

Two-dimensional Computer Modeling of Single Junction a-Si:H Solar Cells

Changwoo Lee, Harry Efstathiadis, James E. Raynolds, Pradeep Halder
Energy and Environmental Applications Center (E2TAC)
College of Nanoscale Science and Engineering
University at Albany, State University of New York
Corresponding author: PHalder@uamail.albany.edu

ABSTRACTS

A two dimensional physically-based computer simulation of single junction pin amorphous silicon solar cells is presented using Sentaurus, TCAD by Synopsys Inc. The simulation program solves the Poisson, the continuity, and the current density equations by using a standard procedure for amorphous materials, including the continuous density of state model, Shockley-Read-Hall and Auger recombination mechanisms, and computes the generation function of electron-hole pairs from the optical parameters of each layer. The dependence of these optical parameters with the photon energy has been included, taking into account the doping level, thickness of each layer and their effect on cell efficiency. The simulator is applied to the analysis of a *pin* single junction a-SiC:H/a-Si:H/a-Si:H solar cell, obtaining results comparable to one dimensional simulation results using AMPS-1D. More advanced simulation models for novel solar cell devices such as tandem cell are in progress, with the aim of achieving an optimal design of solar cells based on amorphous materials or micro-/nanocrystalline layer.

INTRODUCTION

Physically-based computer simulations of thin film photovoltaic devices have received more attention and become increasingly mature over the past two decades since modeling of a-Si:H solar cells started in the early 80s [1-3]. A number of simulation packages such as AMPS-1D, SCAPS-1D, PC-1D, SimWindows, ADEPT-F, AFORS-HET, ASPIN, and ASA have been developed, however, they are limited to one dimensional although they can evaluate solar-cell performance either directly or indirectly.

Two dimensional simulation has become necessary for more precise device simulation in order to model complex

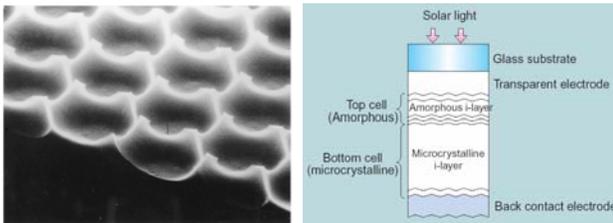


Figure 1. (left) SEM image of texture surface with $14 \mu\text{m}$ spacing of the hexagon [4] and (right) microcrystalline layer in bottom cell of tandem a-Si:H solar cell [5]

devices although one dimensional simulation well describes optical and electrical properties of a-Si:H solar cells on flat substrates. Two important improvements in the device simulation of a-Si:H based solar cells need to be addressed. The first is how to model the textured substrates in complex structured a-Si:H solar cells, which introduces spatial variations through the device. The second development in third generation solar cells is the application of microcrystalline or nanocrystalline silicon, which is not a spatially homogeneous material as shown in [4-5].

In this report, we present the study of doping density and layer thickness effect on electrical behavior of a *pin* single junction a-SiC:H/a-Si:H/a-Si:H solar cell prior to performing two dimensional simulations of a-Si:H solar cell with complex structures in advance.

MODEL DESCRIPTION

For the simulation of a-Si:H solar cells, we used the commercially available software of Sentaurus TCAD, Synopsys Inc. In this session we describe structural and electrical parameters for the device simulation including optical parameters.

A. Optical parameters

In this study, we have used optical constants, which are

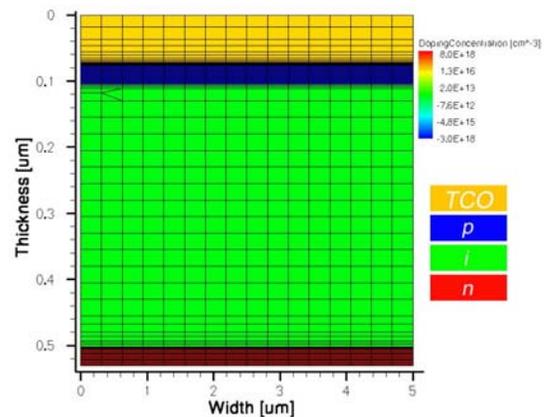


Figure 2. Cross section of single junction *pin* a-Si:H solar cell device with two dimensional mesh configuration shows doping profiles. TCO (top layer)/p-type a-SiC:H/intrinsic absorber layer a-Si:H/n-type a-Si:H.

the refractive index and the extinction coefficient as functions of the wavelength for the layers used in the solar cell, of all individual layers as input optical parameters in the reference [6].

