Proc. 25nd IEEE Photovoltaic Specialists Conference (Washington D.C., april 1996), pp. 901-904, IEEE, New-York, 1996

NUMERICAL MODELLING OF ac-CHARACTERISTICS OF CdTe AND CIS SOLAR CELLS

Alex Niemegeers and Marc Burgelman
Department of Electronics and Information Systems (ELIS), University of Gent, Gent, Belgium

ABSTRACT

A complete electrical characterisation of thin film solar cells necessitates the analysis of capacitance vs. voltage measurements at different frequencies and illumination intensities. We developed a fully numerical device simulation tool for polycrystalline CdTe and $CuInSe_2$ solar cells, which carries out frequency domain calculations. Numerical simulations of *I(V)* and *C(V)* characteristics of CdTe cells are compared with measurements. It is shown that capacitance voltage measurements not only confirm the thesis that a back contact barrier limits the current at high forward bias - they also yield additional information on the CdTe doping in the vicinity of the contact. The numerical model has also been applied to $CuInSe_2$. We indicate that especially the doping profiles which are deduced from *C(V)* data, may be misinterpreted when interface states are present at the heterojunction.

INTRODUCTION

Electrical characterisation and modelling of polycrystalline thin film solar cells includes the interpretation of admittance data, besides current voltage and spectral response analysis. However, the interpretation of capacitance data is not unambiguous, and often less understood. This complicates the construction of complete, self consistent models for the electrical behaviour of thin film cells. The numerical programs which are presently in use do not offer the possibility to model the ac characteristics of heterojunction cells. We developed the fully numerical simulation program, SCAPS-1D (a solar cell capacitance simulator in one dimension), for polycrystalline thin film heterojunction solar cells. Admittance spectra are calculated straightforward for every dc working point for which the dc algorithm converges. Simulations and measurements of *C(V)* data at various frequencies and illumination intensities illustrate that a correct interpretation of admittance data provides valuable information.

NUMERICAL MODEL

We developed the numerical program SCAPS-1D to improve our understanding of admittance measurements of thin film heterojunction solar cells. The program has been written in C code and runs on a personal computer. First, a dc algorithm calculates the dc solution. Then an ac algorithm calculates the complex admittance from the found dc solution.

Steady state algorithm

SCAPS-1D finds numerical solutions of the system of three coupled differential equations constituting the basic semiconductor equations (Poisson equation and continuity equations for both electrons and holes). The boundary conditions at semiconductor-semiconductor interfaces assume that the transport mechanism across the heterojunctions is thermionic emission [1]. Interface recombination is treated following the Pauwels-Vanhoutte theory, developed in ELIS, Gent [2-4]. Traditional models for interface recombination only consider direct recombination terms, i.e. electrons of a given semiconductor can only recombine with holes of the same semiconductor. The Pauwels-Vanhoutte theory accounts also for possible cross recombination terms. The boundary conditions at the metal-semiconductor surfaces assume a Schottky barrier, thermionic emission for the majority carriers and surface recombination for the minority carriers.
To deal with the numerical problems caused by strongly varying exponential functions, an exponentially fitted, finite difference scheme is used [5]. With N nodes, this results in a non-linear set of 3N equations with 3N variables (electrostatic potential and electron and hole quasi Fermi levels). This system is solved, using a Gummel iteration scheme [5]. Convergence is easily achieved, except for the high injection case (high forward bias).

Small signal analysis

Once the dc solution is found, SCAPS-1D calculates the complex admittance for any frequency. The small signal analysis technique is used. This technique solves a linear set of 3N equations with 3N unknowns (the ac amplitudes of the variables). The coefficient matrix is the Jacobian associated with the dc operating point, with some terms on the leading diagonal supplemented by $j\omega$-terms (where j is the imaginary unit). This system is solved directly (not iteratively) and thus the solution is available for arbitrary frequencies [6]. This method is to be preferred to other methods such as successive overrelaxation, since the latter methods only work for sufficiently low frequencies.

