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Special Issue

Modeling Thin-film PV Devices

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Numerical modeling is increasingly used to obtain insight in to the details of the physical operation of thin-film solar cells. Over the years several modeling tools specific to thin-film PV devices have been developed. A number of these tools have reached a mature status and are available to the PV community. Some of the most commonly used programs are presented and the possibilities as well as the shortcomings are discussed. Also, for the different thin-film PV devices (CdTe, CIGS, and, to a lesser extent, amorphous silicon and nano-structured solar cells) an overview is given of modeling efforts and achievements. Copyright © 2003 John Wiley & Sons, Ltd.

INTRODUCTION

Numerical modeling of thin film solar cells evolved from a rather exotic research topic in the early 1980s, to a mature research field and an accepted practice at present. A driving force for this development is the complicated structure of thin-film PV devices. A variety of measurements has been presented to obtain information concerning the internal optical and electronic operation of these cells. However, interpretation of these measurements is often difficult, because of the lack of precise models. Only under certain assumptions and simplifications are analytical descriptions possible. Numerical modeling is a necessity for the realistic description of thin-film PV devices.

In this article, we will present a selection of currently available numerical simulation tools for thin-film solar cells, and discuss their possibilities and limitations. Afterwards, some results obtained with numerical simulation will be presented. We do not claim to give here an exhaustive overview. The aim is to illustrate the purpose and the accomplishments of numerical simulation with some older and recent examples. These examples could provide some guidance to answer some key questions on numerical modeling of thin-film solar cells. Why numerical modeling? Why it is not (yet?) standard for thin films? Are the modeling results realistic? Which models are possible, relevant, necessary? Can numerical simulation lead to better insight into the details of the physical operation of a thin film cell structure? Can the results be trusted? Are numerical experiments relevant as an alternative to real experiments? Can numerical simulation point to critical parameters for the cell performance? Can numerical simulation give hints, or better, recipes for improvement of the cells? Does numerical simulation lead to better cells? Can numerical simulation alone do this job?

NUMERICAL SIMULATION PROGRAMS FOR THIN-FILM PV

Three-dimensional, numerical simulation is now almost indispensable for the design of silicon devices, from discrete transistors and optoelectronic devices to large-scale integration. Highly developed programs include, e.g., tunneling, optics, heat flow and other features. Numerical simulation is routinely performed in developing

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and studying crystalline silicon cells. Amongst the various programs in use, PC1D[1] is more or less a standard in the field. Physical device modeling in thin-film photovoltaics is less developed than for crystalline silicon PV, owing to the more complicated physics involved.

In principle, any numerical program capable of solving the basic semiconductor equations could be used for modeling thin-film solar cells. The basic equations are the Poisson equation and the continuity equations for electrons and holes. The recombination terms, contained in the continuity equations make the problem non-linear.

An ideal thin-film solar cell simulation program should in addition meet all the requirements listed in Table I. It must allow for multiple semiconductor layers; six layers should be considered as a minimum number. It should handle correctly graded materials, in which not only the bandgap E_g, but also other parameters vary with the position x along the depth axis of the device: the electron affinity χ, the effective density of states N_C and N_V, the optical absorption α, ... An alternative to the handling of $E_g(x)$, ... profiles, is to define multiple homogeneous layers; the programs should then allow for several tens of layers. The program should describe correctly the possible discontinuities in the energy bands E_C and E_V at the interface between the layers. The effect of deep energetic states, both in the bulk of the semiconductor layers and at the interfaces, should be treated completely, i.e., both the recombination and the charge contained in these states should be accounted for. Simulation of the relevant electro-optical measurements commonly carried out on thin film solar cells should be possible, this is: not only the *J–V* characteristics, but also the spectral response $Q(\lambda)$ and the capacitance measurements *C–V* and *C–f*, surface photovoltage (SPV), Kelvin probe, transient measurements of current, of voltage, of capacitance (including DLTS), preferably all these as a function of ambient temperature. Also, it should provide convergence at least for the most common thin-film cell structures at normal working conditions. The occurrence of large-bandgap materials in typical thin-film cells can cause problems in this respect. The capability of handling various tunneling mechanisms is becoming increasingly relevant. Finally, when the simulation is fast and user-friendly, a short learning time and the possibility of interactive usage are appreciated benefits.

