

AFORS-HET, Version 2.1, a numerical computer program for simulation of (thin film) heterojunction solar cells

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Abstract: We offer the (open-source on demand) Version 2.1 of AFORS-HET, a numerical computer simulation program for modeling (thin film) heterojunction solar cells. This version now offers a general time dependent (transient state) calculation mode. The time response of the system due to an arbitrary change of the external cell voltage/current and/or illumination can be calculated. It 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/aSiSi/AFORS-HET (note: this link is case sensitive).

Key Words: Simulation, Heterojunction, Experimental Methods, Thin Film.

1 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 electro-luminescence, capacitance/impedance, deep level transient spectroscopy, 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 hetero-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 visualization, storage and comparison of all simulation data. Furthermore, arbitrary parameter variations and parameter fits to the corresponding measurements 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)/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 18% [1].

2 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 arbitrary 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 (IQE, EQE), intensity and voltage dependent surface photovoltage (ID-SPV, VD-SPV), photo- and electroluminescence (PL, EL), impedance spectroscopy (IMP), capacitance-frequency (C-f), capacitance-voltage (C-V), capacitance-temperature (C-T), capacitance/conductance decay (C-t) and electrical detected magnetic resonance (EDMR).

Different numerical modules permit to treat each interface and each layer of the solar cell structure in a different way, in order to account for different experimental situations like using a metal/semiconductor (MS) or a metal/insulator/semiconductor (MIS) front contact.

New measurement 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) MS Schottky- or MIS- front contact interface, (b) drift diffusion or thermionic emission transport across the semiconductor/semiconductor heterojunction interface, (c) coherent or incoherent multiple reflection within the layers in order to calculate the generation rate.

3 Numerical Information

In the following, only the modifications of AFORS-HET, using the improved transient calculation mode, are stated. For general information, see [2,3].

3.1 General transient calculation mode

Arbitrary changes of the external cell voltage or cell current and/or illumination can be specified by loading an external file. The time response of the system during and after the specified perturbations will be calculated. Thus, for example, pulse like illumination profiles can be loaded. Furthermore, small sinusoidal perturbations can be additionally superposed with the transient state. Thus, for example, the transient change of capacitance/conductance due to a pulse like change of the external applied voltage can be calculated. The measurement method of SPV has been expanded in order to account for transient, pulse like laser excitations.

3.2 Defect distribution function

In case of using the transient calculation mode, the Shockley-Read-Hall distribution function $f_i(E, x, t)$, describing the electron occupation probability of each defect, is defined by an extra differential equation:

$$\frac{d}{dt} f_i(E, x, t) = (c_n n(x, t) + e_p(x)) (1 - f_i(E, x, t)) - (c_p p(x, t) + e_n(x)) f_i(E, x, t) \quad (*)$$

n, p are the local electron/hole densities of the conduction/valence band at the position x and time t , $c_{n,p}$ are the electron/hole capture coefficients and $e_{n,p}$ the (thermal plus optical) electron/hole emission coefficients. These differential equations (one for each defect) are solved, using different iteration schemes, which can be chosen by the user:

(a) full explicit calculation scheme, assuming the right hand side of equation (*) to occur at the time point t_i when performing the time discretization.

$$f_{i+1} = f_i + (t_{i+1} - t_i) \{ (c_n n_{i+1} + e_p) (1 - f_i) - (c_p p_{i+1} + e_n) f_i \}$$

(b) full implicit calculation scheme, assuming the right hand side of equation (*) to occur at the time point t_{i+1} when performing the time discretization:

$$f_{i+1} = \frac{f_i + (t_{i+1} - t_i) (c_p p_{i+1} + e_n)}{1 + (t_{i+1} - t_i) (c_p p_{i+1} + c_n n_{i+1} + e_n + e_p)}$$

