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DOI
10.1109/PVSC45281.2020.9300968

Publication date
2020

Document Version
Accepted author manuscript

Published in
2020 47th IEEE Photovoltaic Specialists Conference, PVSC 2020

Citation (APA)
Mazzarella, L., Alcaniz-Moya, A., Kawa, E., Procel, P., Zhao, Y., Han, C., Yang, G., Zeman, M., & Isabella, O. (2020). Strategy to mitigate the dipole interfacial states in (i)a-Si:H/MoOxpassivating contacts solar cells. In *2020 47th IEEE Photovoltaic Specialists Conference, PVSC 2020* (pp. 405-407). Article 9300968 (Conference Record of the IEEE Photovoltaic Specialists Conference; Vol. 2020-June). Institute of Electrical and Electronics Engineers (IEEE). https://doi.org/10.1109/PVSC45281.2020.9300968

Strategy to mitigate the dipole interfacial states in (i)a-Si:H/MoO_x passivating contacts solar cells

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***Abstract*— Electrical simulations show that the dipole formed at (i)a-Si:H/MoO_x interface can explain electrical performance degradation. We experimentally manipulate this interface by a plasma treatment (PT) to mitigate the dipole strength without harming the optical response. The optimal PT+MoO_x stack results in strongly improved electrical parameters as compared to the one featuring only MoO_x and to the silicon heterojunction reference cell. Optical simulations and experimentally measured currents suggest that the additional PT is responsible of very limited parasitic absorption overcompensated by the thinner MoO_x used (3 nm) and by the lower losses in the (i)a-Si:H layer underneath.**

Keywords—(i)a-Si:H/MoO_x solar cells, Dipole layer, Enhanced stability.

I. Introduction

Transition metal oxides (TMOs) are very attractive in c-Si based heterojunction (SHJ) solar cells for their ability to induce efficient carrier selectivity and mitigate parasitic absorption losses resulting in clear current gain [1], [2].

Among TMOs, molybdenum oxide (MoO_x) is promising for applications as hole transport layer (HTL). MoO_x layer, in combination with a thin intrinsic passivation a-Si:H layer and a transparent conductive oxide (TCO) has in fact demonstrated conversion efficiency of 23.3% [3]. However, (i)a-Si:H/MoO_x exhibits a weak thermal stability in air/moisture hindering the carrier selectivity in contrast to conventional SHJ cells. Consequently, devices with TMOs usually suffer from lower fill factor (*FF*) and possibly S-shaped *J-V* characteristics as compared to solar cells with doped silicon carrier selective HTLs. Possible causes of deterioration can be attributed to the decreased work function of MoO_x and deteriorated passivation performances [4]. Some papers [5], [6] report on the formation of a resistive SiO_x thin layer at the (i)a-Si:H/MoO_x that might create a potential barrier limiting the cell performances. Others [7] observe MoO_x reduction triggered by the H effusion from (i)a-Si:H.

In this work we explain the electrical degradation by means of a thin dipole formation, confirmed by electrical simulations. Therefore, we fabricated solar cells introducing a plasma treatment (PT) that mitigates the dipole negative affect, thus confirming the indications from modelling and obtaining high-efficiency devices.

II. Results and Discussion

A. Role of interface dipole

The strong difference of work function (*WF*) between MoO_x and (i)a-Si:H causes accumulation/depletion of holes at this interface with formation of a thin dipole (inset in Fig.1 b) [8].

