

Computer Modeling of *a*-Si:H/*a*-SiGe:H Solar Cells

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Abstract—Current hydrogenated amorphous (*a*-Si:H) and micro-crystalline (μ c-Si:H) silicon solar cells use textured substrates for enhancing the light absorption and (graded) buffer layers in order to improve the overall performance of the cells. The resulting solar cell structures are very complex and for understanding the role of these layers and for further optimization of the solar cell structures computer modeling is a useful tool. In this article we demonstrate the use of integrated electrical and optical modeling to optimize hydrogenated amorphous silicon/silicon-germanium *a*-Si:H/*a*-SiGe:H tandem solar cells. In this article both the bandgap grading profile of the *a*-SiGe:H bottom cell and current matching are optimized

Keywords—current matching, amorphous silicon germanium, bandgap profile, solar cells, modeling

I. INTRODUCTION

One of the most severe limitations of *a*-Si:H solar cells is the light induced degradation (Staebler-Wronsky effect [1]). One way of minimizing the degradation in an *a*-Si:H solar cell is to reduce the thickness of the intrinsic layer. This leads to the multi-junction concept, by stacking several solar cells the thickness of the component cells can be reduced. The efficiency of such a multi-junction solar cell can be increased by applying different bandgap materials for the absorber layers of the component cells as this allows for a better utilisation of the solar spectrum. For the low bandgap absorber layers μ c-Si:H and *a*-SiGe:H are often used [2].

Alloying of *a*-Si:H with Ge reduces the bandgap, allowing its tuning by varying the germanium content. However, the efficiency of *a*-SiGe:H solar cells is limited due to deterioration of the electronic properties of *a*-SiGe:H with increasing Ge alloying and the introduction of large band offsets between the *a*-SiGe:H intrinsic layer and the *a*-SiC:H p-layer and *a*-Si:H n-layer. To overcome some of these problems the bandgap profiling of the intrinsic layer has been introduced [3].

Experimental results show that the width of the profiled region of the intrinsic *a*-SiGe:H layer next to the p-i interface (p-i grading) should be small and the profiled region next to the i-n interface (i-n grading) should be large [5]. In previous work we carried out simulations to further investigate and optimize the performance of solar cells introducing novel designs for profiling the intrinsic layer [6]. Based on these simulations we proposed the modified V type profile, which shows a strong reduction in recombination losses in the intrinsic layer compared to

conventional profiles, such as U and V type.

In this work we optimized the bottom cell in *a*-Si:H/*a*-SiGe:H solar cells. Using a flexible profile design we optimized the bottom cell bandgap profile for the AM1.5 spectrum and the AM1.5 spectrum cutoff below 630 nm. Simulations have been carried out of tandem cells with these optimized bottom cells. To obtain current matching two methods were used, matching of photocurrent and using both optical and electrical simulations to maximize the efficiency of the tandem cell. In both methods the top cell thickness was adapted. We investigated whether the optimized component cell is also the optimal bottom cell structure for the complete tandem cell, we optimized the bottom cell again as a part of the whole tandem structure.

II. SIMULATION MODELS

A. The ASA program

The simulations were carried out with the Advanced Semiconductor Analysis (ASA) program, which has been developed at Delft University of Technology [7]. The main features of the ASA program include: (i) calculation of the light generation profile, which is based on the thin film optics assuming flat interfaces in the device; (ii) models describing a complete density of states distribution as function of energy, which include both the extended and localized (tail and defect) states with corresponding recombination-generation statistics; (iii) calculation of the defect-state distribution in a layer according to the defect-pool models (DPM) [8, 9]; (iv) a model for the tunnel-recombination junction that allows to simulate a multi-junction *a*-Si:H solar cell as one structure. (v) The continuous change (grading) of all input parameters as a function of position in the device can be defined.

Recently new features were implemented into the ASA program that enhance its capability of accurate modeling of hybrid solar cells that are based on crystalline silicon (c-Si) and *a*-Si:H layers. Models describing the dependence of material properties of c-Si such as mobility, doping, lifetime of minority carriers etc., as a function of doping, temperature and electric field were implemented in the ASA program.

