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INTERFACE RECOMBINATION IN AMORPHOUS/CRYSTALLINE SILICON SOLAR CELLS, A SIMULATION STUDY

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ABSTRACT

The paper presents a numerical simulation of the behavior of a-Si:H/c-Si heterojunction solar cells. The simulations address in particular the question of the role of interface recombination for the device performance. It is shown that the critical parameters are the density of interface states at the a-Si:H/c-Si heterojunction and the band bending which is determined by the band offsets and the front contact work function. It is shown that due to the more favorable band bending the structure with the p-type emitter on an n-type c-Si absorber has an intrinsic advantage over the inverse structure. The role of an undoped a-Si:H buffer layer is discussed and it is shown that the front contact TCO/a-Si:H has considerable influence on the band bending in the c-Si wafer and therefore is of crucial importance for the cell performance.

INTRODUCTION

Amorphous/crystalline silicon (a-Si:H/c-Si) hetero-junction solar cells have raised considerable interest offering a low-cost alternative to crystalline silicon solar cells with diffused pn-junctions. Processing is comparatively simple and does not require high temperature steps. The high potential of this technology was recently demonstrated by the Sanyo Group, with an independently confirmed efficiency for a laboratory cell of 20.7 % [1].

A-Si:H/c-Si solar cells consist of a thin layer of highly doped amorphous hydrogenated silicon (a-Si:H), which is deposited on a moderately doped, monocrystalline silicon wafer (c-Si). The low conductivity of doped a-Si:H requires the use of a transparent, conductive layer (TCO) on top of the amorphous emitter, which minimises resistive losses as well as reflective losses. Additionally, high efficiency features such as surface texturing, and the incorporation of a thin intrinsic a-Si:H layer have been used to enhance the efficiency.

The performance of the heterojunction cell critically depends on the recombination at the a-Si:H/c-Si interface. These losses can be suppressed by a strong band bending in the crystalline wafer which leads to an inversion layer at the interface [2] or by a low density of defect states at the interface. Experimentally the density of interface states can be modified by a pre-treatment of the Si wafers which results in different defect state densities at the amorphous/crystalline interface [3,4] or by passivating the defects by deposition of a thin undoped a-Si:H buffer layer prior to the a-Si:H emitter deposition [1].

We report about numerical simulation of the a-Si:H/c-Si heterojunction solar cell addressing in particular the role of interface recombination. The work discusses the influence of (a) the band bending in the c-Si substrate, (b) the use of an intrinsic amorphous buffer layer, (c) the a-Si:H/c-Si interface defect state density and (d) the front contact on the solar cell characteristics.

MODELLING

The one-dimensional, algebraic semiconductor equations have been solved numerically using Shockley-Read-Hall recombination statistics. Recombination at the a-Si:H/c-Si interface can be modeled in two ways: (i) introducing an additional thin, defect rich layer nearby the interface or (ii) modeling the transport across the interface through thermionic emission. The interface defect states can then interact with both semiconductors. In this work the first approach (i) was used for simulation.

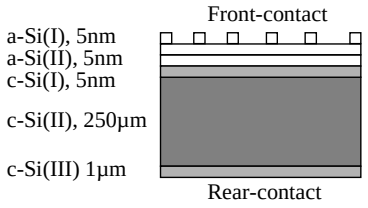

Fig.1: Structure used for modeling the a-Si:H/c-Si heterojunction solar cell. The a-Si:H emitter is split up into two parts, see text below, and the weakly doped c-Si absorber is split up into tree parts: defect rich layer (5nm), absorber (250µm) and back-surface field (BSF) (1µm).

