AFORS-HET, AN OPEN-SOURCE ON DEMAND NUMERICAL PC PROGRAM FOR SIMULATION OF (THIN FILM) HETEROJUNCTION SOLAR CELLS, VERSION 1.2

R. Stangl, M. Kriegel, K. v. Maydell, L. Korte, M. Schmidt and W. Fuhs
Hahn-Meitner Institut Berlin, Kekuléstr.5, D-12489 Berlin

ABSTRACT

We offer the open-source on demand Version 1.2 of AFORS-HET, a numerical computer simulation program for modelling (thin film) heterojunction solar cells. It is distributed free of charge by download via internet: www.hmi.de/bereiche/SE/SE1/projects/aSicSi/AFORS-HET

INTRODUCTION

In order to investigate (thin film) heterojunction solar cells, a variety of different experimental methods are used, ranging from standard solar cell characterization techniques like current-voltage (I-V) or quantum efficiency (EQE, IQE) to more advanced characterization techniques like for example surface photovoltage (SPV), photo- or electroluminescence (PL, EL), capacitance-voltage (C-V), capacitance-temperature (C-T), impedance (IMP), intensity modulated photocurrent spectroscopy (IMPS) or electrically detected magnetic resonance (EDMR).

In order to support the interpretation of such measurements, we developed a numerical simulation tool (**AFORS-HET**, **a**utomat **for** **s**imulation of **het**ero-structures). AFORS-HET not only simulates (thin film) heterojunction solar cells, but also the observable of the corresponding measurement techniques. A user-friendly graphical interface allows the visualisation, storage and comparison of all simulation data. Furthermore, arbitrary parameter variations and parameter fits to the corresponding measurements can be performed. Different numerical modules permit to treat different experimental situations, as for example a metal/semiconductor or a metal/insulator/semiconductor front contact, that can be chosen freely.

Up to now, we used AFORS-HET mainly to simulate amorphous/crystalline silicon heterojunction solar cells of the structure TCO/a-Si:H(n)/a-Si:H(i)/c-Si(p)/a-Si:H(p^+)/Al, where ultra-thin layers (5 nm) of amorphous hydrogenated silicon are deposited on top of a thick (300 µm) crystalline c-Si(p) wafer. Experimentally, we realized efficiencies larger than 17% [1]. In the following, we will demonstrate the capability of the program showing selected results on the characterization of these kind of solar cells.

MODELLING CAPABILITIES

An arbitrary sequence of semiconducting layers can be modelled, specifying the layer and -if needed- interface properties, i.e., the defect distribution of states (DOS). Using Shockley-Read-Hall recombination statistics, the one-dimensional semiconductor equations are solved for thermal equilibrium, various steady-state conditions (specifying the external cell voltage or cell current and the spectral illumination) and for small additional sinusoidal modulations of the external applied voltage/illumination.

Thus, the internal cell characteristics, such as band diagrams, local generation and recombination rates, local cell currents, free and trapped carrier densities can be calculated. A variety of characterization methods can be simulated, i.e.: current-voltage (I-V), quantum efficiency (IQE, EQE), surface photovoltage (SPV), photo-electroluminescence (PEL), impedance spectroscopy (IMP), capacitance-voltage (C-V), capacitance-frequency (C-f) and electrically detected magnetic resonance (EDMR). The visualisation and comparison of all simulated data is possible. Furthermore, since version 1.2, arbitrary parameter variations and multi-dimensional curve fitting of simulated measurements to experimental data can be performed.

Other characterization methods and new numerical modules can be implemented by external users (open-source on demand). So far, the following numerical modules have been developed: (a) The front contact can be treated either as a metal/semiconductor contact (Schottky contact) or as a metal/insulator/semiconductor contact (MIS contact). (b) The transport across each semiconductor/semiconductor interface can be modelled either by drift-diffusion currents or by thermionic emission. (c) The optical generation rate can be calculated taking into accout coherent/incoherent multiple reflections. (d) A specific numerical module for crystalline silicon considers impurity and carrier-carrier scattering.

In Version 1.2 external circuits (serial and parallel resistances and serial capacitance) and multi-dimensional curve fitting algorithms (on up to 4 measurements simultaneously) have been implemented. Furthermore, some characterization methods have been improved and new ones have been added (i.e. EDMR).

