AFORS-HET, VERSION 2.2, A NUMERICAL COMPUTER PROGRAM FOR SIMULATION OF HETEROJUNCTION SOLAR CELLS AND MEASUREMENTS

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ABSTRACT

We offer the new (open source on demand) Version 2.2 of AFORS-HET, a numerical computer simulation program for modeling heterojunction solar cells and measurements. Within this version, several transient state measurements have been implemented. Furthermore, the interface models have been refined and a specific model for crystalline silicon has been implemented, taking the specific temperature and doping dependence of this material into account. Additionally, a multi-dimensional parameter optimization has been implemented, allowing for example to optimize several parameters in order to obtain the maximum solar cell efficiency. AFORS-HET will be distributed free of charge on CD-ROM at the conference site and can also be downloaded 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 or quantum efficiency to more advanced characterization techniques like for example surface photovoltage, photo- and electroluminescence, impedance, capacitance/conductance, photoconductance decay, intensity modulated photocurrent spectroscopy or electrically detected magnetic resonance.

In order to support the interpretation of such measurements, we developed a numerical simulation tool (AFORS-HET, automat for simulation of heterostructures). AFORS-HET not only simulates heterojunction solar cells, but also the observables of the corresponding measurement techniques. A graphical interface allows the visualization, storage and comparison of all simulation data. Arbitrary parameter variations, multi-dimensional parameter-fitting and optimization can be performed.

Up to now, we used AFORS-HET mainly to simulate amorphous/crystalline silicon heterojunction solar cells of the structure TCO/a-Si:H(n,p)/c-Si(p,n)/a-Si:H(p,n)/Al, where ultra-thin (5 nm) a-Si:H layers of amorphous hydrogenated silicon are deposited on top of a thick (300 µm) crystalline c-Si wafer. Experimentally, we realized efficiencies up to 19,8% [1].

MODELLING CAPABILITIES

An arbitrary sequence of semiconducting layers can be modelled, specifying the corresponding layer and interface properties, i.e. the defect distribution of states (DOS). Using Shockley-Read-Hall recombination statistics, the one-dimensional semiconductor equations are solved (1) for thermodynamic equilibrium, (2) for steady-state conditions under an external applied voltage or current and/or illumination, (3) for small additional sinusoidal modulations of the external applied voltage/illumination, (4) for transient conditions, due to general changes of the external applied voltage or current and/or illumination. Thus, the internal cell characteristics, such as band diagrams, local generation and recombination rates, local cell currents, carrier densities and phase shifts can be calculated. Furthermore, a variety of characterisation methods can be simulated, i.e.: current voltage (I-V), internal and external quantum efficiency (QE), transient, pulse length, wavelength, intensity and voltage dependent surface photovoltage (TR-SPV, PD-SPV, WD-SPV, ID-SPV, VD-SPV), spectral resolved photo- and electroluminescence (PEL), transient luminescence (TR-PEL, intTR-PEL), impedance/admittance spectroscopy (IMP, ADM), capacitance voltage (C-V), capacitance-temperature (C-T) and capacitance-frequency (C-f), electrical detected magnetic resonance (EDMR) and transient + quasi-steady-state photoconductance decay (TR-PC, QSSPC).

New characterisation 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) front contact modules: metal/semiconductor Schottky- or Schottky-Bardeen- or metal/insulator/semiconductor contact, (b) interface modules: no interface or drift diffusion or thermionic emission semiconductor/semiconductor heterojunction interface, (c) bulk layer modules: arbitrary layer (standard) or layer of crystalline silicon, (d) optical layer modules: Lambert-Beer absorption or coherent/incoherent multiple reflection.

The capability of the program will be demonstrated showing selected results on the simulation of amorphous/crystalline silicon heterojunction solar cells. All figures shown are direct screenshots of the AFORS-HET program.

SELECTED RESULTS

In the following, ZnO/a-Si:H(n)/c-Si(p)/Al solar cell structures are simulated. The influence of the a-Si:H/c-Si interface state density D_{it} on various characterization techniques is investigated.

Input

Before calculation, an appropriate sequence of semiconducting layers and interfaces has to be defined. For the shown example, the corresponding semiconductor properties, namely of 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 modeled as an optical layer (specifying the measured reflectivity and absorption). The TCO/a-Si:H contact is assumed to be a depleted Schottky contact, whereas the measured barrier height of the contact serves as an input parameter. For the sake of simplicity, the metallic c-Si(p)/Al back contact is assumed to be flatband, with a recombination velocity of 10^7 cm/s.

