AMORPHOUS/CRYSTALLINE SILICON HETEROJUNCTION SOLAR CELLS, A SIMULATION STUDY

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ABSTRACT: Amorphous/crystalline silicon heterojunction solar cells are investigated by means of numerical computer simulations. The paper compares the p/n-type structure, a-Si:H(p)/c-Si(n), with the inverse n/p-type structure, a-Si:H(n)/c-Si(p), in order to clarify which of the two structures has a higher efficiency potential and what might be the intrinsic advantage of one type or the other. It is the main result of the simulations that there are inherent advantages of the p/n-type structure. This is due to mainly three reasons: (1) The higher band offset in the minority carrier band (valence band offset ΔE_{vb}) of about 400-500 meV in case of the p/n-type structure compared to the lower conduction band offset ΔE_{cb} of about 50-150 meV in case of the n/p-type structure, leading to a more efficient suppression of interface recombination. (2) The lower mobility of the minority carriers within the crystalline absorber when using the p/n-type structure (μ_h = 450 cm^2 V^{-1} s^{-1}) instead of the n/p-type structure (μ_e = 1350 cm^2 V^{-1} s^{-1}), leading to a higher open circuit voltage. (3) The higher mobility of the minority carriers within the amorphous emitter when using the p/n-type structure (μ_e » 15 cm^2 V^{-1} s^{-1}) instead of the n/p-type structure (μ_h » 5 cm^2 V^{-1} s^{-1}), leading to a higher short-circuit current. However, using the p/n-type structure and assuming a valence band offset which is too high (approximately ΔE_{vb} > 500 meV), these advantages are overcompensated by a significant loss in the fill factor.

Keywords: c-Si - 1: a-Si - 2: Heterojunction - 3

1. INTRODUCTION

Amorphous/crystalline silicon (a-Si/c-Si) heterojunction solar cells gain increasing interest as a low cost alternative to crystalline silicon solar cells with diffused pn-junctions. Processing is comparatively simple and does not require high temperature steps. High efficiency a-Si/c-Si solar cells have been successfully demonstrated and industrial production has already been announced [1].

Basically, a-Si/c-Si solar cells consist of a thin film of highly doped amorphous hydrogenated silicon (a-Si:H, the solar cell emitter), which is deposited on top of a moderately doped, monocrystalline silicon wafer (c-Si, the solar cell absorber). The moderate sheet resistivity of the doped a-Si:H requires the further use of a transparent, conductive layer (TCO) on top of the amorphous emitter. This minimises resistive losses in current flow to the metal front grid as well as reflective losses of the incident photon flux.

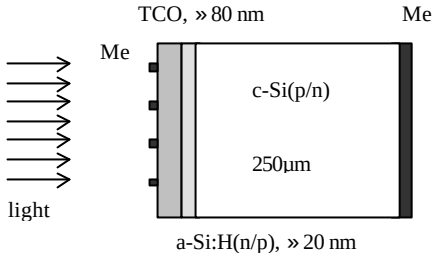

Figure 1: structure of an a-Si/cSi heterojunction solar cell.

Additionally, high efficiency features, such as the use of a back surface field, surface texturing, and the incorporation of a thin intrinsic a-Si:H layer between the emitter and the absorber of the solar cell may be used. The high potential of such a technology was recently demonstrated by the Sanyo Group, reaching an independently confirmed efficiency of 20.7 % [2].

A proper engineering of the crystalline / amorphous heterojunction interface is of crucial importance in order to achieve good a-Si/c-Si solar cell efficiencies. The surface-treatment of the crystalline silicon wafer prior to the emitter deposition is still a matter of debate. In previous work, we obtained the best results on flat and hydrogen-terminated surfaces [3], with surface state densities below of $N_{it}^{cSi} = 10^{12} cm^{-2}$. The incorporation of a thin, intrinsic a-Si:H layer (HIT-structure) has also been reported to enhance the solar cell efficiency [1]. It has been argued that this reduces the density of states in the a-Si N_{it}^{aSi} close to the a-Si/c-Si interface, as the defect density of intrinsic a-Si:H is about three orders of magnitude lower than that of doped a-Si:H.

