation results showed that the a-SiO$_x$(Mo) layer was a large band gap ($\sim2.30$ eV) semiconductor material with good quantum tunneling and field-effect passivation. Furthermore, the results clarified that the barrier height was lowered by the included molybdenum ions, increasing the quantum tunneling probability. Furthermore, the negative charge centers in the a-SiO$_x$(Mo) layer, which was introduced by the included molybdenum ions and oxygen vacancies, played a crucial role in the good field-effect passivation.

### Table 2: Photovoltaic characteristics of the MoO$_x$/n-Si solar cells with different band gaps of the SiO$_x$(Mo) layer

| Band gap of SiO$_x$(Mo) (eV) | $V_{oc}$ (mV) | $J_{sc}$ (mA/cm$^2$) | FF (%) | $\eta$ (%) |
|-----------------------------|--------------|-----------------------|--------|------------|
| 2.28                        | 581.1        | 35.72                 | 81.67  | 16.96      |
| 2.30                        | 581.1        | 35.72                 | 81.45  | 16.91      |
| 2.32                        | 581.2        | 35.72                 | 80.97  | 16.81      |
| 2.34                        | 581.3        | 35.71                 | 79.94  | 16.59      |

### Table 3: Photovoltaic characteristics of the MoO$_x$/n-Si solar cells with different affinities of the SiO$_x$(Mo) layer

| Affinity of SiO$_x$(Mo) (eV) | $V_{oc}$ (mV) | $J_{sc}$ (mA/cm$^2$) | FF (%) | $\eta$ (%) |
|------------------------------|--------------|-----------------------|--------|------------|
| 3.45                         | 581.1        | 35.72                 | 81.81  | 16.98      |
| 3.50                         | 581.1        | 35.72                 | 81.45  | 16.91      |
| 3.55                         | 581.3        | 35.72                 | 79.10  | 16.43      |
| 3.60                         | 582.6        | 35.72                 | 68.99  | 14.36      |

The clarification of the interfacial physical mechanism of the MSHJ solar cells enabled a better understanding of the nature of device physics. We investigated an a-SiO$_x$(In) interlayer that formed naturally between ITO and an n-Si substrate [17, 22, 25–27] during the growth of an ITO film on an n-Si wafer. The a-SiO$_x$(In) interlayer also played multiple roles in the ITO/n-Si heterojunction solar cell and helped produce an outstanding photovoltaic performance. We surmised that the a-SiO$_x$ interlayer included another specific transition metal oxide, for example, VO$_x$ or WO$_x$, which might also form a large energy band gap semiconductor material with a good passivation effect, a high tunneling possibility, and selective contacts.

### 3.4. Electronic Structure and Roles of the Interfacial Region

The device model revealed that there was a strong inversion layer ($p'$) at the surface of the n-Si substrate because of the difference between the work functions of MoO$_x$ and n-Si, as shown in Figure 4. Much higher injection and recombination rates were seen at the n-Si/ITO interface. It was found that the a-SiO$_x$/In interlayer included another specific transition metal oxide, for example, VO$_x$ or WO$_x$, which might also form a large energy band gap semiconductor material with a good passivation effect, a high tunneling possibility, and selective contacts.

The device model revealed that there was a strong inversion layer ($p'$) at the surface of the n-Si substrate because of the difference between the work functions of MoO$_x$ and n-Si, as shown in Figure 4. Such an inversion layer pushed the p/n homojunction, which was the origin of the built-in field on the surface of c-Si. The calculated energy band structure of the interfacial region at equilibrium is shown in Figure 4. A strong p-type inversion layer with a thickness of approximately 200 nm existed near the surface of the n-Si absorber. Additionally, the simulation showed that there was an energy band bending of 0.81 eV, limiting the $V_{oc}$ value of the MoO$_x$/n-Si heterojunction on the surface of the Si substrate. A $V_{oc}$ value is usually correlated with a built-in potential ($V_B$). For the fabricated device, a $V_B$ value of 0.67 V was obtained, as derived from the $1/C^2$–V curve at room temperature, assuming an abrupt junction, as shown in Figure 5. It was clear that the measured value of 0.67 V was close to but smaller than the simulated value of 0.81 V. Considering the other factors of the fabricated device [28, 29], the simulated energy band structure essentially matches that of the fabricated device.