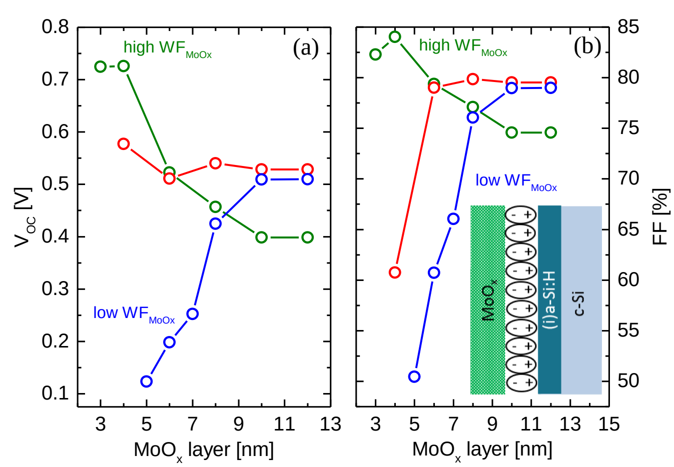

Fig. 1. Simulated (a) V_{OC} and (b) *FF* as function of MoO_x thickness and for different WF_{MoOx}, including the dipole at (i)a-Si:H/MoO_x interface. The inset shows the dipole layer adapted from Ref. [8].

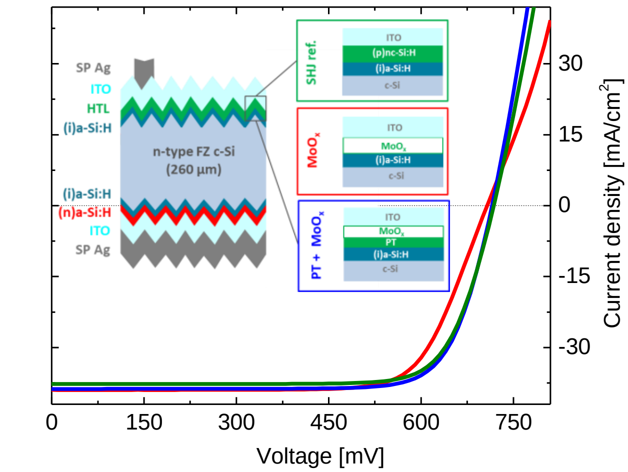

Fig. 2. HTL as depicted in the inset: SHJ reference with 20-nm thick (p)nc-Si:H, 5-nm thick MoO_x and PT+5-nm thick MoO_x.

In fact, those interfacial states strongly affects the band alignment at the a-Si:H/c-Si sides depending on the dipole strength. The dipole energy is a function of MoO_x thickness and depends also on the work function of surrounding materials: MoO_x and (i)a-Si:H [8].

We have calculated the effect of such dipole by using TCAD Sentaurus [9], [10] with *WF* for the MoO_x adapted from Ref. [8] for different layer thickness. The results reported in Fig. 1 confirm that V_{OC} and *FF* strongly depend on MoO_x thickness and WF_{MoOx}. We observe that for higher WF_{MoOx} there is a clear optimal MoO_x thickness around 5 nm as result of the trade-off between dipole and c-Si band bending. On the contrary, if we assume lower WF_{MoOx} values, typically measured for non-stoichiometric MoO_x, the simulated trends progressively change leading to higher *FF* and V_{OC} for thicker MoO_x layers. Hence, such interfacial dipole has a strong impact on positive charge collection highlighting the importance of tailoring the (i)a-Si:H/MoO_x interface.

B. Experimental solar cells results

Based on the abovementioned simulation results, we propose here a strategy to mitigate the negative effect of the dipole. We use a PECVD plasma treatment to modify the layer interaction and make the negative effect of the dipole less strong on electrical parameter.

Therefore, we fabricated SHJ solar cells using three different front HTL stacks and identical electron contact stack at the rear side as depicted in the inset of Fig. 2. (i)a-Si:H and, optionally, a PT, while MoO_x is thermally evaporated from a stoichiometric powder source after reaching a base pressure of 10^{-6} Torr. The contacts are completed with sputtered In_2O_3:Sn (ITO) layers and screen printed Ag cured at 170°C for 40 min.