The modeled structure is shown in fig. 1. The first amorphous layer represents doped a-Si:H. The second layer is either identical to the first one or it represents an intrinsic a-Si:H buffer layer. The resulting thickness of the amorphous emitter is always 10 nm. The defect structure of amorphous silicon is modeled by valence-, conduction band tail states and two dangling bond states. The characteristic energies of this defect distributions depend on the type of doping. In this work we used the set of parameters given in [5,6]. It is a characteristic feature of this parameter set, that the activation energy is 0.8 eV for un-

doped and 0.25 eV for both n- and p-type amorphous silicon. There are less defects in undoped a-Si:H, i.e. dangling bond densities of $5.6x10^{15}$ cm^{-3} (undoped) compared to $5.6x10^{18}$ cm^{-3} (doped). The band gap is assumed to be 1.72 eV, and the electron affinity is set to 3.8 eV.

For the crystalline absorber a doping concentration of 5×10^{16} cm^{-3} and a gaussian defect distribution centered around midgap (defect state densitiy of 5×10^{12} cm^{-3}) is assumed. The front side of the crystalline silicon is modeled by a defect rich surface layer with defect state densities varying from 5×10^{12} cm^{-3} (no additional interface defects) to 2×10^{18} cm^{-3}. At the rear side a highly doped back surface field layer (10^{19} cm^{-3}) is assumed. The material properties are also taken from literature [7,8]. The electron affinity is 4.0 eV, resulting in a conduction band offset of 0.2 eV with the amorphous layer. This is also an upper limit in our measurements [3].

Tab. 1 lists important parameters characterizing the differences between the two structures, n-a-Si:H/p-c-Si and p-a-Si:H/n-c-Si. In c-Si as well as in a-Si:H, 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. Considering minority carrier transport from the c-Si absorber across the a-Si:H/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.

	n/p-type	p/n-type
band offsets	$\Delta E_{cb} = 0.2\,eV$	$\Delta E_{vb} = 0.4\,eV$
c-Si minority carrier mobility	$\mu_e^{cSi} = 1000\,\frac{cm^2}{V\,s}$	$\mu_h^{cSi} = 340\,\frac{cm^2}{Vs}$
a-Si:H minority carrier mobility	$\mu_h^{aSi} = 1\,\frac{cm^2}{Vs}$	$\mu_e^{aSi} = 5\,\frac{cm^2}{Vs}$

Table 1: Important differences in material parameters for n/p- and p/n-type a-Si:H/c-Si solar cell structures.

RESULTS

n/p-type versus p/n-type

Fig. 2 depicts band diagrams for p/n- and n/p-type structures calculated by the above described procedure. Due to the much higher doping level in the amorphous Si most of the built-in voltage appears in the crystalline absorber. The built-in voltage of the p/n-structure is by 200 meV higher than for the n/p structure, because of the broken symmetry due to the different Band offsets in the minority carrier band. Therefore the inversion in the c-Si absorber is more pronounced using a p/n-type structure instead of a n/p-type structure (Fig. 2).

The strong inversion causes a pronounced suppression of interface recombination since only few majority carriers are available for recombination. The open circuit voltage and the efficiency of a p/n-type structure is thus expected to be higher. This has been investigated in detail in [2].

However, if the inversion leads to a degenerated interface, the enhanced band offset causes a transport barrier for the minority carriers. This leads to a strong loss in fill factor and cannot be compensated by the enhanced open circuit voltage. This effect is only critical using a p/n-structure since only in this case a high minority carrier band offset can be expected.