We confine ourselves here to a few one-dimensional programs, readily available to the PV research community, which have been used for numerical simulation work in thin-film solar cells of various types.

AMPS

AMPS (Analysis of Microelectronic and Photonic Structures) was written by S. Fonash and coworkers of Pennsylvania State University.[2] It was engineered to be a very general and versatile computer simulation tool for the analysis of device physics and for device design. The following discussion is based on the Beta. 1·0 version (1997) for the operating system Windows 95 or higher.

With AMPS it is possible to work on several problems simultaneously, and each device (or case as it is called in AMPS) is shown in a separate window. Defining a new problem is an easy task, thanks to a clean and intuitive user interface. In case of doubt the user can rely on the well-written help function. A single device can have up to 30 layers, each layer having its own set of parameters. All parameters (bandgap, effective density of states, mobilities) are independent of temperature. To each layer a total of 50 deep donor and acceptor levels can be assigned, resulting in the possibility of creating an almost arbitrary density of states distribution. The deep

Table I. Critical issues for a thin film PV simulation program

Multiple layers
Band discontinuities in E_C and E_V: ΔE_C and ΔE_V
Large bandgaps: $E_g > 2$–$3{\cdot}7$ eV
Graded bandgaps: $E_g(x)$ and also $\chi(x)$, $N_C(x)$, $N_V(x)$, $\alpha(x)$, ...
Recombination and charge in deep bulk states
Recombination and charge in deep interface states
Simulation of non-routine measurements:
J–V, *C–V*, *C–f*, $QE(\lambda)$, ... all as a function of T
Fast and easy to use

levels can be energetically distributed in the forbidden zone (discrete, uniform or gaussian). In addition it is possible to define exponential band tail states. All properties of a layer are spatially uniform. By adding different layers with gradually changing parameters, however, it is possible to simulate graded junctions.

An issue of AMPS is that wavelengths and corresponding absorption coefficients and spectrum intensities have to be entered manually. The ability to load these parameters from an external file would greatly enhance the user-friendliness of the program. Another downside of AMPS is the limited number of discretization nodes. In the version under discussion this number is 400, which is not enough, particularly when one considers the large number of layers that can be used. A new version of AMPS that can handle up to 3000 nodes is announced at their website.[2] Other new features will be the inclusion of amphoteric states and direct tunneling.

When the definition of the device is completed, the user can choose to simulate $J(V)$ in both light and dark conditions as well as spectral response measurements. Once the case is submitted to the queue, all characteristics will be calculated, and after completion they are saved together with the definition of the device. AMPS is slow in solving the problem when compared with other simulation programs. Therefore it does not encourage an interactive use of the program. The ability to solve several cases simultaneously, combined with a remarkable stability, makes this program more suitable to use in a batch mode.

Once the results are calculated, they can be analyzed with the excellent built-in plotting facility. Simulations with different excitation parameters on a single device, or simulations on different devices can be compared.

A future version of AMPS will include direct tunneling and amphoteric states.

SCAPS

This numerical simulation program is written and maintained at the University of Gen.[3,4] It is designed as a general polycrystalline thin-film device simulator and is mainly used for modeling CdTe- and CIGS/CIS-based solar cells. The discussion is based on version 2·3 for the operating system Windows.

Entering a new problem into SCAPS is straightforward. Up to seven layers can be added to the device and for each layer or contact all physical and electronic properties can be shown and altered inside a separate window. Simple models are used for the temperature dependence of the effective density of states and the thermal velocity, other parameters such as the bandgap and the mobilities are independent of temperature. For each layer up to three deep levels can be defined and in between three layers up to three interface states can be placed. These deep levels can be energetically distributed in the forbidden zone (single level, uniform, gauss or exponential tail). The deep bulk levels can also vary spatially inside the layer (uniform, step, linear or exponentially). All other properties are spatially uniform for each layer and thus several layers must be used if one wants to introduce graded junctions in the device. However, since only seven layers can be defined, this program is not very suitable for graded junctions.

