Numerical Optimization of nc-SiC/SiO_2 Based Transparent Passivating Contacts in Silicon Heterojunction Solar Cells

Karsten Bittkau[1*], Habtamu Tsegaye Gebrewold[1,2], Kaifu Qiu[3], Uwe Rau[1,2], and Kaining Ding[1]

[1]IEK-5 Photovoltaics, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany
[2]Faculty of Electrical Engineering and Information Technology, RWTH Aachen University 52074 Aachen, Germany
[3]Zhejiang Aiko Solar Energy Technology Co., Ltd, 322009 Yiwu, PR China

*Corresponding author: k.bittkau@fz-juelich.de

SUMMARY OF THE ABSTRACT

Silicon heterojunction (SHJ) solar cells that incorporate transparent passivating contact (TPC), based on nc-SiC:H/SiO_2 layer stack, at the front side are currently under investigation due to their combination of transparency, passivation quality, and conductivity. In this work, the potential performance of those TPC solar cells is modeled and investigated. We coupled the finite-element method-based electro-optical device simulator Sentaurus TCAD to a genetic algorithm approach implemented in Python to optimize the thicknesses of the front layer stack. Starting with a configuration that previously showed in experiment an efficiency of 23.8% and short-circuit current density of 40.9 mA/cm², the optimization of front layer thickness results in 24.1% efficiency.

Moreover, we used the Sentaurus TCAD simulations to further improve the device performance by varying the dopant concentration at the rear-side a-Si:H(p) layer and the rear ITO layer. There, an improved carrier extraction could be shown with an efficiency potential beyond 25%.

A detailed analysis will be shown, highlighting the importance of band alignment and the role of defect and band tail states on charge carrier extraction and passivation quality in the TPC-based SHJ solar cells.

APPLICABLE TOPIC AND SUB-TOPIC NUMBER
Topic 1: Silicon Materials and Cells
Subtopic 1.4: Characterisation & Modelling of Si Cells

This work is a numerical study of silicon heterojunction solar cells that apply transparent passivating front contacts. An optimization pathway and a deeper insight into the physical processes of such devices is given.

EXPLANATORY PAGES

AIM AND APPROACH

Silicon heterojunction (SHJ) solar cells provide high open-circuit voltages (V_{OC}) and fill factors (*FF*) due to the passivation of both sides of the silicon wafer. Therefore, the current world record efficiency (η) in silicon-based solar cells is achieved with SHJ technology. Still, one drawback of this technology is the application of hydrogenated amorphous silicon (a-Si:H) thin films as well as transparent conductive oxides (TCO) at the front contact. Those layers suffer from parasitic absorption of incident light resulting in lower short-circuit current densities (J_{SC}) in SHJ solar cells as compared to other technologies.

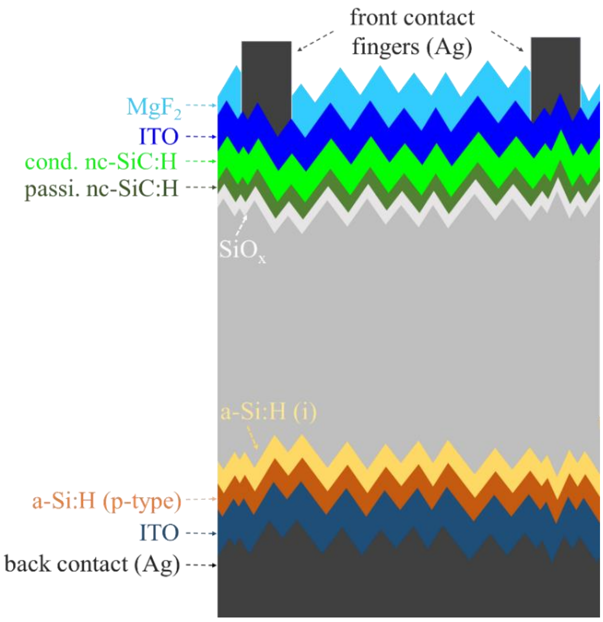

Fig. 1: Layer structure of the SHJ solar cell with TPC front contact.

By replacing the a-Si:H layers at the front contact with a transparent passivating contact (TPC), consisting of a tunneling SiOx layer capped with a nanocrystalline silicon carbide (nc-SiC:H) layer stack (see Fig. 1), it could be shown in previous experimental work that a J_{SC} of more than 40 mA/cm² could be achieved with a conversion efficiency of 23.8%.

This work investigates the TPC solar cell structure numerically by using Sentaurus TCAD and focuses on the further optimization of that structure with the help of a genetic algorithm-based (GA) approach. A detailed analysis of the losses and the physical processes will be outlined.

SCIENTIFIC INNOVATION AND RELEVANCE

Optimizing a solar cell structure is a complex task, as many different aspects interact, partly with contradicting directions. A multiparameter optimization for a full device simulation will lead to huge computational effort. With the help of a genetic algorithm, this effort can be reduced significantly. Within that approach, we considered independently the J_{SC} and the η as fitness parameter in the GA to optimize the front side layer thicknesses, showing different results.