NUMERICAL INFORMATION

AFORS-HET numerically solves the one-dimensional semiconductor equations with appropriate boundary conditions under steady-state conditions and under additional small sinusoidal perturbations. The set of coupled partial differential equations is transformed into a set of nonlinear algebraic equations by the method of finite differences. Up to now, the grid on which the equations are solved is fixed at the beginning of the calculation (fixed x-discretization, non-adaptive meshing), but can be modified by the user, if needed. The free electron density n_i, the free hole density p_i and the cell potential φ_i at each grid point are used as

independent variables. All other variables in the discretized differential equations and boundary conditions are expressed in such a way that they only depend on these independent variables. The resulting nonlinear equations are solved using the Newton-Raphson iteration scheme thereby requiring a good starting solution. If equilibrium conditions are chosen, AFORS-HET can supply a starting solution from analytical approximations. Otherwise the last calculated solution serves as a starting solution for the new boundary conditions to be solved. Alternatively, starting solutions can be saved and loaded. For detailed information see [2, 3]

With the ability to calculate internal cell characteristics (band diagrams, local generation and recombination rates, local cell currents, carrier densities and phase shifts) under various specified external boundary conditions, measurement methods can be defined by a specific variation of the external boundary conditions and some additional post-processing data analysis.

SELECTED RESULTS

In the following, we will demonstrate the capability of the program showing selected results on the simulation of TCO/a-Si:H(n)/c-Si(p)/Al silicon heterojunction solar cells.

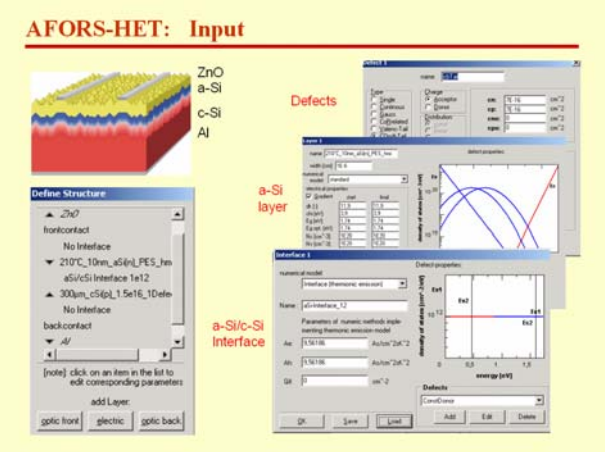

Fig. 1: Screenshots of typical input specifications used for the simulation of TCO/a-Si:H(n)/c-Si(p)/Al heterojunction solar cells. (left) layer sequence, (right) DOS of the a-Si:H(n) layer and the a-Si:H(n)/c-Si interface.

Before the calculation, an appropriate sequence of semiconducting layers and interfaces has to be defined. For the shown example, the corresponding semiconductor properties, namely the a-Si:H(n) thin-film emitter and the c-Si(p) silicon wafer, must be stated. Additionally, the defect distribution of states (DOS) has to be specified for all layers and, if needed, for the interfaces. Furthermore, the boundary contacts have to be specified: For the chosen example, the TCO layer is modelled as an optical layer (specifying the measured reflectivity and absorption). The TCO/a-Si:H(n) contact is assumed to be depleted, whereas the measured barrier height of the contact serves as an input parameter. For the sake of simplicity, the c-Si(p)/Al back contact is assumed to be flatband. Some screenshots of typical input specifications are presented in Fig.1.

The DOS of the a-Si:H/c-Si interface states is assumed to be constant within the bandgap, with a donator/acceptor behavior in the lower/upper part of the a-Si:H band gap, respectively (compare Fig.1).

In order to specify the DOS for the thin film a-Si:H layers, we use photoelectron yield spectroscopy with UV light excitation (UV-PEYS). Thus, the position of the Fermi energy, the density of occupied states in the band gap and the valence band close to the band edge can be measured. Details of the experimental method can be found in [4]. As an example, the measured defect distribution of occupied states for a nominal intrinsic and a n-doped a-Si:H layer is shown in Fig. 2. The measured valence band tail, i.e. the Urbach energy, and the measured occupied dangling bond distribution are used as direct input parameters in AFORS-HET. However, the density of unoccupied states, i.e., the Urbach energy of the conduction band tail, have to be guessed.

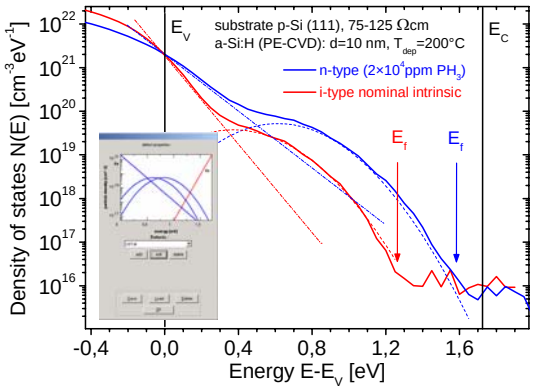

Fig. 2: Measured photoelectron yield spectroscopy data for nominal intrinsic and n-doped a-Si:H. The results are used to specify the defect distribution of states within the thin amorphous silicon layers. The inset shows the corresponding DOS for a-Si:H(n) as used in AFORS-HET.