B. Device structure and input parameters

The structure of a single junction a-Si:H solar cell is TOC/a-SiC:H/a-Si:H/a-Si:H as shown in figure 2. For the baseline structure, transparent conductive oxide (TCO) layer has 75 nm thickness. a-SiC:H has been used for p-layer because the wide bandgap of 1.92 eV and high conductivity results in a high built-in potential, allow more light to reach the absorber layer improving in open circuit voltage as well as short circuit current. Table 1 shows the minimum set of input parameters, which are used in this simulation without any buffer and graded layer in between each layer. For an a-Si:H *pin* solar cell, it is widely accepted that the most important parameter affecting the device properties is the gap states of the films. It is also very important to note that these values are not the absolute values for a-Si:H based materials, but reference.

Table 1. Baseline input parameters used in the simulation

Baseline input parameters			
Layer	p-layer	i-layer	n-layer
Thickness [nm]	25	400	25
Doping concentration [cm^{-3}]	3×10^{18}	10^{14} - 10^{17}	8×10^{18}
Mobility gap [eV]	1.92	1.82	1.82
Electron mobility (min/max) [cm^2/Vs]	10	20	20
Hole mobility (min/max) [cm^2/Vs]	1	2	2
Effective DOS in CB [cm^{-3}]	2.5×10^{20}	2.5×10^{20}	2.5×10^{20}
Effective DOS in VB [cm^{-3}]	2.5×10^{20}	2.5×10^{20}	2.5×10^{20}
Capture cross section [cm^2]			
for electron/hole in valance bandtail		$1 \times 10^{-15}/1 \times 10^{-17}$	
for electron/hole in conduction bandtail		$1 \times 10^{-17}/1 \times 10^{-15}$	
DOS at CB/VB mobility edge [cm^{-3}eV]		$1 \times 10^{21}/1 \times 10^{21}$	
Gap (dangling bond) states			
Model	Standard density of state model (Gaussian distribution function)		
1 st Gaussian defect state density [cm^{-3}]	1×10^{18} (D-like)	4×10^{15} (D-like)	1×10^{16} (D-like)
	Standard deviation [eV]	0.15	0.06
2 nd Gaussian defect state density [cm^{-3}]	1×10^{18} (D-like)	4×10^{15} (D-like)	1×10^{16} (A-like)
	Standard deviation [eV]	0.08	0.06
3 rd Gaussian defect state density [cm^{-3}]	1×10^{16} (A-like)	4×10^{15} (A-like)	4×10^{18} (A-like)
	Standard deviation [eV]	0.08	0.06

*D-like and A-like represent donor-like state and acceptor-like state, respectively

SIMULATION RESULTS AND DISCUSSION

The cell performances of a *pin* single junction a-Si:H, such as open circuit voltage (V_{oc}), short circuit current (J_{sc}), fill factor (FF), conversion efficiency, photo- $I-V$ characteristics, are obtained as a function of thickness and doping concentrations each layer as well as acceptor level of i-layer varying defect density. The electrical properties inside the solar cells such as the distribution of

generation and recombination rates, electric fields and electron and hole concentrations are also obtained.

Figure 3 shows the characteristics of *pin* a-Si:H solar cell as function of p-layer thickness. Thickness of n-layer

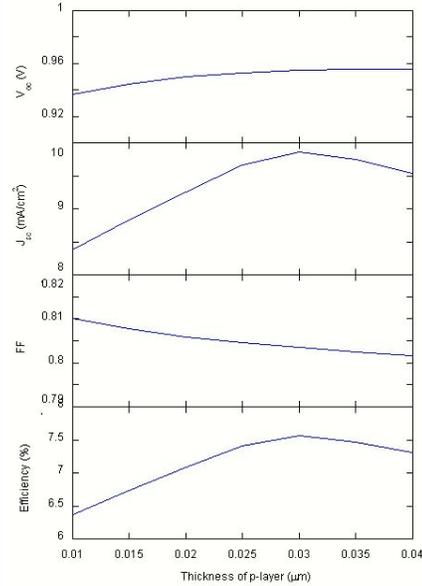


Figure 3. Variation of photovoltaic characteristics of a single junction *pin* a-Si:H solar cell device as a function of p-layer thickness