Furthermore, the doping concentration at the rear side p-doped a-Si:H layer and rear TCO layer was varied to investigate their impact on carrier extraction and passivation. A detailed loss analysis and a pathway to achieve efficiency values beyond 25% will be presented. This demonstrates the potential of this type of solar cells.

RESULTS (OR PRELIMINARY RESULTS) AND CONCLUSIONS

In a first step, we optimized the thicknesses of the front layer stack, i.e., MgF_2, ITO, conductive nc-SiC:H, passivating nc-SiC:H. For this, the device simulation software Sentaurus TCAD was combined with a Python-based genetic algorithm. In that GA, each layer thickness is represented as a gen. A set of genes, i.e., a specific layer thickness combination, forms a chromosome, and a set of chromosomes forms a population of a corresponding generation. For each chromosome, the fitness parameter is calculated, which is either the generated J_{SC} or the conversion efficiency of the solar cell. The fittest chromosomes will be selected for crossover and some mutations to create new offspring. These offspring form the population of the next generation. After some generations, the whole population converges toward the optimal thickness configuration. Table 1 summarizes the solar cell parameters of the experimental results, the initial configuration in the simulation (that mimics the experimental results), and the result from the GA-based optimization with respect to J_{SC} (optical) and η (electro-optical).

Table 1: Solar cell parameters efficiency η, short-circuit current density J_{SC}, open-circuit voltage V_{OC}, and fill factor *FF* for the measured solar cell, the initial simulated solar cell, and the optically and electro-optically optimized solar cell.

	η [%]	J_{SC} [mA/cm²]	V_{OC} [mV]	*FF* [%]
Measurement	23.8	40.9	723	80.4
TCAD Model	23.81	40.92	724	80.39
Optical optimization	23.67	41.40	724	78.98
Electro-optical optimization	24.09	41.14	724	80.89

It can be seen in the results that even though the optically optimized layer configuration generates the highest J_{SC} of 41.4 mA/cm², the highest efficiency does not match the highest short-circuit current density. This is due to a reduced fill factor for the layer stack with the highest J_{SC} caused by too thin conductive layers. With optimized layer thicknesses, a gain in efficiency of ~0.3%abs. could be achieved.

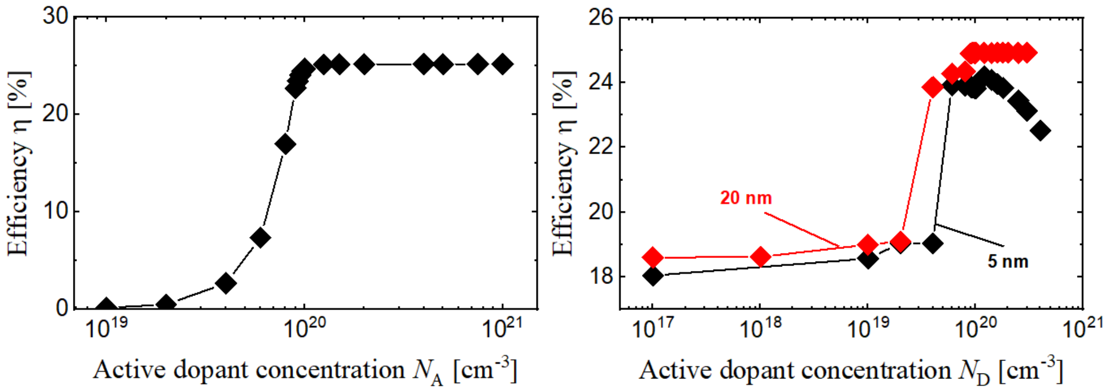

Fig. 2: Power conversion efficiency (η) as a function of active dopant concentration of a-Si:H(p) layer (left) and the rear side ITO layer (right) in TPC-SHJ solar cell for the optimized front contact layers thicknesses. For the ITO variation, a p-layer thickness or 5 nm (black) and 20 nm (red) are compared.

The next step of the optimization is at the rear contact, where the dopant concentration in the p-doped a-Si:H layer as well as in the rear side ITO layer is varied in the simulation model. The results are shown in Fig. 2. The solar cell efficiency saturates at active dopant concentration above 10^{20} cm^{-3} in the a-Si:H(p) layer. This indicates a proper alignment of the valence band of the a-Si:H(p) layer to the conduction band of the ITO above that value. For lower active dopant concentration, however, the defect and tail states in the a-Si:H layers play a stronger role in minority carrier extraction at this contact. Since this is less efficient, it results in less extraction of minority carriers and high surface recombination.

A low active dopant concentration in the ITO layer deteriorates the solar cell performance, similar to the previous case, due to the stronger dependency of carrier extraction on defect and band tail states. At higher carrier concentration in the ITO, a further decrease in efficiency is found after reaching the highest performance. This is due to the negative impact of high carrier concentration on the space charge region and field effect passivation, which can be suppressed by increasing the thickness of the p-doped a-Si:H layer from 5 nm to 20 nm.

According to our computational study, with optimal layer thickness combination at the front side and optimization of carrier extraction at the rear side, a solar cell efficiency above 25% can be achieved. A more detailed investigation will be presented at the conference.