It is still discussed which might be the preferred structure, a-Si:H(n)/c-Si(p) or a-Si:H(p)/c-Si(n). These two heterostructures have distinctively different electronic properties: Considering minority carrier transport across the interface, the low conduction band offset has to be compared with the high valence band offset using p-doped or n-doped c-Si wafers respectively. While the Sanyo group uses a p/n-type structure, a-Si:H(p)/c-Si(n) [1,2], most other groups investigate the inverse n/p-type structure, a-Si:H(n)/c-Si(p) [4]. It is still a matter of debate which of the two types has a higher efficiency potential and what might be the intrinsic advantage of one type or the other. We addressed this question by means of numerical computer simulations, investigating the influence of the corresponding band offsets, interface recombination and the different minority carrier mobilities on the solar cell performance for both types of structure.

2. MODELLING

One-dimensional, fully numerical simulations of the I-V curves and the spectral response have been performed. Poisson´s equation and the continuity equations within the

a-Si and c-Si layers are solved for a given defect state distribution, using Shockley-Read-Hall recombination statistics. In a first approximation, the TCO-layer is modelled by assuming an ohmic metal/a-Si front contact. Light trapping effects (i.e. due to surface texturing) are not considered.

For c-Si, a doping level of $N_{d/a}^{cSi} = 10^{17}\,cm^{-3}$ and a constant defect state distribution of $D^{cSi} = 10^{12}\,cm^{-3}\,eV^{-1}$ was assumed. This corresponds to a minimum minority carrier lifetime of $t^{cSi} = 0.2\ ms$ and a minority carrier diffusion length of $L_e^{cSi} = 840\,mm$ (p-doped) or $L_h^{cSi} = 430\,mm$ (n-doped) respectively. In this case of a high quality absorber, $L_{e/h}^{cSi}$ is always larger than the absorber length (250 µm). The spectral absorption coefficient $a^{cSi}(l)$ was taken from literature [5].

For a-Si, a bandgap of $E_g^{aSi} = 1.8\,eV$, a doping level of $N_{d/a}^{aSi} = 10^{19}\,cm^{-3}$ and an effective density of conduction band / valence band states of $N_{cb/vb}^{aSi} = 10^{20}\,cm^{-3}$ was assumed. The spectral absorption coefficient $a^{aSi}(l)$ was taken from literature [6]. The defect-state distributions within the bandgap are exponential band tail states and Gaussian dangling bond states, also taken from literature [7], i.e. dangling bond states: $N_{A/D}^{db} = 10^{19}\,cm^{-3}$, $s_{A/D}^{db} = 0.15\,eV$, tail states: $N_{A/D}^{tail} = 10^{21}\,cm^{-3}/eV$, $E_A^{tail} = 0.08\,eV$, $E_D^{tail} = 0.17\,eV$, see figure 2. This corresponds to an energetic distance from the Fermi level to the majority-band of $E_F^{aSi} = 0.48\,eV$.

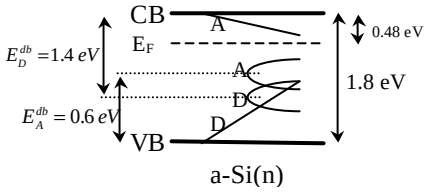

Figure 2: Sketch of the acceptor-like (A) and donor-like (D) defect-state distributions of n-doped a-Si. The energetic distribution of p-doped a-Si is assumed to be symmetrical to n-doped a-Si, i.e. $E_D^{db} = 0.6\,eV$, $E_A^{db} = 1.4\,eV$.

All the simulations presented in this paper accord to the a-Si parameters given above. Depending on the preparation conditions, the properties of the a-Si layers may vary considerably, i.e. $0.2\,eV \le E_F^{aSi} \le 0.5\,eV$. We also performed simulations using very different a-Si parameter, i.e. leading to $E_F^{aSi} = 0.25\,eV$. Qualitatively, this didn't have a strong influence on the main trends to be discussed in this paper.

