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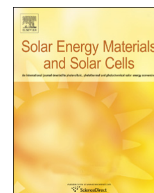

# TCO work function related transport losses at the a-Si:H/TCO-contact in SHJ solar cells

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ABSTRACT

Silicon based heterojunction (SHJ) solar cells show high efficiency enabled through excellent passivation by amorphous silicon (a-Si:H), the use of light trapping schemes and transparent conductive layers. Many different research groups and companies have achieved high open-circuit voltages above 730 mV, but fill factors (*FFs*) at the level of conventional silicon solar cells are rare. One reason for a lower *FF* may be the (p)a-Si:H/TCO-contact, where a Schottky diode results. This can lead to an increased transport barrier adversely affecting the hole collection and thus the FF. The role of TCOs with work functions (WF) higher (tungsten oxide ($WO_x$)) and lower (aluminium doped zinc oxide, AZO) than the standard ITO (indium tin oxide) will be examined experimentally in this paper. The aim of this paper is the proof of concept that WF engineering can improve the contact. Schottky theory with TCO WF values taken from the literature was the main assumption for the simulations and in the case of $WO_x$ at the hole contact, it could be shown that adjusting the TCO WF to (p)-a-Si:H decreases the Schottky barrier height.

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## 1. Introduction

Highly efficient silicon solar cells produced at low cost are one key to a cost-effective renewable energy supply. High efficiency can be reached using silicon hetero-junctions (SHJ) on silicon wafers, where efficiencies of up to 24.7% have been achieved by Panasonic [1].

This is enabled through excellent passivation, the avoidance of direct metal contact to the absorber, and transparent TCO (transparent conductive oxide) layers [2].

Regarding the fill factor (FF), several factors enable a high value of above 80%. One is good passivation at the maximum power point [3]. Another is avoiding transport barriers, which will be addressed in the following regarding the a-Si:H/TCO junction.

In a solar cell device, contact characteristics to metal and TCO electrodes are desired to be ohmic and low resistive. Among others these characteristics are determined by the difference in work function (WF) between a-Si:H and TCO. The WF is the difference between the energy of the vacuum level and the Fermi level ($E_F$). Most TCOs are degenerately doped, with the Fermi level being above the conduction band ($E_C$), whereas for a-Si:H it is within the band gap and close to the $E_C$ for n-type and close to the valence band for p-type.

However, if contact is made between a semiconductor for instance a p-type one and a metal or TCO with a WF lower than the semiconductor, the semiconductor is depleted and a Schottky barrier forms [3–5]. The WF of typical boron-doped amorphous silicon ((p)-a-Si:H) is 5.3 eV [6], i.e. 0.3 eV above the valence band ($E_V$.). For SHJ, ITO (indium tin oxide) with a WF of around 4.7 eV [7] is typically employed, which leads to a Schottky barrier [8]. An important factor determining the width of this barrier is the doping in (p)-a-Si:H [3,9]. For a-Si:H thin film *nip* cells, higher doping leads both to higher $V_{oc}$ as well as to higher FF [10]. Thus, transport (and FF) can be improved by higher doping [11]. However, junction recombination can at the same time increase with higher doping [12,13], leading to a lower $V_{oc}$.

Alloying of doped a-Si:H layers increases the transparency [14], but leads to lower doping efficiency [14,15] and thus to worse transport characteristics [16]. WF engineering could allow the use of more transparent p-layers at no additional cost of higher contact resistance (see e.g. [4]).

Another option could be microcrystalline silicon, which has a much higher doping efficiency [17], resulting in lower contact resistance with the TCO. However, the technological implementation faces the challenge of the amorphous incubation layer occurring before the microcrystalline growth starts [18]. This undesired incubation layer can assume a thickness of several nanometers and leads to a much too high overall thicknesses with respect to parasitic absorption.

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In general, an adjusted work function (WF) is important for the metal/insulator/semiconductor (MIS) gate stacks in transistors as well as for optoelectronic devices that involve a TCO. This includes LEDs [1] and silicon thin film solar cells [2]. For transistors, WF influences the threshold voltage, but carrier transport across the gate stack is not desired. In the case of solar cells, however, the extracted charge carriers move over the a-Si:H/TCO interface. For thin film solar cells, mainly the influence of WF on $V_{oc}$ was investigated [19]. However, for SHJ devices, experimental investigations on this crucial aspect are very seldom [11,20,21].

On the basis of device simulations it could be shown how an adjusted WF allows for lower doping and a lower thickness of doped a-Si:H layers, thus permitting a higher *FF* and $J_{sc}$ without the trade-off of a lower $V_{oc}$ [3]. The aim of this paper is the proof of concept that WF engineering can improve the contact.

Characteristic TCOs with low WF (aluminium zinc oxide (AZO), WF: 3.4–4.5 eV [7]), medium WF (ITO, 4.2–4.7 eV [7]) and high WF ($WO_x$, 5.1–6.4 eV [22]) were selected for comparison. With regard to $WO_x$ the high WF is desired for the p-contact, but there is a trade-off since very high charge carrier densities lead to high parasitic absorption [23]. Alternative TCOs which are In-based and also have high WF could be a solution as well. One example is Zn–In–Sn–O, which showed higher transparency than ITO and a WF of 6.1 eV [24].

All these TCOs have a high charge carrier density and thus show metal-like behaviour while enabling the applicability of the Schottky theory. To address the question of whether WF has any influence in SHJ cells TCO contacts on both n- and p-type a-Si:H were investigated.