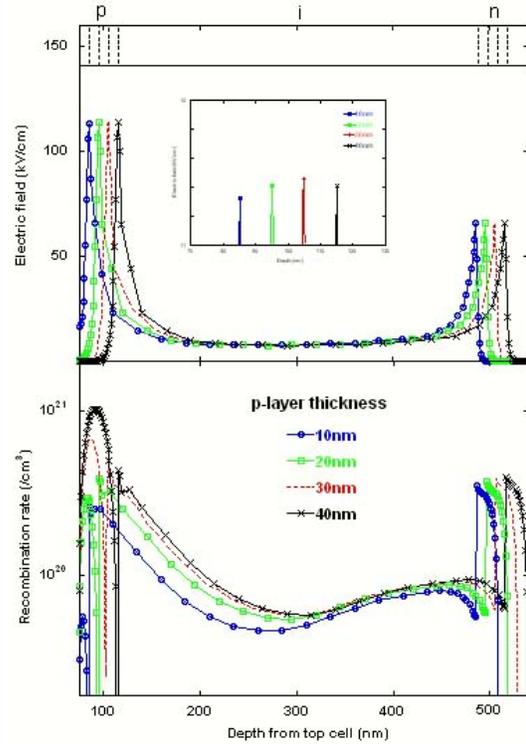


Figure 4. Electric field distribution (top) and recombination rate distribution (bottom) of a *pin* a-Si:H solar cell device for different thickness of p-layer (dash line on top indicates interface in between p/i and i/n layer)

and i-layer are fixed as 25 and 400 nm, respectively. Doping concentration of p-layer and n-layer are also fixed as 3×10^{18} and $8 \times 10^{18}/\text{cm}^3$, respectively. The p-layer with 30nm thickness shows the highest efficiency due to highest short circuit current of the device although fill factor decreases with increasing thickness of p-layer as shown in figure 3. This is because the highest electric field at p/i interface collecting more carriers to the TCO layer although it also has high recombination rate followed by 40nm thickness cell. This result agrees well with Kim et al. although they claimed that the optimum p-layer thickness is 50Å without a buffer layer [7]. We note that 30nm is not necessary to be absolute optimum value for a-SiC:H material, however, it can be considered as a reference.

Figure 5 shows the characteristics of a-Si:H solar cell as a function of acceptor level in p-layer. Doping concentration of n-layer is fixed as $8 \times 10^{18}/\text{cm}^3$. Thickness of p-, i-layer and n-layer are fixed as 25, 25 and 400nm, respectively. Typical value of N_A in the a-SiC:H p-layer is $10^{18}/\text{cm}^3$ or a little higher [8].

In order to collect the maximum number of electron hole pairs generated by absorbed photons, the electric field at the interface should be high, however, the recombination rate will also be high resulting a reduction of efficiency. Thus, there is trade-off between electric field and recombination rate.

Simulation result in figure 5 shows that p-layer over $4 \times 10^{18}/\text{cm}^3$ of N_A has high efficiency due to drastic increase of open circuit voltage of the device, however, it is possibly difficult to achieve higher N_A than that of conventional a-SiC:H material without degradation of the film quality. Figure 6 shows that the electric field distribution (top), generation rate and recombination rate (middle), and electron and hole density (bottom) through the i-layer. As shown in figure, $1 \times 10^{19}/\text{cm}^3$ of N_A in p-layer builds the highest electric field at p/i interface collecting more carriers, which is holes for this case (bottom in figure 6), to the TCO layer although it also has the highest recombination rate over the i-layer. This result well agrees to that of one dimensional simulation results done by Yamanaka et al [9].

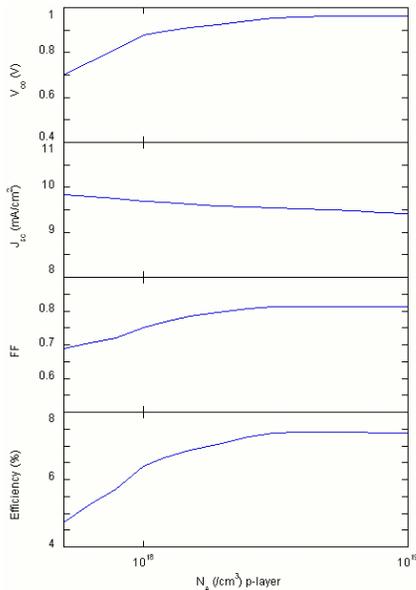


Figure 5. The dependence of a-Si:H solar cell characteristics on the acceptor doping concentration in p-layer.