Recombination in deep bulk levels and their occupation is described by the Shockley–Read–Hall (SRH) formalism. Recombination at the interface states is described by an extension of the SRH formalism,[5] allowing the exchange of electrons between the interface state and the two adjacent conduction bands, and of holes between the state and the two adjacent valence bands.

Excitation parameters are displayed in a separate window, together with the parameters that are necessary for defining the measurements. SCAPS has among the studied simulation programs the largest number of electrical measurements that can be simulated: $J(V)$, $C(V)$, $C(f)$ and spectral response. Each measurement can be calculated for light or dark conditions and as a function of temperature. When solving the desired simulations, the energy band diagram and the charge and currents in the device are shown on screen for each intermediate bias voltage or wavelength. These intermediate solutions can then be saved to a file. When the simulation is completed, the characteristics can be viewed and compared with characteristics from other simulations. This feature makes SCAPS a very interactive program.

ASA

ASA (Amorphous Semiconductor Analysis) was written by M. Zeman, M. Kroon, J. van den Heuvel and others at the Delft University of Technology.[6] It is especially designed for amorphous silicon devices. The following discussion is based on version 3·3 for Windows. Versions for other operating systems are also available.

ASA is the only program discussed here that does not use a graphical user interface for the definition of the problem. In the other programs all cell parameters are shown in windows and can be altered by clicking in the appropriate field. In ASA the problem is defined by writing commands in an ASCII input file. Each command starts with a keyword and is followed by the parameter value. This approach makes ASA far from intuitive. It is difficult to start a new problem from scratch and, even when starting from the default problem file, the manual is often needed.

On the other hand, ASA is a very flexible program. The number of layers as well as the number of discretization nodes is large compared with the other programs. Most parameters can have a spatial distribution inside each layer. Effective density of states, doping densities, mobilities, etc., can be constant in space, graded linearly or exponentially, or can be read from an external file. Since ASA is developed for amorphous silicon, specific recombination models are used. In each layer tail states for both conduction and valence band can be defined. Recombination via these states is calculated with the SRH model. Furthermore, it is possible to define a distribution of amphoteric dangling bond states in the band gap. The recombination–generation statistics for these states is described with the Sah and Shockley model.[7] The Hurkx model[8] for trap-assisted tunneling and a model for enhanced carrier transport in high-field regions are also implemented. Recombination due to dopants or impurities is solely defined by lifetimes, thus no space charge is connected with these deep levels (space charge however is connected with the amphoteric levels).

To simulate a certain measurement, commands have to be entered in the input file. The measurements that can be simulated are $J(V)$, spectral response and $C(V)$ measurements, in light or in dark. ASA also calculates reflection and transmission spectra and it can treat surfaces with multiple smooth and rough (or textured) optical layers. It is allowed to have several simulation commands in a single input file and to change parameters between simulations. It is for example possible to calculate a number of $C(V)$ measurements at different temperatures in one run. Comparing results within the program, however, is not possible, because only one plot can be viewed at once. ASA is therefore more suitable to be run in a batch mode rather than interactively.

PC1D

This program by Basore and coworkers was originally written at Sandia National Labs[9] and was further developed at UNSW, Australia.[1] As it is considered a standard for crystalline Si cells, it is widely spread in the PV research community, and hence also used for thin-film cells, though it is not particularly designed for those cells.

PC1D has a very clean user interface and defining a new problem is simple. For each layer and contact in the device there is a parameter list displayed on screen and, by clicking on a parameter, its value can be altered. Alternatively, the parameters can be changed through a menu system or simply by clicking on the appropriate layer or contact in a schematic diagram of the device, also displayed on screen.