Table 1 lists the main differences in the parameters of the two possible structures a-Si:H(n)/c-Si(p) and a-Si:H(p)/c-Si(n). In c-Si as well as in a-Si, the electron mobilities are generally larger than the hole mobilities. Thus the minority carrier mobilities differ when using a p/n-type or a n/p-type structure, see table 1. Assuming an electron affinity of $E_{ea}^{cSi} = -4.05\,eV$, $-3.90\,eV \le E_{ea}^{aSi(p)} \le -3.95\,eV$, $-3.96\,eV \le E_{ea}^{aSi(n)} \le -4.00\,eV$ [7], [8], and applying Anderson´s rule, a low conduction band offset ΔE_{cb} and a correspondingly high valence band offset ΔE_{vb} is expected ($\Delta E_{cb} + \Delta E_{vb} = E_g^{aSi} - E_g^{cSi}$). This is in accordance with literature, where the observed conduction band offset is between $50meV \le \Delta E_{cb} \le 200meV$ and $150meV \le \Delta E_{cb} \le 250eV$ using an n/p- or an p/n-type structure respectively [8]. Considering minority carrier transport across the a-Si/c-Si heterojunction, a low conduction band offset in case of the n/p-type structure has to be compared with a high valence band offset in case of the p/n-type structure, see table 1. Thus the band offset in the c-Si minority carrier band is of decisive importance. This is the conduction band offset ΔE_{cb} in case of a n/p-type structure and the valence band offset ΔE_{vb} in case of a p/n-type structure.

	n/p-type	p/n-type
c-Si minority carrier band offset	Low $50\,meV \le \Delta E_{cb} \le 150\,eV$	High $400\,meV \le \Delta E_{vb} \le 500\,eV$
c-Si minority carrier mobility	High $m_e^{cSi} = 1350\,cm^2\,V^{-1}\,s^{-1}$	Low $m_h^{cSi} = 450\,cm^2\,V^{-1}\,s^{-1}$
a-Si minority carrier mobility	Low $m_h^{aSi} = [1..5]\,cm^2\,V^{-1}\,s^{-1}$	High $m_e^{aSi} = [10..20]\,cm^2\,V^{-1}\,s^{-1}$

Table 1: main differences of the electronic properties of n/p- or p/n-type a-Si/c-Si solar cell structures.

3. BAND DIAGRAMS AND I-V CHARACTERISTICS

The resulting band diagrams for a p/n- and a n/p-type structure are shown in figure 3, with a c-Si minority carrier band offset of $\Delta E_{vb} = 450\,meV$ and $\Delta E_{cb} = 100\,meV$ respectively. The higher c-Si minority band offset in the p/n-type structure results in larger band bending and thus in a higher built-in voltage in the crystalline absorber ($V_{bi}^{cSi} = 67\,mV$ compared to $V_{bi}^{cSi} = 47\,mV$). Therefore the c-Si majority carrier density at the a-Si/c-Si interface will be much more reduced in case of the p/n-type structure ($n_{e,it}^{cSi} \approx 10^{13}\,cm^{-3}$ compared to $n_{h,it}^{cSi} \approx 10^{16}\,cm^{-3}$ under open-circuit conditions).

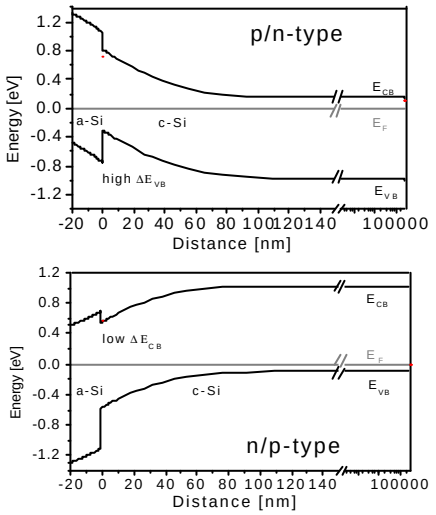

Figure 3: Band diagrams of a p/n- and a n/p-type a-Si/c-Si heterojunction solar cell.

The resultant I-V curves are shown in figure 4, assuming an illumination according to the AM1.5 solar spectrum. Furthermore interface recombination at the a-Si/c-Si heterojunction has been considered by introducing a constant surface state density of $D_{it}^{cSi} = 10^{12}\,cm^{-2}\,eV^{-1}$ at the crystalline interface. The I-V curves neglecting additional surface states ($D_{it}^{cSi} = 10^{8}\,cm^{-2}\,eV^{-1} \cong D_{bulk}^{cSi}$) are compared to the I-V curves assuming additional surface states. The main influence of introducing additional surface states at the crystalline interface is a loss in the open-circuit voltage V_{oc}. Four characteristic features are observed: (1) The loss in V_{oc} due to interface recombination is lower using the

p/n-type structure, (2) the open-circuit voltage is higher using the p/n-type structure, (3) the short-circuit current is higher using the p/n-type structure, but (4) the fill factor is lower using the p/n-type structure. The physical origin of these features will now be examined in more detail.