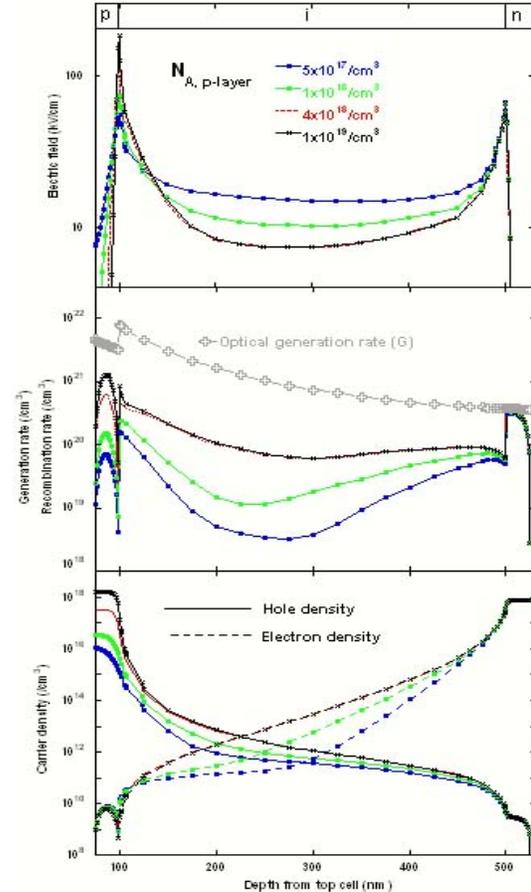


Figure 6. Electric field distribution (top), generation and recombination rate distribution (middle), and electron and hole density of a-Si:H solar cell device for different acceptor levels of p-layer (N_D is fixed as $8 \times 10^{18}/\text{cm}^3$)

distribution (middle), and electron and hole densities (bottom) through the i-layer. As shown in figure, $1 \times 10^{19}/\text{cm}^3$ of N_A in p-layer builds the highest electric field at p/i interface collecting more carriers, which is holes for this case (bottom in figure 6), to the TCO layer although it also has the highest recombination rate over the i-layer. This result well agrees to that of one dimensional simulation results done by Yamanaka et al [9].

The effect of donor level in n-layer on characteristics of *pin* a-Si:H solar cell is shown in figure 7. Doping concentration of p-layer is fixed as $3 \times 10^{18}/\text{cm}^3$. Thickness of p-, i-layer and n-layer are fixed as 25, 25 and 400 nm, respectively. Simulation result shows that increasing N_D over $5 \times 10^{18}/\text{cm}^3$ shows slightly increasing cell efficiency due to increase of open circuit voltage of the device although short circuit current has insignificant effect. This is because electric field in the cell with N_A lower than $4 \times 10^{18}/\text{cm}^3$ is weak to conduct drift current by sweeping photogenerated electron-hole pairs through i-layer as shown in figure 8.

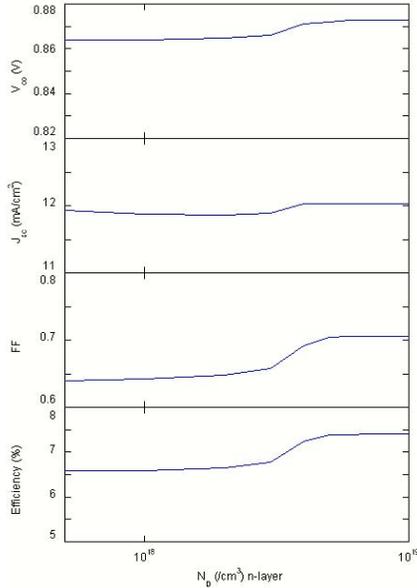


Figure 7. The dependence of a-Si:H solar cell characteristics on the donor doping concentration in n-layer.

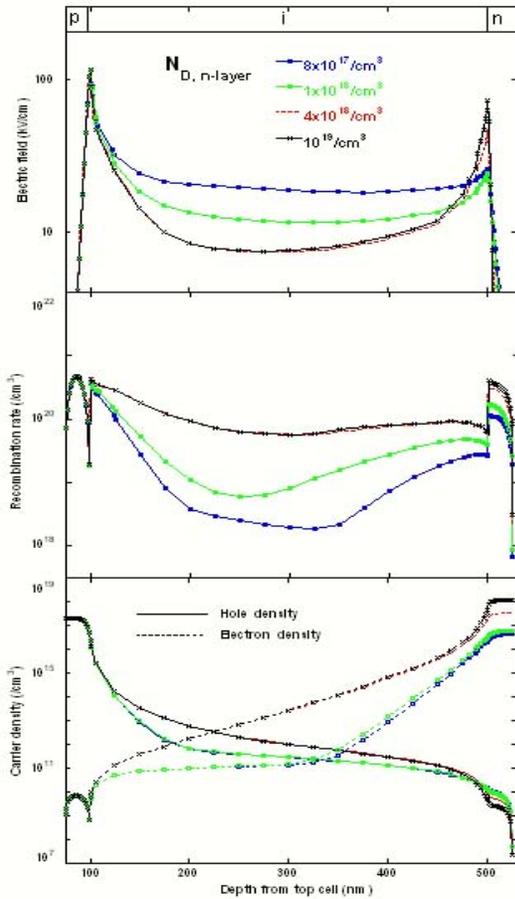


Figure 8. Variation of photovoltaic characteristics of a single junction *p-i-n* a-Si:H solar cell device as a function of n-layer doping concentration

We also have performed the dependence of single junction a-Si:H solar cell efficiency on changing the doping level and defect density in i-layer for the purpose of comparison between AMPS-1D and Sentaurus TCAD.