Being originally developed for (poly)crystalline silicon cells the number of layers is rather limited, only five layers are allowed per device. For CdTe/CdS-based devices this is probably enough provided that the doping of the layers is not graded, but for CIGS based devices this number is almost certainly too low.

All of the most common recombination mechanisms are implemented: Auger, band-to-band and trap-assisted tunneling (Hurkx model).[8] It is not possible to define a general DOS distribution; only one deep level can be specified per layer by giving its position in the forbidden zone and the lifetimes for electrons and holes. Because no densities of deep levels can be given, there is no space charge connected with these levels. This is a problem when modeling II-VI and a-Si solar cells, where the charge contained in deep states can play an essential role.

Besides the standard $J(V)$ and spectral response measurements, transients can also be simulated. Light or bias voltage can suddenly be applied and the effect on the device can be monitored as a function of time. The results of the simulations can be viewed in a separate window and the data can easily be copied and pasted in external programs such as spreadsheets.

Comparison

All the aforementioned programs start from the same equations, but do they lead to the same results? To test this, one needs to enter the same problem and simulate the same measurements in all the programs. This is not

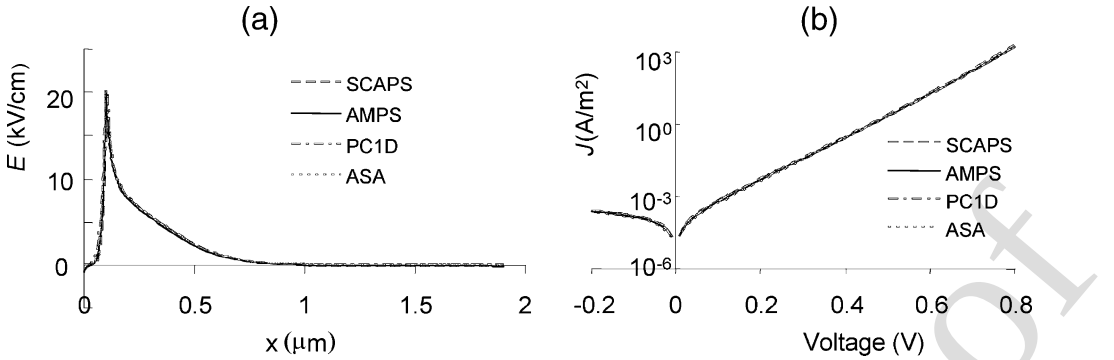

Figure 1. Comparison of simulation results by different simulation programs of a simple test case (an n^+p CdS/CdTe cell with one level of deep states, see text): (a) electric field $E(x)$ when cell is at its maximum power point; (b) dark J–V curves.

an easy task, because each program uses different parameter sets and especially the way impurities and deep dopants are defined differs substantially. Nonetheless, it is interesting to do the exercise, and even a simple example will give an idea about the agreement in results.

The problem under investigation is a CdTe/CdS-like solar cell, with an n^+-type window (bandgap 2·4 eV) and a p-type absorber (bandgap 1·4 eV). The dominant recombination mechanism in the absorber is recombination through one discrete deep defect lying at the intrinsic energy level. The bands are held flat at the back and the front contact. In Figure 1(a,b) two different simulation results are shown. The four curves almost coincide, so it is clear that for this simple example agreement between the programs is very good. Simulations of more complex problems, having more layers, more defects and rectifying contacts, generally continue to agree well, however extreme care must be taken when defining these problems. Critical issues are the way the discretization nodes are placed and the definition of the contacts.

Other programs

Many other numerical simulation programs than those discussed here are in use. SimWindows[10] is a freely available one-dimensional drift/diffusion simulator for semiconductor devices. It can handle tunneling and incorporates internal heat generation in its calculations. ADEPT-F from the group of Jeff Gray, Purdue University[11–13] has been widely used. A version for the Windows operating system is to be issued shortly. The program ASPIN of the University of Ljubljana[14] has been used for CIGS cells and for a-Si cells. A graphical user interface is under construction, and the electrical simulation program will be integrated with the optical modeling of the same group.[5] Recently AFORS-HET was presented by a group of the Hahn-Meitner Institute of Berlin.[16] Other programs were listed by A. Fahrenbruch at a recent NCPV Workshop.[17] Some of these are expensive commercial programs used in silicon microelectronic industry; though in principle also usable for solar cells, they are specially developed for microelectronic devices, and some also implement simulation of Si wafer processing. They often offer true multi-dimensional (two- or three-dimensional) simulation.