25th PVSC; May 13–17, 1996; Washington, D.C.

Possibilities

The program SCAPS-1D finds dc solutions for structures consisting of an arbitrary number of semiconductor layers, with arbitrary doping profiles (as a function of position), with arbitrary energetic distributions of deep donor and/or acceptor levels (single level as well as a uniform, Gauß or tail distribution) in the semiconductor bulk and at the heterojunction interfaces (surface states), for arbitrary light spectra (e.g. the superposition of monochromatic light and AM1.5G bias light). Admittance spectra (within an arbitrary frequency band) can be calculated for every dc working point (bias voltage, illumination and temperature), provided that the dc algorithm converges.
In the following sections, SCAPS-1D will be applied to CdS/CdTe and $CdS/CuInSe_2$ heterostructures.

CdTe BACK CONTACT

It has been shown that a CdTe back contact barrier may be responsible for the frequently observed "roll over" of the *I(V)* characteristics [7]. Here we show that a Schottky barrier at the back contact explains some more special features of the *I(V)* and *C(V)* curves which we measured on SnO_2/CdS/CdTe/Au cells from ANTEC, Germany [8].

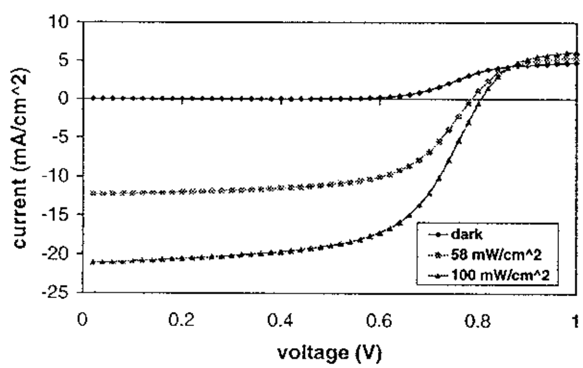

Fig. 1. Measured current vs. voltage of a CdS/CdTe cell from ANTEC for different illumination intensities (AM1.5G spectrum).

I-V curves

Figures 1 shows the light and dark *I(V)* curves of an ANTEC cell, measured in Gent at room temperature. At high forward bias, the current saturates, resulting in "S"-shaped *I(V)* curves. This effect is common in CdTe solar cells, and will be denoted as "roll-over"; it is caused by a Schottky barrier at the CdTe back contact. Besides this roll-over, the *I(V)* curves show another feature which often occurs in CdTe cells, and which will be denoted as "cross-over": at room temperature, the *I(V)* curves corresponding with different illumination intensities all intersect in one point, such that at higher forward bias the illuminated curves lie above the dark curve.

Roll-over

Figure 2 shows the SCAPS-1D simulations of dark and light *I(V)* curves. A good quantitative agreement with the measured *I(V)* curves is obtained with a Schottky barrier height ϕ_B of 0.5 eV (i.e. the energy difference between the metal Fermi level and the top of the CdTe valence band at the contact).

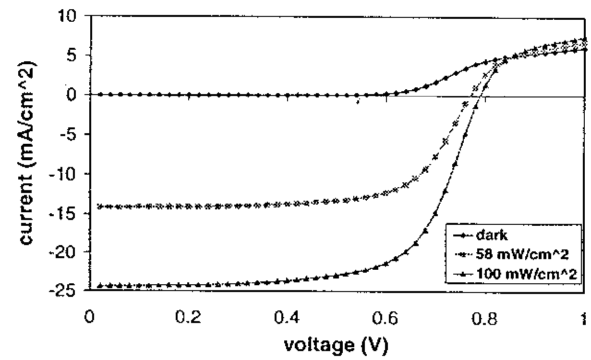

Fig. 2. SCAPS-1D simulation of the current voltage characteristics.