Figure 9 shows simulation results of both AMPS-1D and TCAD, which are a-Si:H solar cell efficiencies as a function of acceptor level in i-layer varying defect density in absorber layer from 10^{15} to $10^{17}/\text{cm}^3$. The reason why we chose this range of defect density is that N_{DB} about $5-6 \times 10^{15}/\text{cm}^3$ is reasonably accepted as initial defect density in quality film and N_{DB} between 2×10^{16} and $6 \times 10^{16}/\text{cm}^3$ is "stabilized" defect density which is in equilibrium after illumination [10,11]. Electrical and structural parameters used in simulation remains same as baseline parameters in table 1 excluding defect densities of i-layer. Simulation result shows that decreasing N_{DB} clearly shows higher efficiency due to low recombination rate through i-layer.

It also has been reported that truly intrinsic or slight p-type absorber layer has high stabilized cell efficiency than weak n-type absorber layer in which typical a-Si:H film of i-layer shows [10-12]. As shown in the inset of figure 9 (bottom), cell efficiency increases by increasing N_A as close as defect density in i-layer due to the improvement of the carrier distribution through the i-layer although the effect is not significant for our simulation. The results of AMPS-1D and Sentaurus TCAD are in good agreement although there is a little difference in cell efficiency as a result of a different method of light illumination.

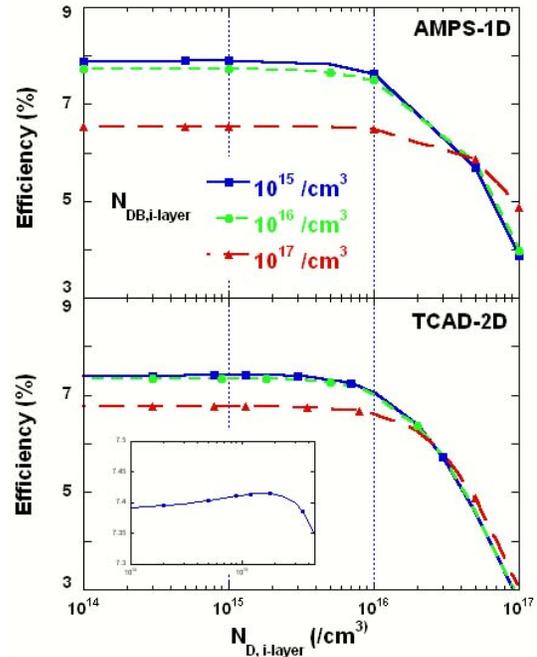


Figure 9. The dependence of a-Si:H solar cell efficiency on the defect density in i-layer as function of acceptor doping concentration in AMPS-1D (top) and Sentaurus-2D (bottom)

CONCLUSION

Results of the first version of a two dimensional computer simulation, which is designed to optimize amorphous silicon solar cells, are presented using the standard density of state model for continuous density of state modeling of dangling bond in amorphous material. Simulation results shows that high doping concentration of the p- and n-layer results high electric field although recombination rate is also high, resulting high carrier density increase short circuit current. In addition, the effect of N_A and N_{DB} in absorber layer on solar cell performance has been analyzed suggesting weak p-type doping of i-layer improvement of stabilized cell efficiency. Simulation results very well agree with one dimensional simulation results in AMPS-1D although there is some value difference caused by different optical modeling.

More advanced versions of the simulator are in progress, with the aim of obtaining optimized cell parameters such as electrical as well as structural parameters.

FUTURE WORKS

Our future works is to perform two or three dimensional computer simulation of single junction micro-/nanocrystalline-Si solar cell in order to find proper models of the nanocrystallinity, columnar grains, and defective grain boundaries in the solar cell. Finally, we will perform computational device simulation on a-Si:H based tandem or multijunction solar cells consisting of $\mu\text{-c}/\text{nc-Si:H}$ layer in order to optimize electrical and structural parameters achieving improvement of cell efficiency as well as stability of the device.

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