Polycrystalline thin-film solar cells properly require the use of two- or even three-dimensional programs because of grain boundaries and non-planar interfaces. Grain boundary effects seem to be more prominent in CdTe cells than in CIGS cells. Though one-dimensional problems effectively average the effect of grain boundary states over the bulk, they have been surprisingly successful. Also, transition to two or three dimensional will increase substantially the number of input parameters, many of which are presently not well known. In a simpler approach, pseudo-two-dimensional simulation is obtained by combining one-dimensional physical simulation, e.g., with one of the programs discussed here, with network-like (SPICE) treatment of other dimensions. In its simplest form, such a two-dimensional program treats the monolithic series integration of thin film cells in a module by lumping all the physics of the 'elementary unit cell' in one exponential diode law, to be specified by the user. While the direct link with cell physics is lost in this way, there is a tremendous gain in speed and interactivity when it comes to designing the series integration. An example is the Module Design

Table II. Some simulation programs for thin-film PV

	AMPS	SCAPS	ASA	PC1D
Maximum number of layers	30	7	Unlimited	5
Band discontinuities ΔE_C, ΔE_V	All programs use the Anderson model: $\Delta E_C = \Delta\chi$ and $\Delta E_V = \Delta\chi + \Delta E_g$			
Graded bandgaps	No	No	Yes	No
Deep bulk states	50	3	4	No charge
Deep interface states	No	Yes	No	No
Charge in deep states	Yes	Yes	Yes	No
Simulation of non-routine measurements	No	C–V C–f	C–V	Transients
Numerical robustness (convergence)	++	OK	++	OK
Speed	−	+	++	++
User friendliness, interactivity	+	++	−	++

Simulator.[18] A similar network approach, combined with an analytical effective medium model, was used by Karpov *et al*. to simulate the effect of nonuniformities and small-area defects.[19]

In Table II, some features of the simulation programs described in Sections 2·1 to 2·5 are summarized. Though none of the programs described perfectly matches all the criteria of Table I, all of them are very useful in modeling thin film solar cells. It is no surprise that they perform better for the materials and types of problems they were originally designed for.

SIMULATION OF THIN-FILM SOLAR CELLS: RESULTS

CdTe solar cells

Preliminary simulation work was done by Lee[20,21] in which the adverse effects of several recombination mechanisms was looked at (CdS/CdTe interface, grain boundaries). In recent work,[22] some starting simulation parameters for the CdTe solar cell modeling were described (a CdTe-baseline) as well as for the CIGS cell. A nice simulation study by Fahrenbruch[23] describes the role of the thin (0·1 μm) CdS layer between the TCO and the CdTe. It shows that the high electric field and the low hole density, present in the CdS, reduce the recombination in its bulk and at its interfaces. Moreover, from comparison with measured samples, it follows that the CdS/CdTe interface behaves better than a TCO/CdTe interface in terms of recombination.

Most of the numerical simulation on CdTe solar cells is focused on the anomalous behavior of the $J(V)$ curves at forward bias: so-called roll-over and cross-over. While these effects are mainly seen at voltages above V_{oc}, their origin should be described correctly in order to predict the influence on the cell efficiency. The first contributions to explain the roll-over phenomenon always started from analytical expressions referring to the blocking back contact on the *p*-type CdTe in series with the principal CdS/CdTe junction.[24] An analytical model was suggested by Niemegeers[25] capable of explaining a cross-over behavior: an extra current contribution of minority carriers (electrons) across the back contact under illumination. This kind of behavior is seen in simulations,[26] and also in the case of highly doped CdTe with high back-contact barrier.[27,28] Some special cases are also illustrated: McMahon[28] illustrates an example of an S-shaped curve and Fahrenbruch[27] demonstrates how the predicted back-contact barrier is no longer present in the case of a thin and lowly doped CdTe.