Based on the energy band structure, we could see that the valence band and conduction band offsets were 0.46 eV and 0.71 eV, respectively. Both energy barriers induced by the band offsets and the electric field at the interface could separate electron-hole pairs due to the high degree of band bending [30, 31]. In our device, quantum tunneling played an important role in the explanation of the charge carrier transport. The tunneling probability for the charge carriers was strongly influenced by the height of the barrier, the thickness of the barrier, the barrier shape, and many other factors [25, 32–36]. The valence band offset of 0.46 eV offered a relatively low potential barrier for the holes. Hence, the tunneling probability for the holes increased significantly. As expected, the increased tunneling probability for the holes could directly lead to a higher $J_{sc}$.

Furthermore, the conduction band offset of 0.71 eV resulted in a high potential barrier for the electrons, restricting their transport. Moreover, the negative charge centers repelled electrons to the backside of c-Si due to field-effect passivation. We found that the SiO$_x$(Mo) layer was a desirable material that was suitable for hole transport while preventing electron transport, thus obtaining a high

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Therefore, the \(a\)-SiO\(_x\)(Mo) interfacial layer offered a strong field-effect passivation and high quantum tunneling probability, which was of great significance for the output performance of MSHJ solar cells. The \(a\)-SiO\(_x\)(Mo) interlayer enabled holes to be more easily transported by assisted tunneling, and it repelled electrons on the other side of the layer with Coulombic force, thereby indicating that it was a promising material for heterojunction solar cells. Liu et al. investigated the band arrangement and charge transfer when the interfacial interaction varied on the BiVO\(_4\)/WO\(_3\) heterostructure semiconductor material [37]. One can find that the charge transfer internal mechanism of the interfacial layer in the heterojunction needs to explore furthermore. This interfacial material of MSHJ is open to further research; although, we could independently prepare an \(a\)-SiO\(_x\)(Mo) layer at the time of this research.

4. Conclusions

By employing a simple process, we fabricated a MoO\(_x\)/\(n\)-Si solar cell that achieved good performance with an \(\eta\) of 13.94\%, an open-circuit voltage of 569.96 mV, a short-circuit current density of 32.10 mA cm\(^{-2}\), and a high FF of 76.21\%. We found that a 3.5 nm ternary-like hybrid layer of \(a\)-SiO\(_x\)(Mo) formed between the MoO\(_x\) and the \(n\)-Si
substrate, and that the hybrid layer might have played a vital role in the good performance of the MSHJ solar cells. The subsequent simulation results demonstrated that this interfacial layer SiO\textsubscript{x}(Mo)\textsubscript{1} was a Mo-based semiconductor material with a wide optical band gap of \(\sim 2.30\) eV and negative charge centers with densities in the range of \(10^{11}-10^{12}\) cm\textsuperscript{-2}. The interfacial layer SiO\textsubscript{x}(Mo)\textsubscript{2} played the role of passivation in the MoO\textsubscript{x}/n-Si device. The negative charge centers played dual roles in both the quantum tunneling and field-effect passivation processes, resulting in the excellent transport characteristics of the majority charge carriers and the effective suppression of the minority charge carrier recombination. The improved performance, the clarification of the physical mechanism, and the superiority of the fabrication process indicated that the MSHJ solar cells would have appealing prospects in mass production. Finally, the clarification of the interfacial layer SiO\textsubscript{x} as the anode interfacial layer, “Molybdenum and tungsten oxide: high work function wide band gap contact materials for hole selective contacts of silicon solar cells,” Solar Energy Materials and Solar Cells, vol. 142, pp. 34–41, 2015.

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