Modeling of Polycrystalline Thin Film Solar Cells

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Abstract. This paper describes modeling polycrystalline thin-film solar cells using the program AMPS-1D[1] to visualize the relationships between the many variables involved. These simulations are steps toward two dimensional modeling the effects of grain boundaries in polycrystalline cells. Although this paper describes results for the CdS/CdTe cell, the ideas presented here are applicable to copper-indium-gallium selenide (CIGS) cells, as well as other types of cells. Results of these one-dimensional simulations are presented: (a) the duplication of experimentally observed cell parameters, (b) the effects of back-contact potential barrier height and its relation to stressing the cell, (c) the effects of the depletion layer width in the CdTe layer on cell parameters, and (d) the effects of CdS layer thickness on the cell parameters. Experience using the software is also described.

TYPES OF MODELS

Many types of models are used in PV to apply theory, visualize relationships, and, occasionally, even to predict results. A short list of these includes electronic (e.g., semiconductor band diagrams), materials (diffusion in layered and polycrystalline materials), and optical (light absorption in layered structures). This paper is focused on the computer simulation of photoelectronic junction transport mechanisms that seek to explain the behavior of thin film polycrystalline solar cells. In particular, the program called AMPS-1D, written by Steve Fonash and others[2] is described with its application to the polycrystalline (PX) CdS/CdTe cell. Some of the ideas here are applicable to CIGS cells as well

WHAT GOOD IS A MODEL?

Because of the complexity of simultaneous solution of the transport and continuity equations for electrons and holes for a two terminal device, only the simplest of cases can be done symbolically. For more complex devices., solutions may be best obtained numerically (and perhaps can only be), giving considerably more flexibility and speed. Because of the relatively large number of variables involved, the output (e.g, V_{OC}, ff) may not be unique for these more complex systems, even if most (but not all) of the variables can be specified accurately. In my opinion, the major value of such models is not in prediction, but as an *experimental tool* for:

1. visualization of the fields, potentials, currents, regions of high recombination, and effects of light and dark on transport,

[1] AMPS-1D is a one-dimensional semiconductor transport computer simulation program written under the direction of Prof. S. Fonash at Pennsylvania State Univiversity, with the support of the Electric Power Research Institute.

[2] e.g., P. Chatterjie, P.J. McElheny, and S.J. Fonash, J. Appl. Phys. **67**, 3803 (1990).

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2. identifying parameters that have strong or weak effects on the cell operation,
3. as a source of ideas that can be tested experimentally (and the methods of testing),
4. parameter gathering, checking, and adjustment, and
5. "what if" expeditions and reality checking.

Modeling must be used with a good deal of physical insight and caution, and always be cross checked with experiment, and with more specific theory-based models

MODELING RESOURCES

Table 1 is a brief (certainly not exhaustive) list of some of the electronic transport modeling programs available commercially and from Universities.

Table 1. Modeling programs. Medici is the only program on this list that handles tunneling. (1D = one dimensional).

1D	Source	Platform	≈ $	Comment
AMPS-1D	Fonash–Penn State U	PC, unix	free	user friendly, trapping OK
ADEPT	Gray, Schwartz, Lee–Purdue	PC, Solaris	free	no trapping
PC-1D, v. 3	Basore–U. South Wales	PC	$100	Used to model Si and III-V's no trapping
SimWindows	D. Winston-U of CO	PC	nominal	no trapping
2D				
PISCES IIB	Dutton, Chen–Stanford	unix	$300 Univ.	trapping, can add on Fortran modules. ($2500 commercial)
Medici	Tech. Modeling Assoc., Inc.	unix	$20,000	transients, tunneling
ADEPT 2D	Gray, Schwartz, Lee–Purdue	PC	free	no trapping

My own experience with AMPS shows the following good points:

1. Very intuitive and straight forward graphical user interface, with many variables.
2. Excellent and quick plotting facility.
3. Reasonably fast (25 min/case at 300 MHz, 64 MB RAM)—faster with more RAM.
4. Data sets generated are very comprehensive (CB, VB, E_{Fn}, field, recombination, generation, n, p, trapping, J_n, J_p, J_{total}, light, and dark J-V, and more).
5. Free.

The following aspects could be improved:

1. Queuing cases does not work satisfactorily with Windows NT on my system. Apparently queuing does work with Windows 95.
2. Only 8 points in the spectral response. More points on Unix version.
3. No provision for external series resistance (e.g., grids), tunneling, or internal reflectance (e.g., at the CdS/CdTe interface).
4. Exporting data must be done one data-pair set at a time.