After the specification of all internal cell parameters, one has to to define the external parameters (temperature, illumination and external cell voltage or cell current through the boundary). Then, the internal cell characteristics (band diagrams, local generation and recombination rates, local cell curents, local free and trapped carrier densities) and the resulting total cell current or cell voltage can be calculated.

As an example, the room temperature equilibrium band diagrams (no illumination, zero external cell voltage) of a TCO/a-Si:H(n)/a-Si:H(i)/c-Si(p)/Al solar cell, assuming two different TCO/a-Si:H(n) barrier heights, V_{bi} of 0 and 0.4 eV, are shown in Fig.3. The TCO/a-Si:H(n) contact critically influences the solar cell performance. If ultra-thin layers of amorphous silicon are used (thickness < 10 nm), a depleted contact changes the band bending in the crystalline silicon absorber (see Fig.3). This will significantly reduce the open-circuit voltage of the solar cell (see Fig.4 and Fig.5).

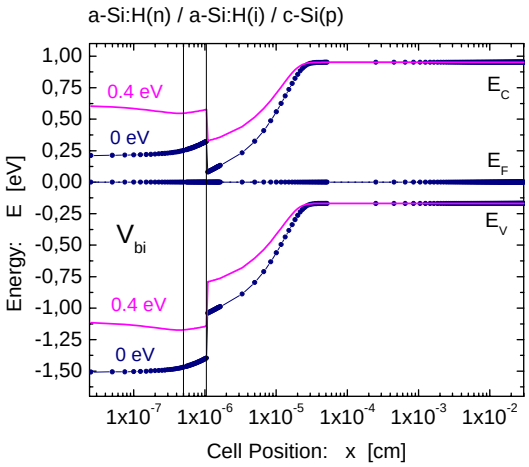

Fig. 3: Simulated equilibrium band diagrams of a TCO/5nm_a-Si:H(n)/5nm_a-Si:H(i)/c-Si(p)/Al solar cell for a TCO/a-Si:H(n) barrier height V_{bi} of 0 eV and 0.4 eV.

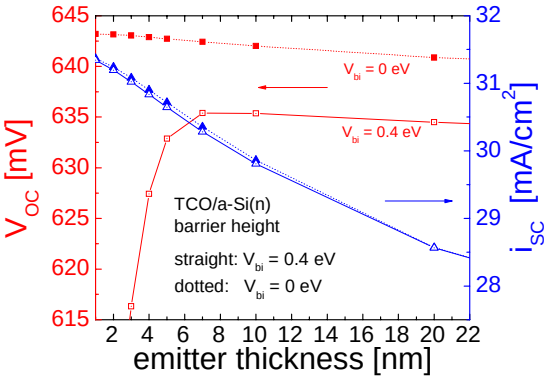

Fig. 4: Simulated open-circuit voltage and short-circuit current of TCO/a-Si:H(n)/c-Si(p)/Al solar cells as a function of the a-Si:H(n) emitter thickness, assuming a TCO/a-Si:H(n) barrier height of 0 eV and 0.4 eV.

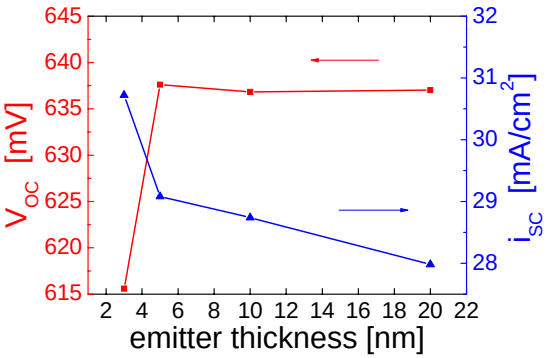

Fig. 5: Measured open-circuit voltage and short circuit current of TCO/a-Si:H(n)/c-Si(p)/Al solar cells as a function of the a-Si:H(n) emitter thickness.

That means, there exists an optimum emitter thickness, depending on the TCO/a-Si:H(n) front contact. A thick emitter, on the one hand, results in a loss in short-circuit current, as the recombination in a-Si:H(n) is quite high. On the other hand, if the emitter gets too thin, there is a significant loss in open-circuit voltage due to the TCO/a-Si:H(n) contact.

This finding is presented in Fig.4, where the simulated open-circuit voltage, Voc, and short-circuit current, Isc, of TCO/a-Si:H(n)/c-Si(p)/Al solar cells are plotted as a function of the a-Si:H(n) emitter thickness. If there is no TCO/a-Si:H(n) barrier height (ohmic contact, V_{bi} = 0 eV), the a-Si:H(n) emitter should be deposited as thin as technologically possible, see Fig.4. However, if a barrier height is assumed, Voc suddenly drops at a certain emitter thickness (see Fig.4). The sudden drop of Voc is also observed experimentally (see Fig.5).