Measurements on various CdTe cells, however, showed that the cross-over effect has some more specific features: (1) extra current under illumination, which is too high to be simply an extra current created through illumination; (2) wavelength dependence; and (3) time dependence. These features led to a series of new models. In all these models, the first feature is explained in terms of a current transport mechanism which is changed under illumination (going from a lowering of resistivity in a certain region to the hindering of a certain recombination path). The effect is seen clearly in apparent *QE* measurements at forward bias, resulting in values above unity. The second feature stressed the importance of different regions of the CdTe cell (CdS layer, region near back contact,). The third feature points in the direction of deep defects, with slowly varying occupation (its modeling asks for a time-dependent approach). The anomalies in the *QE* curves at forward bias, seen in measurements of

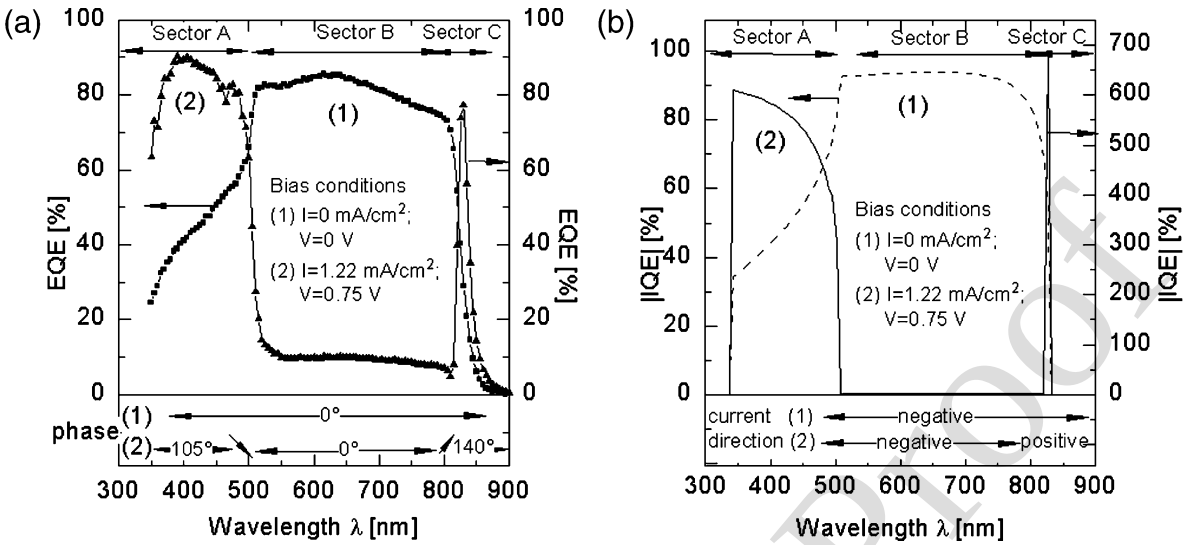

Figure 2. Measurement of external QE (a) and simulation of internal QE in SCAPS (b) of QE at 0 V and 0·75 V for a CdTe solar cell. Extra information on the cell and simulation parameters is available elsewhere[29]

Antec cells, were described by introducing the change of charge state of deep defects in CdS (effect at $\lambda < 520\,\text{nm}$) and CdTe (effect at $\lambda \simeq 850\,\text{nm}$)[29,30] (Figure 2). A model based on measurements on BP cells was proposed by Agostinelli.[31,32] The model uses a light-dependent bulk barrier, formed by an intrinsic CdS between the ITO and an *n*-type CdTe layer (effect at $\lambda < 520\,\text{nm}$).

The fact that in the CdS/CdTe simulations the fill factor gets too low when trying to reach the measured V_{oc} (by including extra recombination centers) has been mentioned by Fahrenbruch,[27] and a solution was suggested by using an intermixing CdS_xTe_{1-x} region.