Roll-over can be explained with a two diode model. According to standard theory, the majority carrier current transport through the CdTe back contact diode is limited either by thermionic emission, or by drift and diffusion in the contact space charge layer, or a combination of these. Thermionic emission alone cannot explain the measured slope of the *I(V)* curves at high forward bias (of the solar cell; i.e. negative bias for the contact diode), since a current limited by thermionic emission results in a saturation current independent of voltage at high forward bias. Beyond the roll-over point however, the measured *I(V)* curves show a slope, which decreases exponentially with temperature. The assumption of a shunt conductance at the contact [7] explains the slope of the *I(V)* curves, but not its temperature dependence. It is more satisfying to assume that the current transport across the CdTe back contact is limited by drift and diffusion. In that case, the saturation current is proportional to both the electric field at the metal contact (which depends on the voltage over the contact diode) and the Boltzmann factor $\exp(-q\phi_B/kT)$, explaining the observed voltage and temperature dependence of the saturation current.

Cross-over

A more exotic feature of the *I(V)* curves is the fact that at high forward bias, the illuminated curves lie above the dark curve, and the curves intersect in one point. Simulations with SCAPS-1D indicate that minority carrier (electron) recombination at the metal/CdTe surface may be responsible for this. This electron recombination current is proportional to the illumination intensity, and has to be added to the dark saturation current of the back diode (in other words, at a given voltage, the total recombination current under illumination is higher than in the dark); this is negligible at low bias, but, under certain conditions, it may become comparable to the back contact saturation current at higher bias. An analytical treatment of this effect will be published elsewhere [9].

C-V curves

Simulations point out that the *C(V)* measurements of the same ANTEC cell confirm the assumption that the back contact limits the current at high forward bias.

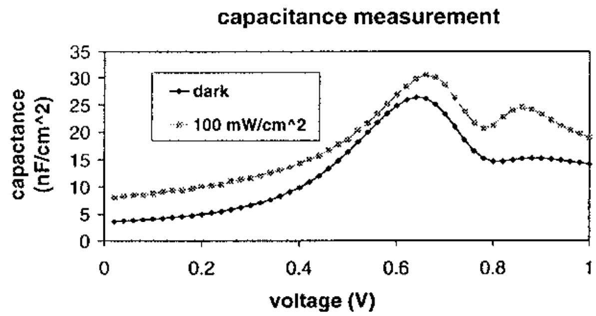

Fig. 3. Capacitance measurement of the same cell as in Figure 1.

Voltage dependence of the dark capacitance

From Figure 3, one can see that at low voltage, the capacitance increases with voltage. It then goes through a maximum, quickly drops and goes through a second maximum. Beyond this second maximum, the capacitance slowly decreases with voltage. Simulations using SCAPS-1D qualitatively give the same results (Figure 4; ϕ_B = 0.5 eV). This behaviour is also explained by the assumption of a back contact barrier. In the dark, when the solar cell is forward biased, the back contact diode is always reverse biased.

At low voltage however, the current is much smaller than the saturation current of the contact diode: therefore, there is no voltage drop over the contact; the applied voltage entirely drops over the CdS/CdTe junction. Consequently, the measured capacitance equals the junction capacitance C_j: it increases with voltage, and the slope of the $1/C(V)^2$ curve is determined by the CdTe doping profile in the vicinity of the CdS/CdTe junction.

At high voltage, the current is limited to the saturation current of the contact diode; the CdS/CdTe junction voltage remains constant, and all additional applied voltage drops over the contact diode. The measured capacitance is then the contact capacitance C_c : it decreases with applied voltage (an increasing forward applied voltage being an increasing reverse voltage for the contact diode), and the slope of the $1/C(V)^2$ curve is determined by the CdTe doping profile in the vicinity of the metal/CdTe contact.