B. Optical Simulations

For the optical simulations the GENPRO2 program was used [10]. This program takes the scattering of the incoming light at the rough interfaces into account and assumes an incoherent light propagation in the cell. The amount of light that is scattered

at an interface is described by the haze parameter. The haze is defined by the ratio between the diffuse fraction of the light and the total amount of light. Four haze values are used for one interface, the haze for reflection at the interface in the first and second medium and the haze for the transmission from the first to the second and from the second to the first medium. The haze for the reflection and transmission can be calculated from [11]:

$$H_R = \frac{R_d}{R_t} = 1 - \exp\left[-\left(\frac{4\pi\sigma_{rms}n_0}{\lambda}\right)^2\right] \quad (1)$$

$$H_T = \frac{T_d}{T_t} = 1 - \exp\left[-\left(\frac{4\pi\sigma_{rms}C|n_0 - n_1|}{\lambda}\right)^3\right] \quad (2)$$

Here R_d and T_d are the diffuse reflectance and transmission, R_t and T_t are the total reflectance and transmission, σ_{rms} is the root mean square roughness, n_0 and n_1 are the refractive indices of the first and second media, C is a constant and λ is the wavelength. For C an appropriate value for asahi TCO is 0.5 [12].

The angular distribution function for the scattered light defines the amount of diffuse light that is scattered in each direction. In general this function will be wavelength dependent. for simplicity we will assume a normalized \cos^2 .

Scattering is taken into account at the TCO/p interface, the p/i interfaces of the top and bottom cell, the i/n interfaces of the top and bottom cell the n/p interface of the tunnel recombination junction and the n/Silver interface. It is assumed for simplicity that there is no scattering within the graded layers.

C. Tandem Solar Cell structure

The simulated tandem solar cells consist of p-i-n-p-i-n solar cells on glass covered with a surface-textured transparent conductive oxide (TCO). The p-layers are 10 nm thick a -SiC:H layers with a bandgap of 1.90 eV. The intrinsic layer of the top cell consists of an a -Si:H layer with a bandgap of 1.75 eV. The n-layers are 20 nm thick a -Si:H layers with a bandgap of 1.75 eV. The intrinsic layer of the bottom cell is a graded a -SiGe:H layer with a minimal bandgap of 1.50 eV and a maximal bandgap of 1.70 eV. The profiling of the p-i grading started with the bandgap of 1.70 eV and continued linearly towards the minimal mobility gap. When a U type profile is used the p-i grading is followed by an intrinsic a -SiGe:H layer with a constant bandgap of 1.50 eV. The i-n grading is profiled from 1.50 eV to 1.70 eV. In order to optimize the profiling of the intrinsic layer we used a flexible profile design, in which the intrinsic layer was divided in four individually graded parts. We have chosen two positions in the intrinsic layer at which we varied independently the mobility gap (Bg1 and Bg2) from 1.70 eV and 1.5 eV in steps of 0.05 eV as is illustrated in Fig. ?? . The total thickness of the intrinsic layer was kept constant at 150 nm. A 300 nm thick aluminum layer is used as the back contact. For simulation of tandem cells the tunnel-recombination junction was included in the simulation so the tandem solar cell is simulated as one structure.

D. Input Parameters

The characteristic energy of the valence band tail (E_{v0}) for material with a bandgap of 1.50 eV is 50 meV, and 45 meV for

the intrinsic material with a bandgap of 1.70 eV. For material with a bandgap in between the value of E_{v0} is linearly interpolated. The defect density for all simulations was calculated using the defect-pool model [9]. The other input parameters for the simulations were obtained from [13, 14].

In the optical simulations the linearly graded layers have been substituted with a stepwise profile, using steps of 0.05 eV. The optical constants for these layers were determined experimentally by measuring the wavelength dependent (complex) refractive index of layers with a corresponding Tauc gap. The generation rate profile in the tandem solar cell was calculated using the AM1.5 spectrum. The bottom cells were optimized for both AM1.5 and AM1.5 cutoff below 630 nm.

III. OPTIMIZATION OF THE a -Si:H/ a -SiGe:H TANDEM CELLS

A. Optimization of the a -SiGe:H bottom cell

To optimize the bandgap profile of the intrinsic a -SiGe:H layer a series of simulations was conducted varying the bandgap at two positions of the intrinsic layer as illustrated in Fig. ?? . The efficiencies as a function of Bg1 and Bg2 for AM1.5 and AM1.5 cutoff below 630 nm are shown in Fig. 2. The optimal profile for the AM1.5 spectrum is the profile with Bg1 1.65 eV and Bg2 1.70 eV. The optimal profile for the AM1.5 spectrum cutoff below 630 nm has a Bg1 and Bg2 of 1.70 eV.

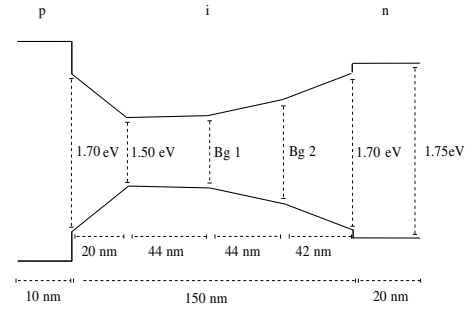


Fig. 1. Schematic profile design for optimization. Shown are two bandgap profiles of the simulated combinations of Bg1 Bg2. Bg1 and Bg2 were varied independently between 1.5 eV and 1.80 eV in steps of 0.05 eV.