CIGS solar cells

The bandgap of the $Cu(In,Ga)Se_2$ absorber depends on the Ga to In ratio, and can be varied between 1·02 eV (pure $CuInSe_2$) and 1·68 eV (pure $CuGaSe_2$).[33] This makes the CIGS cell suitable for bandgap grading. Simulation software can help to predict the optimum bandgap profile. The beneficial effects of bandgap grading were investigated by T. Dullweber *et al.*[33–36] It was found experimentally that back-surface bandgap grading could improve the efficiency of the cell and these results were verified by numerical device modeling.[35] The effects of bandgap grading at the junction were also considered, both experimentally and numerically.[36] It was concluded that V_{oc} depends on the bandgap at the junction while J_{sc} depends on the minimum bandgap in the absorber, so it should be possible to optimize both V_{oc} and J_{sc} independently of each other. A theoretical study on bandgap grading, using AMPS, was also presented by C.H. Huang.[37] A variety of bandgap profiles (not graded, single-graded and double-graded band gaps) were simulated and the solar cell characteristics were considered. The best efficiencies were obtained for cells with a thin inverted surface layer at the junction and a bandgap gradient at the back surface.

Another interesting topic of recent CIGS research is the influence of the heterojunction interface properties on cell characteristics. Guidelines for an efficient heterojunction solar cell were found by R. Klenk,[38] using SCAPS, hereby numerically confirming conclusions from earlier work by Pauwels and Vanhoutte.[5] Johnson *et al.*[39] compared CIGSS cells with a CdS window and cells with a Cd-doped CIGS surface (Cd PE, 'partial electrolyte'). Experimental *J–V* curves were fitted with AMPS, resulting in information about the deep defect distribution in the absorber (see Figure 3).

Rau and Schmidt[40] discussed the role of the intrinsic ZnO layer on the device performance. Although the addition of such a layer is less favorable for the band alignment, it is seen that the cell characteristics do

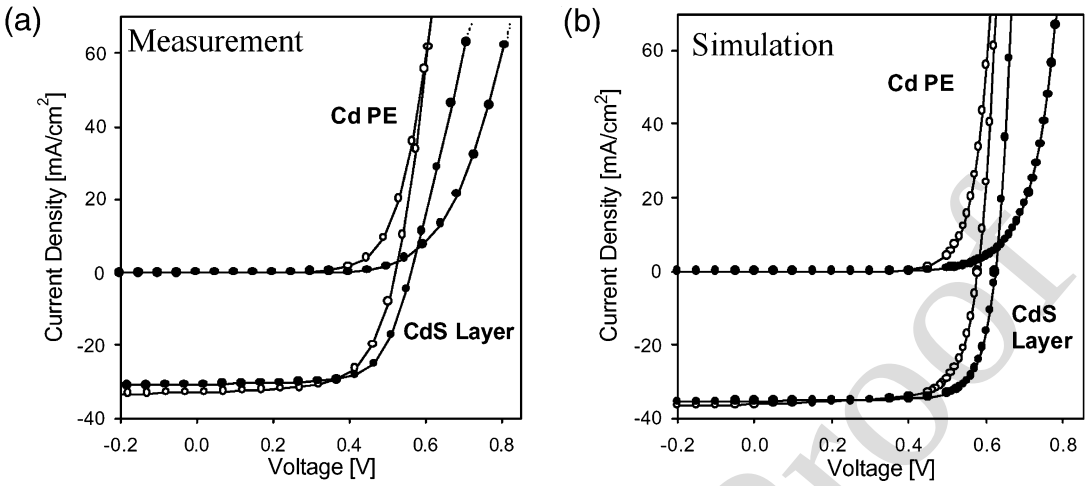

Figure 3. *J–V* characteristics of a Cd-PE ('partial electrolyte') device (open symbols) and a device with a CdS layer (full symbols). Actual measurements on the left-hand side and simulations on the right-hand side[39]

improve. A model to explain this is proposed and verified by the use of SCAPS. It is concluded that the series resistance of the *i*-ZnO layer prevents electrical inhomogeneities from dominating the open-circuit voltage of the entire device.