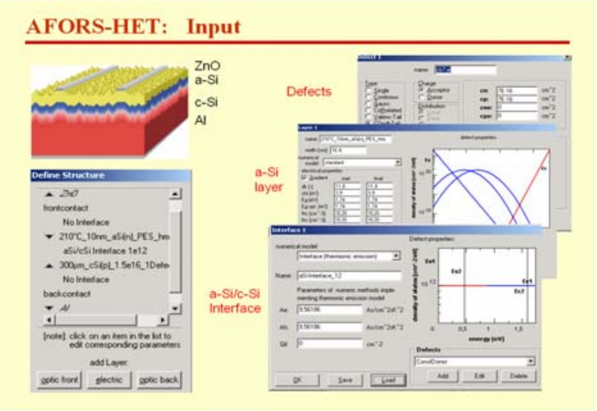

Fig. 1: Typical input specification used for the simulation of ZnO/a-Si:H(n)/c-Si(p)/Al silicon heterojunction solar cells. (left) layer sequence, (right) density of states (DOS) of the a-Si:H(n) layer and the a-Si:H/c-Si interface.

Calculation of cell results

After specification of the external cell parameters (temperature, illumination and cell voltage or cell current) the internal cell results, such as local recombination rates, carrier densities, currents, band energies, etc., can be calculated either under steady-state (DC) conditions or for each time step due to an arbitrary change of the external cell parameters, using the general transient (TR) calculation mode. In case of using small additional sinusoidal perturbations (AC calculation mode) the phase shift and the amplitude ratio of all these quantities can be monitored.

As a simple example, the equilibrium band diagram of a ZnO/a-Si:H(n)/c-Si(p)/Al silicon heterojunction solar cell is shown (Fig.2). If the a-Si:H/c-Si interface state density is in the range 10^{10} cm^{-2} $\leq D_{it} \leq 10^{12}$ cm^{-2}, it does not affect the equilibrium band bending. However, it affects the open-circuit voltage of the solar cell (compare Fig. 3) as long as $D_{it} \geq 10^{10}$ cm^{-2}, thus it cannot be neglected.

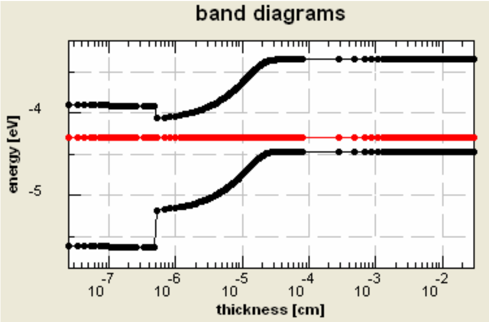

Fig. 2: Equilibrium band diagram of a ZnO/a-Si:H(n)/c-Si(p)/Al silicon heterojunction solar cell.

Parameter variations can be performed, specifying input parameter to vary and output parameter to monitor.

Furthermore, characterization methods (measurements) can be simulated, just by varying external parameters like in a real experiment, and by performing some post processing data analysis with the resulting internal cell results. So far, the following measurement methods have been implemented: *DC-mode characterization methods:* I-V, QE, SPV, PEL, QSSPC, EDMR, *AC-mode characterization methods:* IMP, ADM, C-V, C-T, C-f, *TR-mode characterization methods:* TR-SPV, TR-PEL, intTR-PEL, TR-PC. Other characterization methods may be added or personally adopted by external users (open-source on demand).

Steady-state (DC) characterization methods: current voltage (I-V), photoluminescence (PL)

Varying the external cell voltage at a given illumination, the resulting total cell current can be calculated (I-V). The amount of emitted photons (PL) due to radiative band to band recombination can be calculated from the splitting of the quasi Fermi energies within the cell, using the generalized Planck equation [2].

The solar cell performance of ZnO/a-Si:H(n)/c-Si(p)/Al silicon heterojunction solar cells critically depends on the a-Si:H/c-Si interface state density D_{it}. An interface state density of $D_{it} = 10^{12}$ cm^{-2} reduces the open-circuit voltage of the solar cell by an amount larger than 100 mV, see Fig. 3. Open-circuit photoluminescence proofs to be a fast and non-destructive characterization method, which is quite sensitive to D_{it} and requires no contacting [3]. An increasing interface recombination due to a higher D_{it} quenches the photoluminescence signal, see Fig. 4.