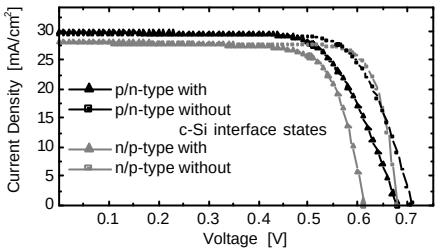

Figure 4: I-V curves of p/n-type (dark lines) and n/p-type (bright lines) a-Si/c-Si heterojunction solar cells, assuming (triangles) and neglecting (squares) additional surface states at the crystalline interface.

4. INFLUENCE OF BAND OFFSETS

In order to study the influence of the band offsets on the solar cell performance, we first hypothetically assume equal carrier mobilities for a-Si as well as for c-Si (i.e. $m_{e,h}^{cSi} = 900\ cm^2\ V^{-1}\ s^{-1}$, $m_{e,h}^{aSi} = 10 cm^2 V^{-1} s^{-1}$). In this case, the c-Si minority carrier band offset remains the only difference using a n/p- or a p/n-type structure. The additional influence of the different magnitude of the minority carrier mobilities is explicitly considered below. It does not change the general tendency, that a higher c-Si minority carrier band offset leads to a more effective suppression of interface recombination at the a-Si/c-Si heterojunction.

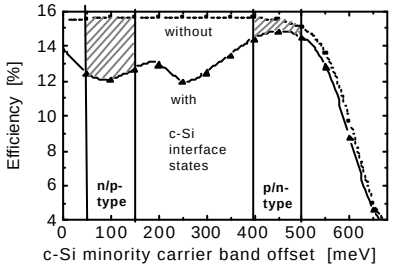

Figure 5: Dependence of the a-Si/c-Si solar cell efficiency on the band offset in the c-Si minority carrier band, assuming (straight line) and neglecting (dotted line) additional surface states at the crystalline interface. The loss in efficiency due to the enhanced interface recombination is highlighted for a n/p- and a p/n-type structure (shaded area).

Neglecting additional surface states at the crystalline interface ($D_{it}^{cSi} = 10^8\ cm^{-2}\ eV^{-1} \cong D_{bulk}^{cSi}$), the solar cell efficiency (open-circuit voltage, short-circuit current and filling factor) is more or less independent of the c-Si minority carrier band offset. This behaviour arises from the fact, that a change in the band offset does not lead to a change of the barrier for the c-Si minority carriers to overcome the heterojunction. This means that the distance of the minority carrier quasi-Fermi energy to the minority band plus band offset remains approximately constant. A higher band offset is compensated by a stronger band bending in the crystalline absorber. However, if the band offset exceeds a value of about 500 meV, it can no longer be compensated, since the minority band approaches the minority carrier quasi-Fermi energy. This results in a strong loss in the fill factor and thus in solar cell efficiency, see figure 5. The critical value for the band offset depends substantially on the properties of the amorphous emitter.

The situation changes significantly if additional surface states at the crystalline interface are considered ($D_{it}^{cSi} = 10^{12}\ \mathrm{cm}^{-2}\ eV^{-1}$). This leads to an additional interface recombination at the a-Si/c-Si heterojunction. The solar cell efficiency will be reduced, basically due to a loss in the open-circuit voltage compared to the case, where the additional surface state density of the crystalline wafer had been neglected, see figure 5 and figure 6. Indeed, additional interface recombination cannot be neglected, since there is experimental evidence, that a low surface state density of the crystalline wafer is of crucial importance [3]. It becomes obvious that the c-Si minority carrier band offset has a strong influence on the effectiveness of this additional recombination channel. As is shown in figure 5 (figure 6) the cell efficiency (the open-circuit voltage) is less strongly reduced in case of the p/n-type structure, where the band offset is high. In case of a high band offset (p/n-type structure) the inverted surface at the crystalline interface is able to suppress interface recombination, since only few majority carriers are available for recombination. The open-circuit voltage and consequently the solar cell efficiency is therefore not severely diminished.