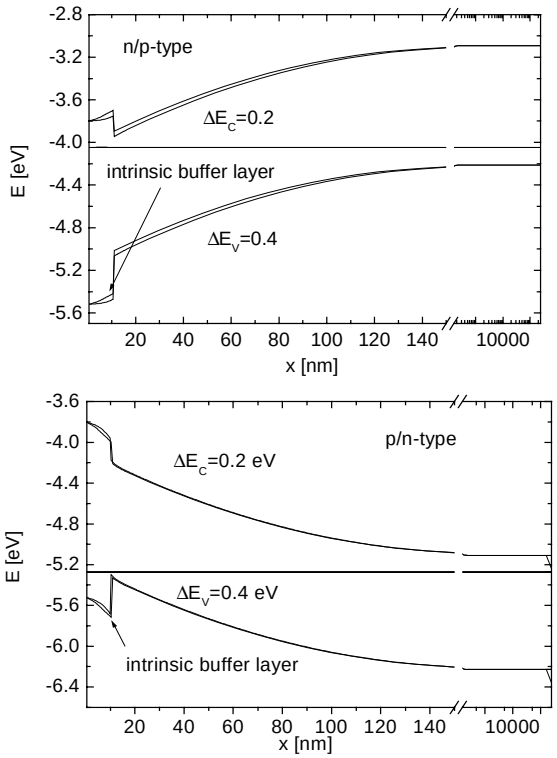

Fig. 2: Band diagrams for p/n- and n/p-type a-Si:H/c-Si structures, with and without an intrinsic a-Si:H buffer layer

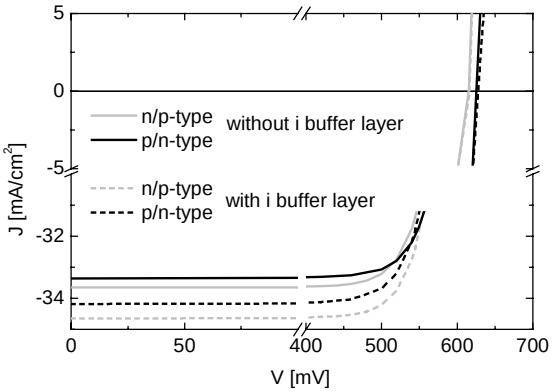

Fig. 3: Current voltage characteristics for n/p- and p/n-type with and without intrinsic buffer layer. Notice the horizontal and vertical breaks within the figure.

Typical current voltage characteristics for structures without assuming an enhanced density of c-Si interface states are simulated for both types of structures with and without an intrinsic amorphous buffer layer (Fig. 3). If an intrinsic amorphous buffer layer is inserted between the

doped amorphous silicon and the crystalline silicon the change in band bending is not significant (Fig. 2). The intrinsic buffer layer has a reduced density of defect states. Therefore interface recombination should be reduced. The following characteristic features are observed:

(a) The intrinsic layer enhances the short circuit current in both cases (Fig.3). As shown in Fig. 4 the amorphous layer is not electronically dead. The recombination rate is always less than the generation rate and in the intrinsic layer the recombination is significantly reduced.

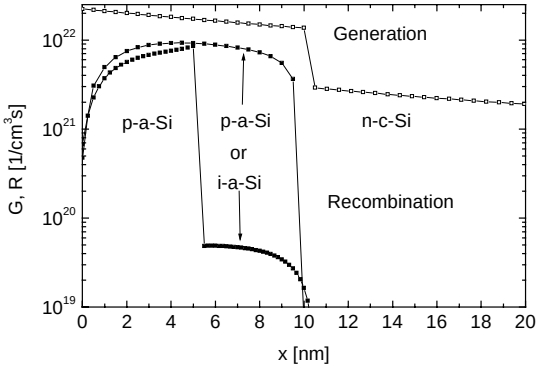

Fig. 4: Recombination rates at short circuit for a simulation with 5nm p-a-Si:H + 5nm i-a-Si:H and a simulation with 10nm p-a-Si:H. The generation rate is also given.

(b) The short circuit current of the n/p-type structure is slightly larger than for the p/n-type structure (Fig. 3). Note that this observation is not generally valid. In the present case it has been assumed that the diffusion length in c-Si is of the same order as the absorber thickness. In this case a higher short circuit current is expected using the n/p-structure, as the c-Si diffusion length L_n is larger than L_p, However, if $L_{n,p}$ is much larger than the wafer thickness D_W all the minority carriers in the absorber are collected, independent whether the absorber is n- or p-type. In this case the charge carrier collection in the amorphous layer determines the difference in the short circuit current. As the diffusion length is higher for the p-type a-Si:H the blue response and also the short circuit current will then be higher for the p/n-type structure (Fig. 5).