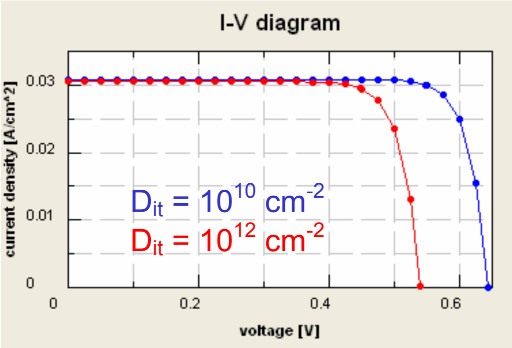

Fig. 3: current-voltage characteristic under AM1.5 illumination of ZnO/a-Si:H(n)/c-Si(p)/Al solar cells with different a-Si:H/c-Si interface state densities D_{it}.

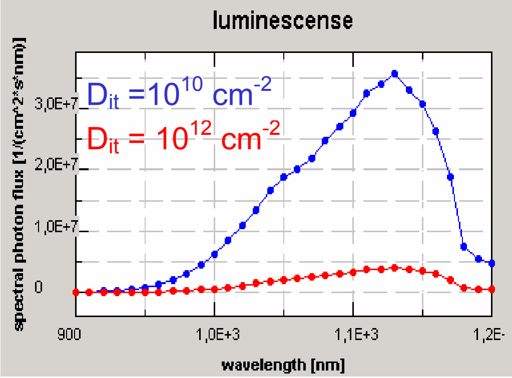

Fig. 4: photoluminescence spectra of ZnO/a-Si:H(n)/c-Si(p)/Al solar cells with different a-Si:H/c-Si interface state densities D_{it}, using a monochromatic excitation at a wavelength of 900 nm and an intensity of 10^{17} photons cm^{-2} s^{-1}.

Sinusoidal (AC) characterization methods: impedance (IMP), conductance (C-T)

Small additional sinusoidal perturbations of the external cell parameters are treated with the help of complex numbers. If a small additional sinusoidal (AC) external voltage signal is superposed to the DC cell voltage, the phase shift and the amplitude ratio between the AC cell voltage and the AC cell current can be calculated as a function of the perturbation frequency. The conductance $G(\omega)$ / capacitance $C(\omega)$ of the system at given frequency ω can be calculated from the real / imaginary part of the AC cell current:

$$G(\omega)=\frac{\mathrm{Re}\{\tilde{j}_{ext}\}(\omega)}{\tilde{V}_{ext}} \qquad C(\omega)=\frac{1}{\omega}\frac{\mathrm{Im}\{\tilde{j}_{ext}\}(\omega)}{\tilde{V}_{ext}}$$

The impedance of a ZnO/a-Si:H(n)/c-Si(p)/Al silicon heterojunction solar cell is also very sensitive to the interface state density D_{it}, if operated under open-circuit conditions [4]. For higher D_{it}, 10^{10} $cm^{-2} \leq D_{it} \leq 10^{12}$ cm^{-2}, the resonance frequency (maximum of the phase shift) is shifted towards higher frequencies, see Fig. 5. Contrary, if operated in the dark or under short-circuit conditions, the sensitivity to D_{it} is low: For example, the temperature dependent conductance in the dark changes only for $D_{it} > 10^{12}$ cm^{-2}, see Fig. 6. This is related to a change of the equilibrium band bending [5].

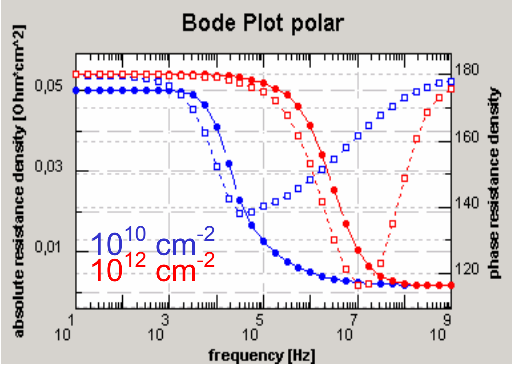

Fig. 5: frequency dependent open-circuit impedance of ZnO/a-Si:H(n)/c-Si(p)/Al solar cells with different a-Si:H/c-Si interface state densities D_{it}.