Internal photoemission and surface photovoltage measurements suggest that the TCO/a-Si:H(n) contact is depleted [5, 11]. From the simulation, an optimum emitter thickness of roughly 7 nm is found for V_{bi} = 0.4 eV. For a lower/higher V_{bi} the optimum emitter thickness is accordingly lower/higher, respectively.

As already mentioned, AFORS-HET can also simulate measurement methods, i.e. current-voltage (I-V), quantum efficiency (IQE, EQE), surface photovoltage (SPV), photo-electro-luminescence (PEL), capacitance-voltage (C-V), capacitance-temperature (C-T), impedance (IMP) and electrically detected magnetic resonance (EDMR). If one simulates such a measurement, the external parameters of the program (temperature, illumination, cell voltage or total cell current) are varied in accordance to the specific measurement set-up. Arbitrary internal or external cell parameters are collected and post-processed in order to produce the desired measurement output. Version 1.2 of AFORS-HET is modulized in a way, that other measurement methods can be implemented or personally adapted by external users (open-source on demand).

As an example, the simulation of internal quantum efficiency (IQE) shall be discussed. The IQE is calculated by varying the wavelength of a monochromatic illumination, which is superposed on a specified bias illumination (i.e. the AM1.5 solar spectrum). The increase of the short-circuit current due to the superposed monochromatic illumination is collected as a function of the wavelength. The measurement output of IQE is the amount of electrons driving this additional short circuit current divided by the amount of monochromatic photons being absorbed within the electronic active layers of the solar cell structure.

Fig.6 and Fig.7 show the simulated and measured IQE for TCO/a-Si:H(n)/c-Si(p)/Al solar cells for different a-Si:H(n) emitter thicknesses. Here, the measured reflection and absorbtion loss in the TCO front contact has been used as an input parameter in AFORS-HET. It is also possible to simulate these losses directly, using the advanced optical numeric module of AFORS-HET.

For ultra-thin emitter layers (< 10 nm), the blue response of the IQE increases (see Fig.6 and Fig.7). The effective diffusion length within a-Si:H(n) is therefore on the order of a few nm only.

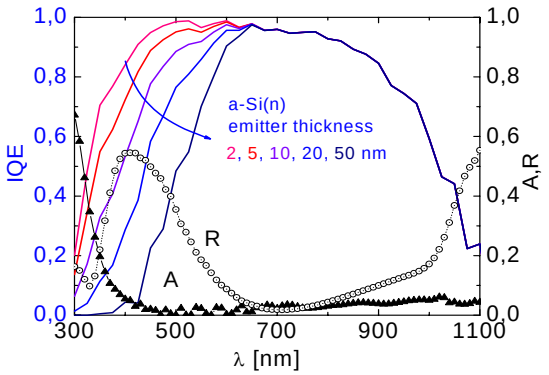

Fig. 6: Simulated IQE of various TCO/a-Si:H(n)/c-Si(p)/Al solar cells, with different a-Si:H(n) emitter thicknesses. The measured TCO front contact reflection and absorbtion loss has been used as an input parameter in AFORS-HET.

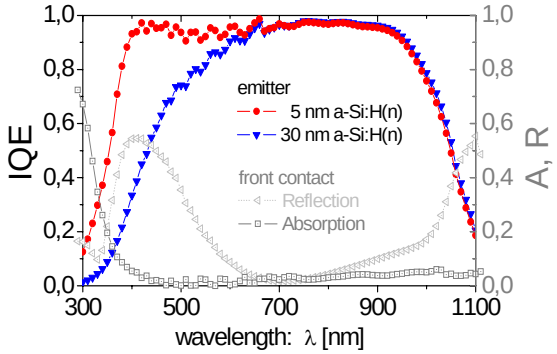

Fig. 7: Measured IQE and TCO front contact reflection and absorbtion loss of TCO/a-Si:H(n)/c-Si(p)/Al solar cells, for two different a-Si:H(n) emitter thicknesses.

CONCLUSION

Up to now, the program AFORS-HET has been mainly used in order (1) to evaluate maximum obtainable efficiencies for amorphous/crystalline heterojunction solar cells, (2) to derive design criterea for those solar cells and (3) to develop measurement methods for monitoring the a-Si:H/c-Si interface recombination and to measure the corresponding a-Si:H/c-Si interface density of states D_{it}. The corresponding results have been published in [6-11]. AFORS-HET will be further developed and is available free of charge via internet. If you want to participate in the development process, please don´t hesistate to contact us under

www.hmi.de/bereiche/SE/SE1/projects/aSicSi/AFORS-HET (please note: this link is case sensitive)

ACKNOWLEDGEMENTS

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