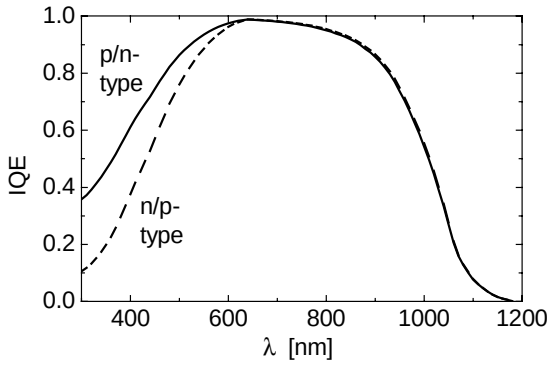

Fig. 5: Internal quantum efficiency calculated for a p/n- and a n/p-type structure for the case $L_{n,p}$ >> D_W (τ = 0.2 ms).

(c) The open circuit voltage in the p-a-Si:H/n-c-Si structure is enhanced compared to the inverse structure (Fig. 3). This is not due to the higher built-in potential, but due to the lower mobility of the minorities in the absorber, which reduces the dark saturation current [2]. The influence of the i-layer on the open circuit voltage is negligible.

Despite of the variations in open circuit voltage and short circuit current, the overall solar cell efficiency η is not very different for the different cell structures investigated so far. It amounts to about 17%. Remarkable differences in the behavior of the two structures (p/n-type or n/p-type) emerge when recombination via defects at the crystalline interface are taken into account.

If interface recombination via defect states at the a-Si:H/c-Si heterojunction plays a role, the open circuit voltage is significantly reduced. This effect is much less pronounced for the p/n-type structure than for the n/p-type structure: Excluding the intrinsic a-Si:H buffer layer, and varying the c-Si interface state density, V_{oc} is reduced from 627 to 580 mV (p/n) and from 611 to 487 mV (n/p). Compare also Fig.7 for the inclusion of the i-layer.

This effect is due to the higher inversion in the p/n-type compared to the n/p-type structure, as seen in Fig. 2. There are fewer majority carriers available at the interface with which the minorities of the c-Si can recombine. For the n/p-type structure the inversion is not strong enough to reduce the recombination rate significantly if there is a high density of interface states. This result was obtained for a defect concentration of 2×10^{18} cm^{-3} which corresponds to a projected density of 10^{12} cm^{-2} at the interface. Similar results were obtained in [2] where we model the interface with 10^{12} cm^{-2} interface states and used the thermionic emission model for transport across the interface. This shows that the reported results are independent of the details of the model used for the simulation, compare also [9]**.**

Influence of front contact

Up to this point we assumed flatband conditions at both contacts, rear and front side. This means, that within the scope of the Anderson model, the work function W of the metal coincides with the sum of the electron affinitiy χ and the difference E_c - E_f of the conduction band and the Fermi level of the adjacent semiconductor before bringing the two materials into contact. If W deviates from the flatband value, charges flow into the metal in order to equilibrate the Fermi levels of the metal and the adjacent layer.

In the following we study the influence of the front contact. Using the a-Si:H parameters specified, the front contact work function has to have a value W = 4.05 eV (n-a-Si:H emitter) or W = 5.27 eV (p-a-Si:H emitter) in order to achieve flat band conditions. However, the electron affinity of typical TCO materials (ZnO, ITO) is about 4.4 eV. Therefore assuming Andersons model the amorphous layer will always be depleted due to the front contact (350 meV for n-a-Si:H and 870 meV for p-a-Si:H). Although these values must not be true due to the inadequacy of Andersons model, a depletion due to the front contact cannot be excluded, see [10], where the front contact of a n-a-Si:H/p-c-Si structure is investigated in

detail. As an example we compare flatband conditions (W = 4.05 eV) to a front contact with W=4.4 eV for a n-a-Si:H/i-a-Si:H/p-c-Si structure, see Fig. 6 and Fig. 7.