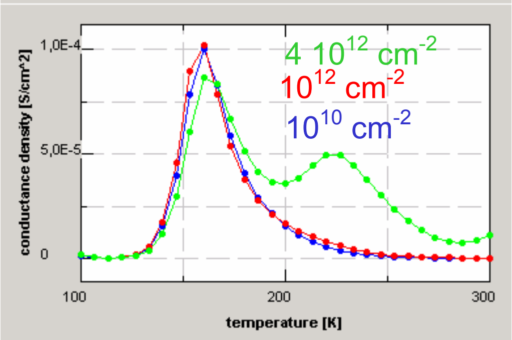

Fig. 6: temperature dependent conductance in the dark of ZnO/a-Si:H(n)/c-Si(p)/Al solar cells with different a-Si:H/c-Si interface state densities D_{it}, using an AC frequency of 10 kHz.

Transient (TR) characterisation methods: surface photovoltage (TR-SPV), luminescence (TR-PL)

The time response of the system due to an arbitrary change of the external parameters can be calculated by loading a transient "*.ttd" file, which specifies these changes. For example, the rise and decay behaviour of the SPV signal or of the spectral integrated PL signal due to a short monochromatic laser pulse can be simulated.

If a monochromatic laser pulse at a wavelength of 900 nm is used to excite ZnO/a-Si:H(n)/c-Si(p)/Al silicon heterojunction solar cells, the excess carrier generation takes place in the c-Si(p) wafer only. Thus the a-Si:H/c-Si interface recombination can be effectively probed. The SPV signal basically monitors the change of surface band bending due to an excess carrier generation / recombination [6], whereas the PL signal is directly related to the excess carrier generation / recombination. If using a 10 ns laser pulse, both signals do not reach steady-state conditions during the pulse. However, the decay behaviour of the two signals takes place in another time domain. It is within the ms range for the SPV decay (Fig. 7) and within the 100 ns range for the PL decay (Fig. 8). Not only the initial values right after the pulse but also the transient decay critically depends on the a-Si:H/c-Si interface state density D_{it} (compare Fig.7 and Fig. 8).

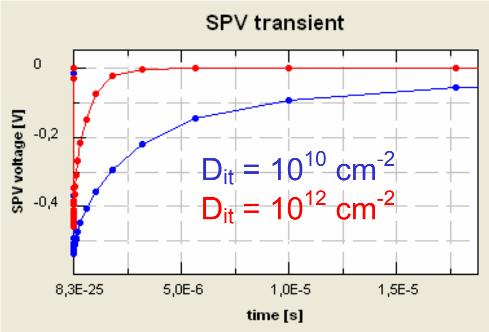

Fig. 7: transient surface photovoltage (SPV) rise and decay of ZnO/a-Si:H(n)/c-Si(p)/Al solar cells with different a-Si:H/c-Si interface state densities D_{it}, using a 10 ns monochromatic excitation pulse, 1 ns steep, 900 nm wavelength and an intensity of 10^{17} photons cm^{-2} s^{-1} during the pulse.

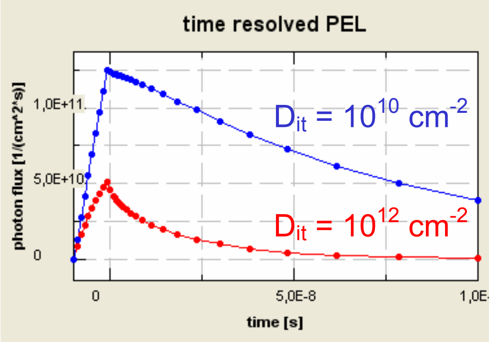

Fig. 8: transient photoluminescence (PL) rise and decay of ZnO/a-Si:H(n)/c-Si(p)/Al solar cells with different a-Si:H/c-Si interface state densities D_{it}, using a 10 ns monochromatic excitation pulse, 1 ns steep, 900 nm wavelength and an intensity of 10^{17} photons cm^{-2} s^{-1} during the pulse.

CONCLUSION

The capabilities of AFORS-HET, Version 2.2, i.e. the new feature of transient mode characterization methods have been described. Up to now, the program AFORS-HET has been mainly used in order to (1) evaluate maximum obtainable efficiencies for amorphous/crystalline solar cells, (2) derive design criteria for these kind of solar cells, (3) develop measurement methods for monitoring the a-Si:H/c-Si interface recombination. AFORS-HET will be further developed (open-source on demand) and is available free of charge via internet.

Acknowledgement

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