Fig. 2 shows illuminated *J-V* curves and Fig. 3 the corresponding electrical parameters for various HTLs, respectively. The cell with only MoO_x (red) exhibits lower V_{OC} and *FF* (708 mV, 74.2%) originated from the S-shape *J-V* curve as compared to SHJ reference cell (green). Treating the (i)a-Si:H layer with PT, before the MoO_x layer deposition, helps to progressively recover the electrical properties with an optimum at 130 s of PT time with measured V_{OC} of 715 mV

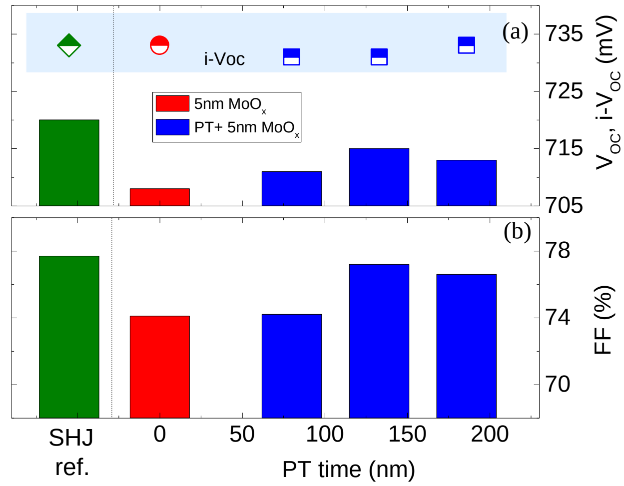

Fig. 3. Measured i-V_{OC}, V_{OC}, *FF* measured on solar cells with various HTL stacks (cell area 3.92 cm^2).

and *FF* above 77%. In Fig. 4, we report the MoO_x thickness optimization using the optimized PT. The results show that MoO_x layer thickness can be reduced down to 3 nm in the presence of PT without V_{OC} loss (715 mV) and with a progressive gain in *FF* up to 77.7%. The optimum MoO_x thickness is in agreement with the trend observed in our simulations discussed above. The device endowed with the optimized PT + MoO_x stack reaches *FF* equal to the SHJ reference cell with only 5 mV losses in V_{OC}. Such an effect is ascribed to the positive presence of the PT that counteracts the dipole effect of MoO_x and (i)a-Si:H layers. The cells are stable and we do not observe performance degradation of electrical parameters after three months of air exposure.

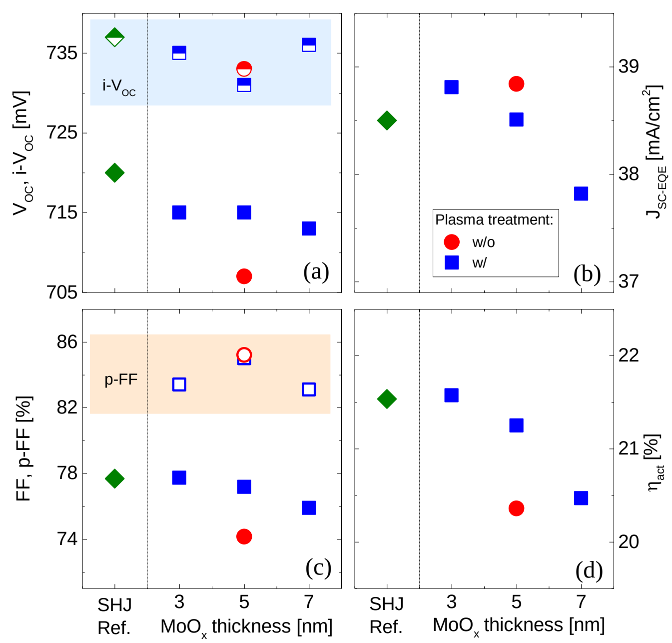

Fig. 4. Solar cell parameters with different MoO_x thickness and constant PT compared to SHJ ref. (a) V_{OC} and i-V_{OC}, (b) $J_{SC\text{-}EQE}$, (c) *FF* and p-*FF*, and (d) η_{act}. Note that all the cells (except the SHJ ref.) feature an unintentionally thicker ITO (90 nm) that reduces J_{SC} by ~0.55 mA/cm^2.