Despite these last comments, AMPS is an excellent contribution to the field of photovoltaics, for both professionals and advanced students.

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DEFINITION OF THE PROBLEM

Ideally a modeling procedure for CdS/CdTe cells might progress from a simple 1D layered structure with no grain boundaries to a 2D approximation of one cylindrical grain, for which grain boundaries play a role.

The 1D layered structure treated here is shown in Figure 1, with the CdTe subdivided into layers to simulate the grading of acceptor density (and possibly lifetime) thought to be inherent in the polycrystalline cells.

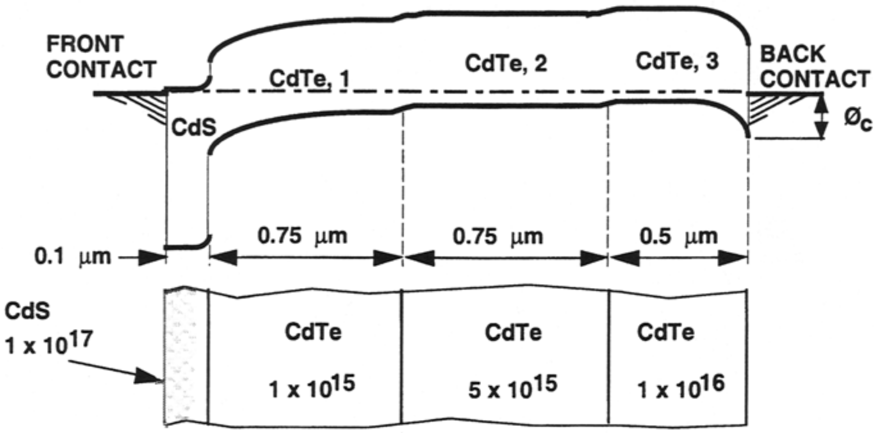

FIGURE 1. Band diagram and layer structure for "basis" case.

To extend this the two dimensions, a cross section of a more realistic polycrystalline device is shown in Figure. 2, where interdiffusion of S and Te at the CdS/CdTe interface and grain boundaries, as well as Cu diffusion from the back contact, is included. Since each CdTe grain is roughly cylindrical,the cell can be approximated by a system of idealized grains, one of which shown in Figure. 3. One could then proceed to model the 2D grain of Figure 3, using the insight provided by the previous results for 1D to gain insight to the effects of polycrystallinity. To study the cell "system" one would appropriately combine the results for a variety of grain sizes.

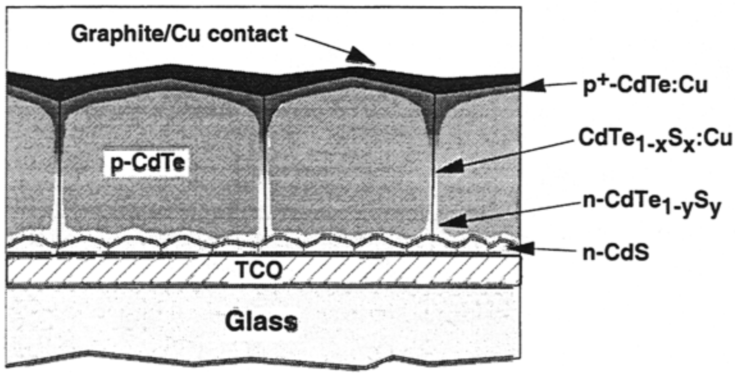

FIGURE 2. Polycrystalline CdS/CdTe schematic cross-section.

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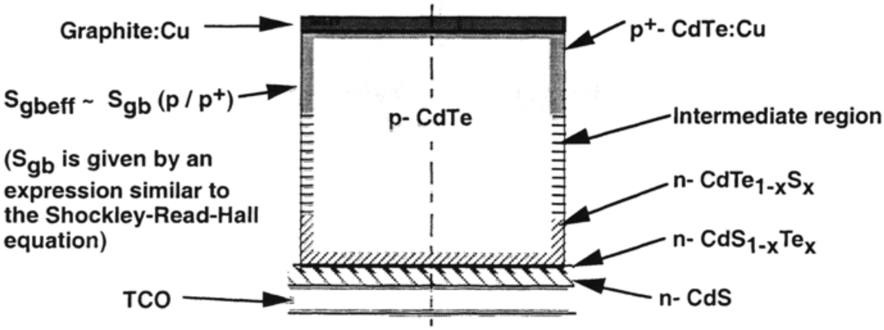

FIGURE 3. "Single grain" schematic cross-section.