At intermediate voltages, the applied voltage is divided between the CdS/CdTe junction and the contact, and the measured capacitance is the series connection of the junction and the contact capacitances. This series connection is smaller than either of the two capacitances. If the width of the intermediate voltage region is not too narrow, the measured *C(V)* curve will exhibit a minimum between two maxima, as the measured capacitance varies from C_j over (C_j in series with C_c), to C_c.

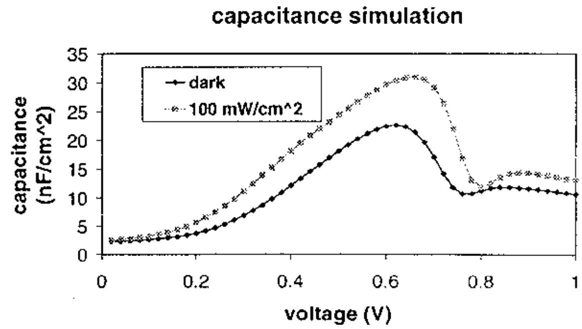

Fig. 4. SCAPS-1D simulation of the capacitance vs. voltage characteristics in the dark and under illumination (the same simulation parameters as for Figure 2 were used).The junction doping profile and the doping concentration in the vicinity of the back contact were deduced from the measurements.

In Figure 5, simulated *C(V)* curves are shown, where the barrier ϕ_B is constant, and the acceptor concentration in the vicinity of the back contact is varied as a parameter. This shows that C(V) measurements at high forward bias can give information about the CdTe doping at the contact .

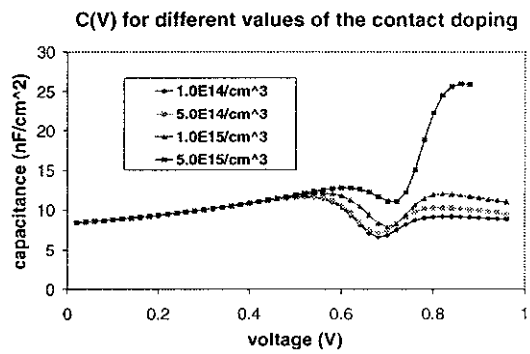

Fig. 5. SCAPS-1D simulation of the capacitance of a CdTe cell. For all curves, the junction doping equals $10^{15}/cm^3$ and the Schottky barrier height 0.5 eV. The parameter is the doping concentration in the vicinity of the back contact.

Light dependence of capacitance

Another feature of the *C(V)* characteristics, correlated with the occurrence of a back contact barrier, is the light dependence of the capacitance. Under illumination, the light current passes through the back contact as a forward current, forward biasing the back contact. For voltages between 0 and 0.6 V, the total cell current is approximately constant (see Figure 1) and equal to the light current . In this voltage region, the back contact is forward biased, and the voltage drop over the contact remains constant (since the current flowing through it remains constant). The applied voltage entirely drops over the junction since the back contact is not limiting the current. It is the junction capacitance that is measured in this region. The voltage over the junction equals the sum of the applied voltage and the voltage drop over the back contact. This means that in the mentioned voltage range, the light *C(V)* curve equals the dark *C(V)* curve, translated to the left (see Figure 4). This effect is more pronounced as the light current becomes larger compared to the contact diode saturation current. It only partially explains the measured light dependence of the capacitance.

INTERFACE STATES AT CdS/CIS INTERFACE

Walter et al. [10] properly stated that the interpretation of doping profiles, deduced from *C(V)* measurements, should be treated with care. They presented a model to explain the role of oxidation on the performance of CdS/CIS solar cells. This model assumes that acceptor like interface states are present at the CdS/CIS heterojunction.

With our SCAPS-1D programme, we simulated a similar junction: we assumed a uniform shallow doping density of 10^{15} /cm^3 in the CIS layer and 10^{17} /cm^3 in the CdS layer, and acceptor-like deep interface states with density 10^{12} /cm^2 (lying in the middle of the interface gap).