$J_{SC\text{-}EQE}$ progressively increases by thinning the MoO_x layer but it is still limited by the 90-nm thick ITO on the front that shifts the antireflection pick away from the optimum wavelength with an estimated current loss of ~0.55 mA/cm^2. The J_{sc} values extracted from experimental EQE curves in Table 1 with 75 nm front ITO layer clearly show the benefit of MoO_x with 39.36 mA/cm^2. We expect to increase further current density by reducing the ITO front thickness down to 65 nm.

TABLE I. EXPERIMENTAL $J_{SC\text{-}EQE}$ CURVES FOR THREE CELLS WITH DIFFERENT HTL. THE CALCULATED CONTRIBUTIONS ARE GIVEN FOR WAVELENGTH BELOW/ABOVE 650 NM.

HTL (75nm ITO)	**Experimental $J_{SC\text{-}EQE}$ (mA/cm^2)**		
	300-650 nm	***650-1200 nm***	***total***
SHJ ref.	13.49	23.03	38.52
MoO_x	15.44	23.96	39.44
PT+ MoO_x	15.29	24.08	39.36

To better quantify the parasitic losses and the potential current generated we performed optical simulations using GenPro4 [11]. Fig. 5 reports the current parasitically absorbed in each layer on the illuminated side of the cells. As expected, the SHJ ref. cell with 20-nm thick (p)nc-Si:H exhibits the highest front losses (-4 mA/cm^2) as compared to the device with 5-nm thick MoO_x (-2.83 mA/cm^2).

The current gain is mainly given by the use of less absorptive MoO_x HLT and partially by the use of a thinner ITO layer that gives a net gain of +0.2 mA/cm^2.

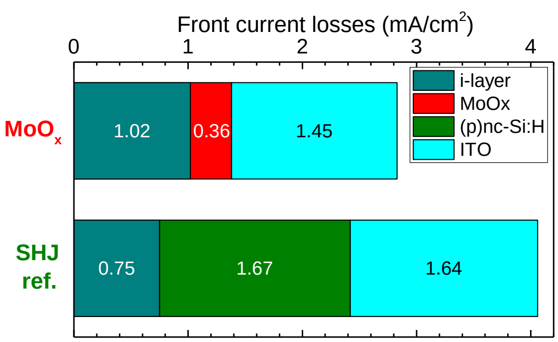

Fig. 5. Simulated current losses parasitically absorbed in each front layer. The ITO thickness is reduced to 65 nm for the cells with 5-nm thick MoO_x and (p)buffer + MoO_x (3.75 nm + 3 nm) while it is kept at 75 nm for the SHJ ref. cell.

III. SUMMARY

In this work we discuss the critical role of the (i)a-Si:H/MoO_x interface for high performance solar cells. We suggest the formation of a thin dipole that depends on *WF*s of adjacent layers and on MoO_x thickness. Electrical simulations confirm that V_{OC} and *FF* strongly depend on the trade-off between the dipole and the c-Si band bending.

The innovation of our approach is that we can deposit MoO_x layers in a wider operational range by introducing a PECVD plasma treatment. This buffer can *(i)* mitigate the interaction of MoO_x with (i)a-Si:H and *(ii)* strongly support the charge transport ascribing this to the reduction of the dipole strength. The optimized plasma treatment gave a S-shape-free *J-V* curve with *FF* comparable to the SHJ reference device. Further thickness optimization demonstrated that the MoO_x layer can be further reduced down to 3 nm with no electrical losses by the presence of the PT. This result is in agreement with the simulated optimal MoO_x thickness for *FF* maximization. Finally, both optical simulations and experimental EQE showed that the proposed approach consisting of PT + MoO_x (3.75 nm + 3 nm) results in very limited losses as compared to the cell with only MoO_x.

Our method could be tested also with other TMOs suitable for both hole-selective and electron-selective contacts.

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