INPUT PARAMETERS

The input parameters for the one-dimensional case of Fig. 1, treated in the following, may be separated into two groups:

Group 1: Relatively well known, once structure is defined (e.g., thicknesses, band gaps).

Group 2: Not well known. It is likely that modeling will help determine the ranges of magnitude for these parameters, e.g., carrier densities (n, p), lifetimes [τ (or recombination center parameters: N_r, E_T, σ_n, σ_p)], contact potential barrier height ($\O_c$, front and back), and CdS/CdTe interface recombination.

For simplicity, in this particular series of simulations it is assumed that there is a Schottky diode at the back contact, there is no recombination at the CdS/CdTe interface, and there is no Transparent Conducting Oxide (TCO) window. The latter two items can be added easily. Also assumed are an (approximately) AM1.5 spectrum, and optical absorption data for PX CdS and CdTe[3]. A lifetime model of recombination is used for this preliminary work. An alternate "discrete state" model is also available, which introduces Shockley-Read-Hall recombination that accounts for trapping at the recombination centers, but this would add more variables.

The procedure has been to set as many as possible of the Group 1 variables according to experimental data and to use educated guesses for the rest. The effects of the Group 2 variables are then determined by studying the variations induced by changing one variable at a time. Some of them have rather small effects for the regions of parameter space of interest and can be set, while others are pivotal and may require some experimental verification.other than just J_{sc}, V_{oc} and ff.

All the modeling here disregards the effects of grain boundaries, except for optical absorption coefficient data. This is because it would introduce too much more complexity at this time, and the 1D modeling results appear to be valuable by themselves, especially for some parts of the cell, as we will see.

MODELING RESULTS

The first thing that was done with AMPS was to try to match existing cell parameters (un-stressed cells) using a combination of published values (e.g., optical absorption), measured quantities (e.g., CdTe thickness, n and p), and best guesses (e.g., lifetimes), as

shown in Figure 1. The target was 25 mA, 0.85 V, ff = 0.750 and 15.8%. By varying parameters, especially the electron lifetime and the depletion layer width in the CdTe, a good

[3] Optical absorption data was obtained from D. Albin at NREL (1997).

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fit for J_{SC} and ff for the unstressed cell was obtained. The V_{OC}, however resisted attempts to independently reduce it to a more widely observed target, possibly indicating that a another loss mechanism, such as CdS/CdTe interfacial recombination, should be incorporated into the model.

The optimization was done with the aid of a set of output-variable trend plots (J_{SC}, V_{OC} and ff) for each input variable. These plots indicated that some input variables had little effect on one or two of the output variables, while others had an unexpectedly large effect.

Front Contact and CdS Layer

1. The lifetime in the CdS has little effect for any but the highest CdS doping levels because the high field there sweeps the carriers out before they can recombine.
2. The surface recombination velocity at the contact/CdS interface also has little effect on J_{SC} except for the case when the front contact barrier height is larger than the difference between the valence band and the Fermi level, reducing or inverting the electric field there.
3. Increasing the CdS thickness has virtually no effect on V_{OC} and ff, but J_{SC} decreased linearly over the range of 0.01 μm to 0.1 μm, as expected.
4. Decreasing the electron density in a 0.1 μm CdS layer from 10^{17} to 10^{15} cm^{-3} increased J_{SC} by 2 mA/cm^2. Again there is virtually no effect on V_{OC} and ff.

CdTe Layer

1. Decreasing the hole density in the CdTe layer with a corresponding increase in depletion layer width from 0.16 to 1.55 μm ($\approx 5 \times 10^{16}$ to 5×10^{14} cm^{-3}) caused a 2 mA/cm^2 increase in Jsc, due to increasing electric field aided collection of photogenerated carriers. On the other hand, since this field is reduced by forward bias, for large depletion layer widths, there was considerable decrease in light-generated current (J_L) with increasing bias, causing Voc and ff to decrease. The efficiency decreased 1.5 percentage points over this range of depletion layer widths.
2. The other major controlling variable is the minority carrier lifetime (τ) which was increased over the rather narrow range from 0.8 to 3.2×10^{-10} sec. resulting in increases in J_{SC} of 1.2 mA/cm^2 and V_{OC} of 0.11 V. The ff was relatively constant except at the ends of the ranges where the change was ± 0.022.