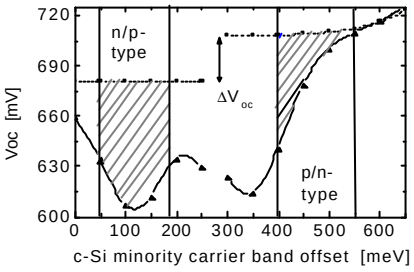

Figure 6: open-circuit voltage of a-Si/c-Si solar cell as a function of the c-Si minority carrier band offset, assuming (straight line) and neglecting (dotted line) additional surface states at the crystalline interface.

In figure 6, we additionally included the influence of the different carrier mobilities (i.e. $m_e^{cSi} = 1350\mathrm{cm}^2\ V^{-1}\ s^{-1}$, $m_h^{cSi} = 450\mathrm{cm}^2\ V^{-1}\ s^{-1}$, $m_e^{aSi} = 15\,\mathrm{cm}^2\ V^{-1}\ s^{-1}$, $m_h^{aSi} = 5\,\mathrm{cm}^2\ V^{-1}\ s^{-1}$). Neglecting additional surface states at the crystalline interface, a higher open-circuit voltage is observed, using the p/n- instead of the n/p-type structure (indicated as ΔV_{oc} in figure 6). This effect is not related with the higher c-Si minority band offset of the p/n-type structure. It results from the different minority carrier mobilities in the crystalline absorber as will be further outlined.

5. INFLUENCE OF ABSORBER MINORITY CARRIER MOBILITY

In the following, additional surface states at the crystalline interface are neglected. Figure 7 shows the dependence of the maximum achievable open-circuit voltage for the p/n- and the n/p-type structure on the absorber quality (the defect density in the crystalline wafer). The resultant minority carrier diffusion length due to the different minority carrier mobilities are indicated for both types of structure. The open-circuit voltage V_{oc} of a p/n-type solar cell (exhibiting a lower minority carrier mobility of $m_h^{cSi} = 450\mathrm{cm}^2\ V^{-1}\ s^{-1}$) is always higher compared

to a n/p-type solar cell (exhibiting a higher minority carrier mobility of $\mu_e^{cSi} = 1350 \mathrm{cm}^2 V^{-1} s^{-1}$). The difference ΔV_{oc} depends on the quality of the absorber, with $\Delta V_{oc} \leq 30 mV$, see figure 7.

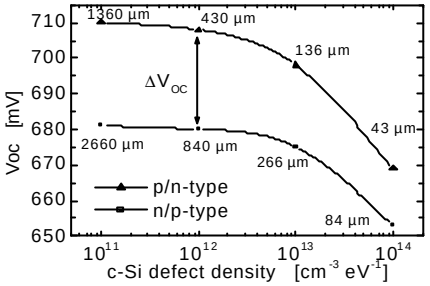

Figure 7: open-circuit voltage of a p/n- and a n/p-type a-Si/c-Si heterojunction solar cell as a function of the absorber quality (c-Si defect density and minority carrier diffusion length), neglecting additional surface states at the crystalline interface.

Under open-circuit conditions a significant part of minority carriers will recombine at the metal/c-Si back contact of the solar cell. A lower minority carrier mobility reduces this effect. The splitting of the quasi-Fermi energies within the crystalline absorber and thus the open-circuit voltage will then be enhanced. A good passivation of the back contact of the solar cell (i.e. by means of a back surface field), will not only enhance the achievable V_{oc}, but also reduce the difference ΔV_{oc} between the p/n- and the n/p-type structure.

Contrary, under short-circuit conditions, assuming equal emitter qualities, a lower c-Si minority carrier mobility leads to a smaller short-circuit current, if the absorber quality is poor. However, this effect ($\Delta I_{sc} \leq 1 mA cm^{-2}$) is by far overcompensated by the different emitter quality due to the different a-Si minority carrier mobilities, as will be further outlined.