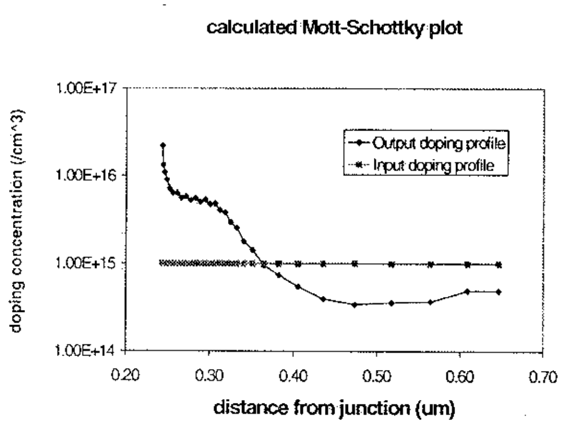

Fig. 6. CIS doping profile, deduced from the slope of the simulated $1/C^2$ vs. V curves. The figure shows a spatially varying doping concentration. However, the absorber was assumed to be uniformily doped.

SCAPS-1D calculated the $1/C^2$ curve and deduced the CIS doping profile from its slope. In contrast to the assumed uniform CIS acceptor density, the apparent acceptor concentration shows a steep rise towards the junction (Figure 6). This phenomenon has to be ascribed to the presence of interface states. We thus indicate that *C(V)* curves can easily be misinterpreted as soon as interface states are present.

CONCLUSIONS

A numerical tool for the simulation of dc and ac characteristics of heterojunction solar cells has been developed. It provides realistic simulation of CdS/CdTe solar cells, explaining some special features such as roll over, cross over and voltage dependence of the capacitance. It can be used for reliable interpretation of doping profile measurement as is illustrated for CdS/CIS cells.

ACKNOWLEDGEMENTS

We acknowledge ANTEC for the supply of the CdS/CdTe cells, the Belgian NFWO (M. Burgelman, research associate) and the Belgian IWT (A. Niemegeers, research engineer).

REFERENCES

[1] S.M. Durbin and J.L. Gray, "Considerations for modelling heterojunction transport in solar cells", *Proceedings of the first WCPEC*, p.1746 (1994).

[2] H. Pauwels and G. Vanhoutte, "The influence of interface states and energy barriers on the efficiency of heterojunction solar cells", *Journal of Physics D: Applied Physics*, vol. 11, p. 649 (1978).

[3] A. Niemegeers, M. Burgelman and A. De Vos, "On the CdS/$CuInSe_2$ conduction band discontinuity", *Applied Physics Letters*, vol. 67, p. 843 (1995).

[4] M. Burgelman, A. De Vos and A. Niemegeers, "Device simulation of polycrystalline heterojunction solar cells", *Proceedings of the 12th European PVSEC*, Amsterdam, p. 1557 (1994).

[5] S. Selberherr, "*Numerical Analysis of Semiconductor Devices*", Springer-Verlag, Wien, p. 150 (1984).

[6] S.E. Laux, "Techniques for Small-Signal Analysis of Semiconductor Devices", *IEEE Trans. on Electron Devices*, vol. ED-32, p. 2028 (1985).

[7] G. Stollwerck and J.R. Sites, "Analysis of CdTe Back-Contact Barriers", *Proceedings of the 13th European PVSEC*, Nice, p. 2020 (1995).

[8] D. Bonnet, H. Richter, K.-H. Jäger, "The CTS Thin Film Solar Module - Closer to Production", *Proceedings of the 13th European PVSEC*, Nice, p. 1456 (1995).

[9] A. Niemegeers and M. Burgelman, to be published.

[10] T. Walter, D. Hariskos, R. Herberholz, V. Nadenau, R. Schäffler and H.-W. Schock , "On the role of oxidation on the performance of Cu(In,Ga)$(S,Se)_2$ polycrystalline thin film solar cells", *Proceedings of the 13th European PVSEC*, Nice, p. 1999 (1995).