In Table I the optimized grading profiles are compared to conventional U and V type profiles. In the table “modified V_{AM} ” is the optimal grading profile for the AM1.5 spectrum and “modified V_{630} ” is the optimal bandgap grading profile for the AM1.5 spectrum cutoff below 630 nm. The p-i grading of the V type profile is 20 nm thick and starts from a bandgap of 1.70 eV and is continued linearly to 1.5. The i-n grading continues linearly over a thickness of 130 nm to a bandgap of 1.70 eV. The p-i grading of the U type profile is again 20 nm thick and starts from a bandgap of 1.70 eV and is continued linearly to 1.5. The i-n grading continues linearly over a thickness of 130 nm to a bandgap of 1.70 eV. The bandgap From this table it can be seen that the efficiencies for the modified V type profiles are equal and higher than the efficiencies for the U and V type profile. The profiling of the p-i grading started with the bandgap of 1.70 eV and continued linearly towards the minimal mobility gap over a

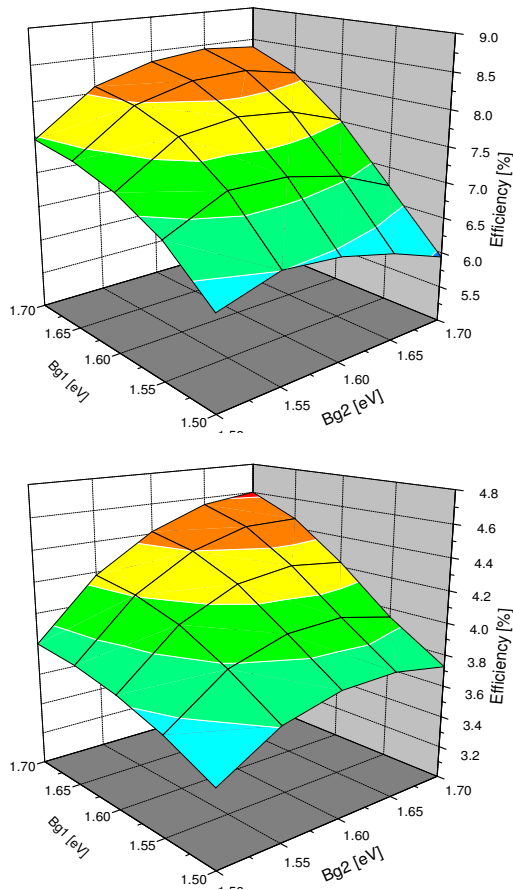


Fig. 2. Top: Efficiency of the bottom cell as a function of Bg1 and Bg2 under AM1.5 illumination. Bottom: Efficiency of the bottom cell as a function of Bg1 and Bg2 under AM1.5 illumination cutoff below 630 nm.

TABLE I
SOLAR CELL PARAMETERS FOR VARIOUS GRADING
PROFILES UNDER THE AM1.5 SPECTRUM

| | V_{oc} [V] | FF[-] | eff[%] | J_{sc} [A/m ²] |
|--------------------------|--------------|-------|--------|------------------------------|
| modifiedV _{AM} | 0.65 | 0.69 | 8.4 | 187 |
| modifiedV ₆₃₀ | 0.66 | 0.69 | 8.4 | 183 |
| V | 0.62 | 0.64 | 7.9 | 197 |
| U | 0.58 | 0.54 | 6.2 | 197 |

distance of 20 nm.

B. Current Matching in a-Si:H/a-SiGe:H solar cells

To obtain current matching the structure of the bottom cell was taken constant and the thickness of the intrinsic layer of the top cell was varied. Two methods were used, matching of photocurrent and matching the top cell current to obtain maximal efficiency. For the first method it is enough to simulate the optical generation in the tandem structure to compare the total amount of charge generated in the intrinsic layers of the top and bottom cell. The other method requires both optical and electrical simulations.

Figure 3 shows the efficiency as a function of top cell thickness. In these simulations the modifiedV_{AM} type profile and the modifiedV₆₃₀ type profile were used as bottom cells. To show how the top cell thickness relates to the matching of the photocurrents, the photocurrent generated in the top and bottom cells are shown. The figure shows that matching the photocurrent results in a thicker top cell, however, the efficiency is not much reduced (0.2% for both profiling schemes). The maximal efficiency of a tandem cell with the modifiedV_{AM} type profile is 10.2% and the maximal efficiency of a solar cell with the modifiedV₆₃₀ type profile is 10.1%.