6. INFLUENCE OF EMITTER MINORITY CARRIER MOBILITY

The minority carrier lifetime t in the a-Si emitter (estimated from the net recombination rate U and the minority excess carrier concentration Δn to $t = \Delta n / U$) amounts approximately to $t \approx 1.5\, 10^{-12} s$. This corresponds to a minority carrier diffusion length of $L_e^{aSi} \approx 8 nm$ (p-doped) or $L_h^{aSi} \approx 4 nm$ (n-doped). These values are smaller than the emitter thickness (20 nm). Thus most of the minority carriers, which are created within the amorphous emitter, will recombine.

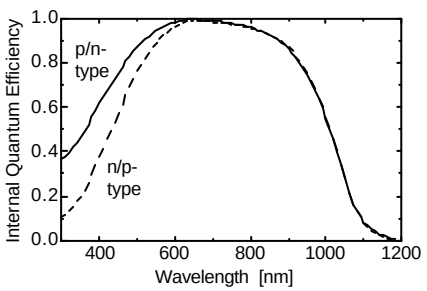

Figure 8: Internal quantum efficiency (IQE) of a p/n- and a n/p-type a-Si/c-Si heterojunction solar cell, neglecting additional surface states at the crystalline interface.

A higher minority carrier mobility within the amorphous emitter therefore directly contributes to the short-circuit current: The amount of minority carriers, which are created in the emitter and are able to pass the a-Si/c-Si heterojunction is enhanced. This results in a higher short-circuit current when using a p/n-type structure, independent of the quality of the crystalline absorber. This effect is also clearly visible comparing the internal quantum efficiency (IQE) for both types of a-Si/c-Si solar cells (figure 8). In the spectral range, where a significant part of photon absorption takes place in the emitter ($300 nm \leq l \leq 600 nm$), the p/n-type structure clearly has the higher IQE.

7. CONCLUSION

Our model calculation showed that there are intrinsic advantages of a p/n-type structure with respect to a n/p-type structure for a-Si/c-Si heterojunction solar cells: (1) Interface recombination at the a-Si/c-Si heterojunction will be suppressed more efficiently due to the higher band offset in the c-Si minority carrier band; (2) higher open-circuit voltages can be reached due to the smaller c-Si minority carrier mobility; (3) higher short-circuit currents can be obtained due to the higher a-Si minority carrier mobility. However, in case of the p/n-type structure, if the band offset ΔE_{vb} is too large, all these effects are overcompensated by a strong loss in the fill factor and thus in solar cell efficiency.

Furthermore, it must be stated that this simple simulation study neglects some technological aspects. Besides of the minority carrier mobility, equal emitter qualities have been assumed. In the comparison of the two structures therefore differences in the absorption spectra, band gaps and defect state densities regarding p-doped a-Si with respect to n-doped a-Si have not been considered.

8. ACKNOWLEDGEMENT

This work was partially supported by the Bundesministerium für Bildung und Forschung (BMBF contract # 01SF0012)

REFERENCES

[1] M.Taguchi, K.Kawamoto, S.Tsuge, T.Baba, H.Sakata, M.Morizane, K.Uchihashi, N.Nakamura, S.Kiyjama, O.Oota, Prog. Phot. Res. 8 (2000), 503.

[2] H.Sakata, T.Nakai, T.Baba, M.Taguchi, S.Tsuge, K.Uchihashi, S.Kiyama, Proc. 20th IEEE PVSEC (2000), 7.

[3] A.Froitzheim, H.Angermann, L.Elstner, W.Füssel, K.Kliefoth, J.Knechthel, M.Schmidt, N.Sinh, H.Weiser, W.Fuhs, Proc. 16th Eur. PVSEC, (2000), 1580.

[4] N.Jensen, R.Hausner, R.Bergmann, J.Werner, U.Rau, Prog. Photovolt. Res. Appl., to be published (2001).

[5] P.Sladek, M.Theye, L.Chahed, J. Non Cryst. Solids 363 (1993), 164.

[6] M.Green, M.Keevers, Prog. Phot. Res. 3 (1995), 189.

[7] R.Schropp, M.Zeman, Amorphous and Microcrystalline Silicon Solar Cells, Kluwer Academic Publishers (1998).

[8] M.Rösch, R.Brüggemann, G.Bauer, 2nd World PVSEC, (1998), 964.