(c) analytical calculation scheme, by analytical integration of (*), assuming the local particle densities n_{i+1}, p_{i+1} :

$$f_{i+1} = f^{DC}(n_{i+1}, p_{i+1}) - \{ f^{DC}(n_{i+1}, p_{i+1}) - f_i \} e^{-(t_{i+1} - t_i) (c_p p_{i+1} + c_n n_{i+1} + e_n + e_p)}$$

with f^{DC} being the steady-state (DC) distribution function of the final state which is to be reached after all transient perturbations have finished:

$$f^{DC}(n, p) = \frac{(c_n n + e_p)}{(c_p p + c_n n + e_n + e_p)}$$

(d) steady-state calculation scheme as a first approximation for the transient defect distribution function

$$f_{i+1} = f^{DC}(n_{i+1}, p_{i+1})$$

The DC steady state solution of the initial state (before the transient perturbations occur) is used as a starting solution f_{i_0} . Using one of the iteration schemes sketched above, the electron/hole density $n_{i+1}(x), p_{i+1}(x)$ and the potential $\varphi_{i+1}(x)$ is iteratively solved for each time step specified, as described in [2,3]. In case of small sinusoidal (AC) perturbations being additionally superposed with the transient state, the program applies small additional sinusoidal perturbations after each time step. The AC steady-state distribution function is used as a first approximation in order to determine the phase shift and the amplitude of the AC cell current and the AC cell voltage.

4 Selected results

In the following, the capability of AFORS-HET is demonstrated by showing selected results on the simulation of TCO/a-Si:H(n)/c-Si(p)/Al silicon heterojunction solar cells. All figures shown are direct screenshots of AFORS-HET. For a

sufficiently dense time discretization, all calculation schemes sketched above lead to the same results.

4.1 Voc transient due to a pulse like excitation

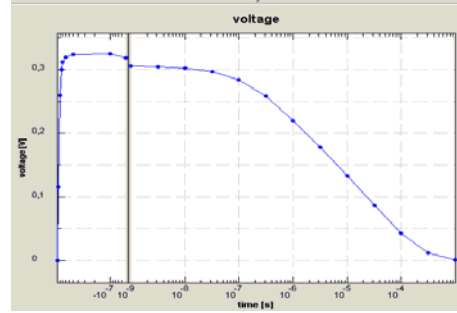


Figure 1: Change of open circuit voltage of an a-Si(n)/c-Si(p) heterostructure, due to a laser pulse, lasting for 1 μ s (monochromatic illumination, 900 nm wavelength, 10^{12} photons $\text{cm}^{-2}\text{s}^{-1}$ during the pulse, $t=0$: end of pulse).

4.2 Capacitance transient due to a voltage switch

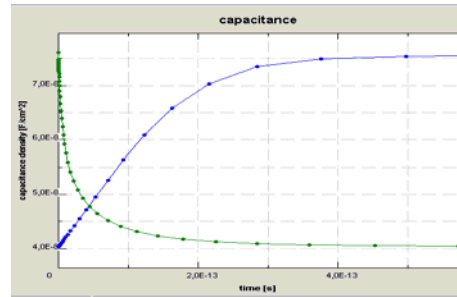


Figure 2: Change of capacitance of an a-Si(n)/c-Si(p) heterostructure, due to a sudden external voltage switch from 0 to 0.5 V (decreasing capacitance) or vice versa (increasing capacitance), assuming one single defect at midgap in c-Si(p).

5 Summary

The new transient-mode capabilities of Version 2.1 of AFORS-HET have been described. The program now allows for arbitrary transient perturbation profiles, like for example a pulse like illumination. In addition, the transient capacitance/conductance decay can be monitored. Up to now, the program AFORS-HET has been mainly used in order (1) to evaluate maximum obtainable efficiencies for amorphous/crystalline solar cells, (2) to derive design criteria for these kind of solar cells, (3) to develop measurement methods for monitoring the a-Si:H/c-Si interface recombination, see references in [3]. AFORS-HET will be further developed (open-source on demand) and is available free of charge via internet.

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7 References

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