## 2. Experimental: Assembly of samples

The test structures (shown in Fig. 4) were manufactured in the following way: The planar FZ wafers were of n- and p-type with a base resistivity of 1 Ω cm. On the front side 10 nm intrinsic amorphous silicon ((i)a-Si:H) was deposited by PECVD, followed by 12 nm (p)a-Si:H deposited by PECVD for n-type base and phosphorus doped for p-type base, respectively. On the backside, 10 nm (i)-a-Si:H is followed by 12 nm of doped layers with respective doping to form a high-low-junction. The (n)-a-Si:H was deposited with a gas phase doping of 1100 ppm and a silane to phosphine ratio of 75. The doping of the (p)a-Si:H was realized with 2300 ppm in the gas phase and a silane to diborane ratio of 36.

These high layer thicknesses are not optimal for solar cell applications, but allow selective contacts with low surface recombination after sputtering and enable one to focus on transport effects at the a-Si:H/TCO contact. On the front and on top of the doped a-Si:H a TCO interlayer was sputtered with 20 nm of AZO, ITO and $WO_x$, respectively. AZO was MF sputtered in Ar atmosphere in an ATON Twin Mag [25] at 200 °C from a ceramic target ($2\%_{cat.wt}$ Al in ZnO) at a pressure of $8.9 \times 10^{-3}$ hPa. ITO was reactively DC magnetron sputtered in an Oxford Instruments System 100 Pro with 1% $O_2$ in Ar from a ceramic target (In/Sn ratio of 9:1) at a heater set point of 100 °C and at a pressure of $2.7 \times 10^{-3}$ hPa. $WO_x$ was reactively DC magnetron sputtered with 10.3% $O_2$ in Ar from a metallic tungsten target [23] at a pressure of $5 \times 10^{-2}$ hPa in the VIP tool originally developed to coat absorbers for solar thermal power plants [26] with no additional heating.

This thin TCO interlayer was capped with 55 nm of ITO and sputtered in the same way as written above to assure comparably low sheet resistance. In addition, this ITO layer leads to similar optical properties of the ITO/TCO/a-Si:H stacks for all three variations. Since the set temperature is 100 °C for the last ITO deposition, the thermal budget is reckoned to be negligible compared to the post deposition annealing performed at 180 °C which is done to remove sputter damage.

The front side was metallized by deposition of 50 nm titanium (Ti), 50 nm palladium (Pd) and 5000 nm silver (Ag) by e-gun and a subsequent lift-off of a photolithographically pattered photo-resist for the groups with AZO and ITO interlayer and cured at 180 °C for 10 min to remove the damage induced by sputtering. The group with a $WO_x$ interlayer was screen printed and cured at 230 °C for 6 min. The back side metallization consists of 50 nm Ti and 50 nm Pd followed by 1000 nm evaporated Ag.

## 3. Results and discussion

### 3.1. Simulation: Influence of WF on n- and p-type a-Si:H

With *Sentaurus TCAD* the influence of WF on the contact was simulated assuming that the dominating transport path would tunnel over the Schottky barrier. The doping of the amorphous silicon moves the $E_F$ away from mid gap and decreases the activation energy of a-Si:H ($E_{act}$). This was one variable input parameter for the simulation. The TCO is modelled as a transparent metal with the WF at the interface ($WF_{IF}$). The second variable input parameter was thus the $WF_{IF}$ with energy levels ranging from the $E_C$ to the $E_V$ of a-Si:H. Fig. 1 depicts the simulated *FF* as a function of the TCO WF at the (p)a-Si:H emitter and the (n)a-Si:H back surface field (BSF). For a good electron contact (called "n-contact" in the following) the WF should be low, much like it is expected for the selected AZO. Thus, the TCO WF should correspond to the WF of the (n)a-Si:H (4.2 eV) or even better, approach the conduction band of the (n)a-Si:H (3.9 eV). For the hole contact (denoted "p-contact") the WF should be high, much like the selected $WO_x$, and should match the WF of the (p)a-Si:H (5.3 eV) or even the valence band (5.6 eV). Furthermore, a low activation energy and thus higher doping of the a-Si:H layer ($E_{act}$ of 200 vs. 300 meV) make the *FF* less dependent on the WF and in the case of small WF, mismatch leads to a higher *FF*. If a high doping can be achieved in solar cell devices, then no increase in series resistance due to the a-Si:H/TCO contact is expected and the TCO WF would have no influence on *FF*. However, a higher (p)a-Si:H doping increases the defect density in the amorphous layer and can reduce the $V_{oc}$ [12,27]. So besides varying the doping of the a-Si:H layer, adapting the TCO WF to (p)a-Si:H and (n)a-Si:H, respectively, is another possibility for improving the *FF*.

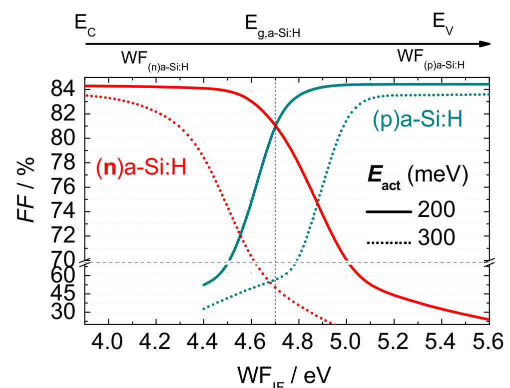


**Fig. 1.** Simulated *FF* as a function of $WF_{IF}$ and a-Si:H doping ($E_{act}$). The *x*-axis corresponds to the band gap of a-Si:H, as indicated above the plot. On the left the corresponding energy of the conduction band of a-Si:H ($E_C$)can be seen with respect to vacuum energy, whereas the right side corresponds to the valance band ($E_V$) energy.

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