Recently, a baseline model for CIGS and for CdTe cells was proposed by Gloeckler *et al.*[22] Although the model incorporates only the minimum number of layers and a minimum of deep defect distributions, it serves as an excellent starting point for more specific and more complete simulations.

Amorphous silicon solar cells

Several physical mechanisms specific to amorphous silicon solar cells have triggered the early development of specialized numerical modeling of thin-film PV devices.[41] First there is the complicated electronic structure of a-Si:H material, with a high density of states distributed in the bandgap, and complicated occupation statistics governing their charge and their contribution to recombination. Second, multiple-junction solar cells have long been common, because the versatility of the a-Si:Ge:C:H materials system allows for bandgap engineering, and because the rather low efficiency and stability of single-junction cells makes multi-junctions almost obligatory. It is therefore not a surprise that features such as bandgap grading and tunnel-recombination junctions are supported in numerical simulation programs dedicated to a-Si, e.g., ASA. And third, a-Si having a rather large bandgap for PV applications, the cells suffer from too low a current. This is a driving force for a careful design of the optical properties of the cell. The use of anti-reflection coatings, optical texturizing, etc., indeed finds more application in a-Si cells than in, e.g., CIGS cells. Also, there is a stronger need for optical modeling of a-Si cells. This specialized subject however is somewhat beyond the scope of this article, and we refer the reader to the excellent overview given in the book by Schropp and Zeman.[6]

Nano-structured solar cells

Modeling of dye-sensitized, nano-structured solar cells[42] is complicated for two reasons: the geometry of the nano-porous TiO_2 network is very complicated, and the molecular processes of excitation, injection and recombination exceed the framework of solid-state semiconductor physics, on which all simulation programs discussed here are based. In ETA cells, the absorbing organic dye monolayer is replaced by an extremely thin absorber (ETA),[43] and the electrolyte is replaced by a wide-gap *p*-type semiconductor ('hole conductor'). While these cells could in principle be completely described by semiconductor physics, the difficulties connected with

the geometry and the nanometer distance scale remain the same. First attempts to simulate the behavior of such extremely thin unit cells have been published.[44,45] The description of a complete macroscopic ETA cell as a network assembly of nano-sized elementary cells was recently presented.[45]

CONCLUSION

From these discussions it is clear that many complicated physical mechanisms govern the operation of thin-film PV devices; also, a quantitative understanding of these cells is definitely beyond intuition and simple analytical models. Numerical modeling has been developed and applied with several purposes: educational illustration of specific physical mechanisms, a tool to interpret advanced measurement on complicated cell structures, design and optimization of advanced cell structures, etc. It is clear that numerical simulation can lead to better insight into the details of the physical operation of a thin-film cell structure. However, this goal will not be reached by only simulating the form of one measured *J–V* characteristic. To get confidence in a proposed model, as many different characteristics, in as many different conditions as possible should ideally be simulated and compared with measurements. This pleads for an extended measurement program, as described in the introduction of Section 2. The large quantity of parameters needed for simulation (50 seems to be a minimum) is a real concern. An exhaustive exploration of a 50-dimensional parameter space is definitely out of reach. This means that numerical modeling needs input from specialized measurements of layers and specially prepared structures to fix as many as possible parameters with some level of confidence. Also, choosing a parameter set to simulate a measurement is not a blind job which can be left to a computer, but requires physical insight and feeling, and if possible also the application of simple, analytical or numerical 'sub-models', which describe the gross action of part of the parameters (e.g., at the back contact of a CdTe cell). If one can be confident that a numerical model and a parameter set give a realistic quantitative description of a cell, the model can be used for numerical experiments to explore the influence of some critical parameters, and finally to obtain hints for improvement of the cells. The examples discussed illustrate that numerical modeling is on its way to reach this ambitious goal. At the same time it is clear that numerical modeling alone is not sufficient to obtain better cells.

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