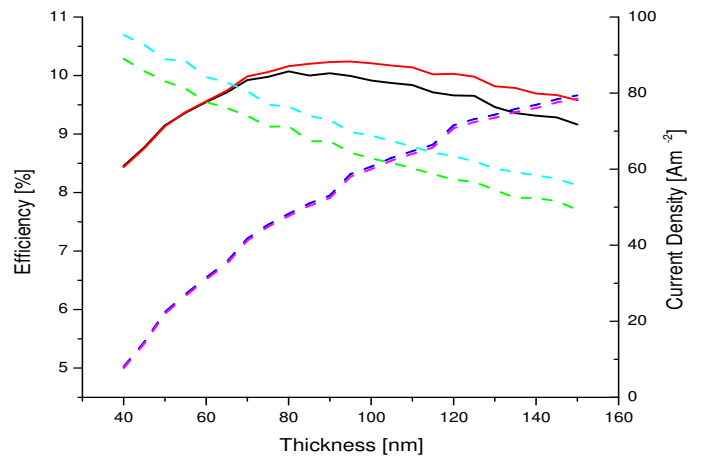


Fig. 3. Efficiency as a function of top cell thickness. red: The efficiency of the tandem cell with the modifiedV_{AM} type profile as a function of top cell thickness. black: The efficiency of the tandem cell with the modifiedV₆₃₀ type profile as a function of top cell thickness. dashed purple: photocurrent of the top cell for the tandem cell with the modifiedV_{AM} type profile. dashed light-blue: photocurrent of the bottom cell for the tandem cell with the modifiedV_{AM} type profile. dashed blue: photocurrent of the top cell for the tandem cell with the modifiedV₆₃₀ type profile. dashed green: photocurrent of the bottom cell for the tandem cell with the modifiedV₆₃₀ type profile.

The optimal profile to use as a bottom cell in a tandem cell structure can, however differ from this profile as the spectrum for the bottom cell will not be the same as the spectra for which the bottom cells were optimized. Therefore the same profiling schemes were applied in simulations of a tandem structure.

C. Optimization of a-Si:H/a-SiGe:H tandem cells

Using optical and electrical simulations to match the current the tandem cell was optimized by Bg1 and Bg2 in the bottom cell. The results are shown in Fig. 4. According to these simulations Bg1 and Bg2 should be 1.50 eV and 1.70 eV respectively for the best efficiency. For this profile (modifiedV_{tandem} type profile) the efficiency was 10.7% which is 0.5% higher than the maximal efficiency with the modifiedV_{AM} type profile and 0.6% higher than the maximal efficiency with the modifiedV₆₃₀ type profile.

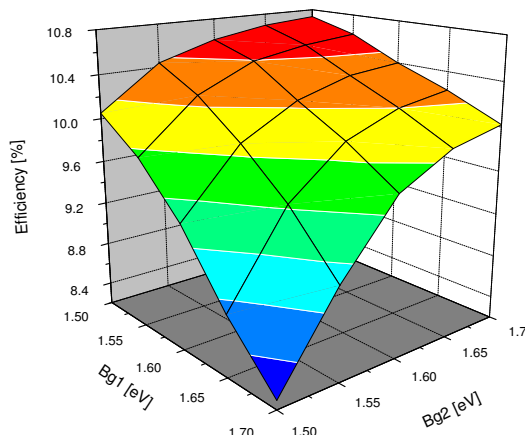


Fig. 4. The efficiency of the tandem cell as a function of Bg_1 and Bg_2 .

IV. CONCLUSIONS

Simulations of various bandgap grading profiles for *a*-SiGe:Hsolar cells have been carried out. Optimized grading profiles have been found which for the AM1.5 spectrum (modified V_{AM} type profile) and the AM1.5 spectrum cutof below 630 nm (modified V_{630} type profile). The optimized profiles have a higher efficiency than conventional U and V type profiles.

In order to optimize *a*-Si:H/*a*-SiGe:Htandem solar cells simulations have been carried out of tandem cells with the modified V_{AM} type and the modified V_{630} type profile. Two methods for current matching were investigated, matching of the photo current and using both optical and electrical simulation to find the top cell thickness that gives the highest efficiency. It was found that matching the photocurrent results in thicker top cells than using both optical and electrical simulations, however, the efficiency was not much affected by the current matching method.

Simulations of *a*-Si:H/*a*-SiGe:Htandem cells showed that the optimal bottom cell grading profile differs from the seperately optimized component cells.

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