Back Contact

Two of the possible explanations for the effects of stressing (heat and/or bias) are (a) a potential barrier ($Ø_c$) exists at the back contact and its magnitude is changed by stressing, and (b) the high level of Cu in the CdTe near the back contact diffuses away into the bulk of the CdTe, lowering the carrier density there and perhaps decreasing tunneling at the contact. Modeling the first explanation for a 2.1 μm thick cell gives the relationships in Figure 4a; at about $Ø_c = 0.45$ eV the barrier starts to drop the efficiency strongly. A 6.6 μm thick cell with $Ø_c = 0.5$ eV behaves very similarly to the one in Figure 4a. The thick (thin) cell has $J_{SC} = 25.0$ (25.0) mA/cm^2, $V_{OC} = 0.950$ (0.936) V, ff = 0.697 (0.706), and efficiency = 15.1 (15.0) %. In the thin cell the back contact barrier is essentially another solar cell that is bucking the main junction. A small amount of light gets through to it and so it produces a reverse voltage ($\approx$ 14 mV). In the thick cell virtually no carriers are generated at the back contact and the reverse voltage is negligible, but there is more recombination because of the greater thickness of the CdTe layer.

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The J-V curves of the stressed models in Figure 4b are very similar to some of the observed stressed cells, even having the slightly depressed V_{OC} values observed for the higher values of $\emptyset_C$. Such a barrier might arise from a thin interlayer of Cu_xTe between the CdTe and the graphite:Cu contact. Such a barrier to CdTe has been reported by several researchers.[4] In addition, many phases of Cu_xTe exist, depending on small variations of x.

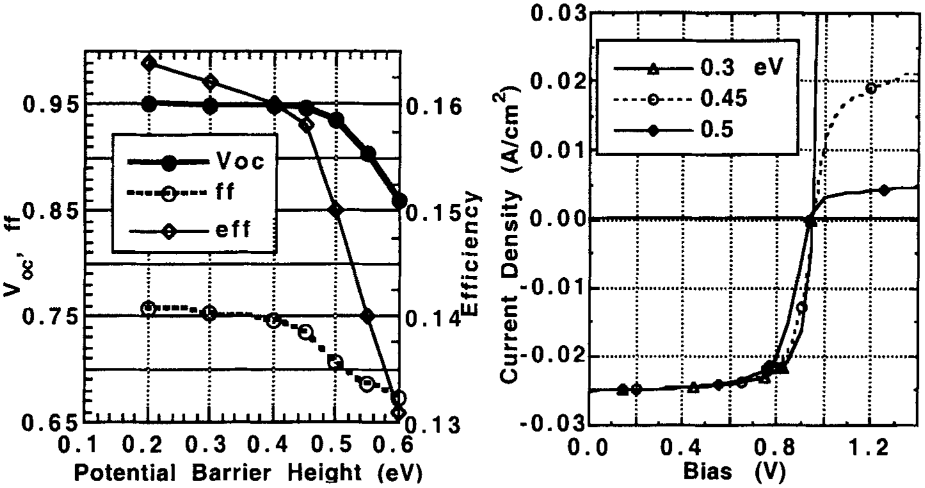

FIGURE 4. (a) Photovoltaic parameters for the #21 series vs. barrier height (AM1.5). (b) AM1.5 J-V characteristics of the cases of (a) for various barrier heights.

PROGNOSIS AND FUTURE WORK

The largest hurdle to getting useful results from AMPS is dealing with the large number of variables involved and gaining some perspective of their effects. Once a satisfactory set of input variables is determined, it is relatively simple to find the effects of variables, one at a time. While the analysis presented here used only three target quantities (J_{SC}, V_{OC} and ff) other, readily accessible experimental data such as spectral response and V_{OC} vs. temperature would allow the model to be considerably refined. The user-friendly quality of AMPS greatly assists this process because one can quickly see the results from so many perspectives (currents, bands, fields, recombination, to name a few).

Some interesting future directions are: (a) comparison of lifetime and recombination center descriptions (carrier trapping), (b) determining the effects of an i-layer at the CdS/CdTe junction, (c) the effects of interfacial recombination, (d) the addition of a transparent conducting oxide layer, and (e) interaction of CdS layer thickness and electric field there.

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[4] Garth Jensen, Materials Research Society, Spring 1993. Awam, G.R. et al. 7th E.C. Photovoltaic Solar Energy Conference. Proc. (1987) p. 1000-4

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