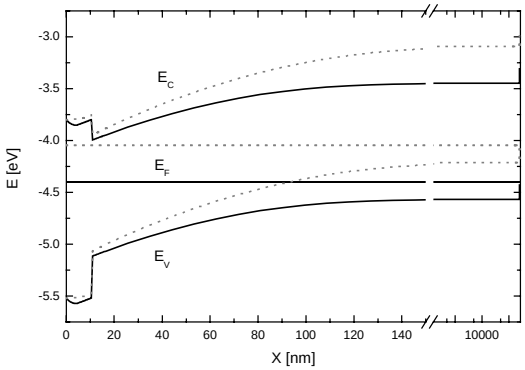

Fig. 6: Banddiagrams for the n/i/p-type structure with different front contact work functions W: an ohmic contact (flatband, W = 4.05 eV, dotted lines) and a Schottky contact (W = 4.44 eV, straight lines). Note the different Fermi level positions E_c - E_f at the interface.

The higher work function shifts the Fermi level at the a-Si:H/c-Si interface towards midgap (Fig. 6). As the amorphous layer is very thin, there are not enough carriers in this layer to equilibrate the Fermi levels to the value of the layer without contacts. Therefore the whole layer gets depleted, that is the difference of the majority band to the Fermi level changes drastically. In amorphous silicon the Fermi level is determined through the trap states, mainly the tail states, where most of the doping charge is stored. In our simulation the charge carrier concentration for the doped emitter layer changes from 10^{17} cm^{-3} (without contacts) down to 10^{12} cm^{-3} after contact with the metal.

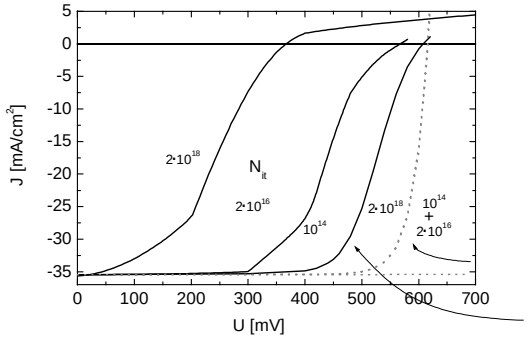

Fig. 7: Current voltage characteristics for a n/i/p-type structure with an ohmic front contact (flatband, work function W = 4.05 eV, dotted lines) and a Schottky front contact (W = 4.4 eV, straight lines). The varied parameter is the density of the c-Si interface states N_{it} [cm^{-3}].

The observed shift of the Fermi level at the interface towards midgap will enhance interface recombination, as the band bending in the crystalline absorber is reduced. The influence on the solar cell characteristic is shown in Fig.7. We varied the interface state density at the crystalline surface in the range from 10^{14} to 10^{18} cm^{-3} for flatband and depletion conditions at the front contact. For flatband conditions, the open circuit voltage is reduced for high interface state densities like already discussed. If the front contact leads to depletion, the Schottky front contact counteracts with the n/p junction. Even if there are no interface states, the IU-characteristic changes (Fig.7). If interface states are introduced they are much more effective for recombination and strongly reduce the fill factor and the open circuit voltage.

A good design for a-Si:H/c-Si solar cells will try to minimize the a-Si layer thickness in order to reduce the high recombination losses in the emitter. However, as shown above, this requires a properly chosen front contact which drives the front surface into accumulation. If this is not the case a thinner a-Si:H layer will enhance recombination losses due to a-Si:H/c-Si interface recombination.

Conclusion

The simulation of a-Si:H/c-Si solar cells indicates a pronounced influence of interface recombination on solar cell performance. The p-a-Si:H/n-c-Si structure reduces interface recombination due to higher band bending of the absorber at the interface. For thin emitter layers the front contact will influence the a-Si:H/c-Si interface recombination. If the front contact drives the a-Si layer into depletion the interface recombination will be enhanced. This effect is even stronger for thinner emitter layers.

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