NUMERICAL MODELING OF GRADED BAND GAP CIGS SOLAR CELLS

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ABSTRACT

The high efficiency reported recently by NREL for CIGS solar cells demonstrates the potential of band gap grading in producing high efficiency thin film solar cells. In order to reap the full benefits of this design strategy, a clear understanding of the fundamental device physics of these structures is needed. The purpose of this paper is to examine the role grading of the band gap plays in achieving high conversion efficiencies. To aid in this examination, a detailed numerical device simulation program, ADEPT, is used.

INTRODUCTION

Graded band gap CIGS solar cells have proved to be very efficient. This increase in efficiency over that of CIS solar cells is attributed to an increase in open circuit voltage due to the larger band gap near the junction and an increase collection efficiency caused by the built-in electric field that results from the band gap grading. While this simple explanation is useful in understanding the basic device performance, a complete understanding of the physics of graded cells is needed in order to fully understand cell performance and to design and fabricate even higher efficiency cells.

Here, issues affecting cell performance are discussed and examined using ADEPT (A Device Emulation Program and Tool), a detailed numerical device simulation program developed at Purdue University.

ADEPT

ADEPT [1] and its developmental predecessors [2] have been used to model a wide variety of photovoltaic devices. It has been demonstrated to be a useful tool for interpreting the performance of existing solar cells. The accuracy of ADEPT in predicting cell performance depends on several factors. In well understood material systems, such as crystalline silicon and gallium arsenide, the predictive ability of detailed device simulation codes is quite good. In thin film devices such as CIS and CdTe, the predictive ability of these codes is not as good. Basic characterization of these materials is still an active area and is complicated by variations in the material parameters resulting from different fabrication methods and even different facilities. In a graded band gap structure these difficulties are even more severe.

In order understand these issues, it is necessary to examine the assumptions used in creating a detailed numerical model of a thin film solar cell.

Semiconductor Equations

ADEPT generates a numerical solution to a set of three coupled partial differential equations commonly referred to as the semiconductor equations. These are Poisson's equation and the hole and electron continuity equations and are shown below for steady state isothermal conditions.

\[ \nabla \cdot D = q(p - n + N) \]  \hspace{1cm} (1)

\[ \nabla \cdot J_p = q(G - R) \]  \hspace{1cm} (2)

\[ \nabla \cdot J_n = -q(G - R) \]  \hspace{1cm} (3)

Coupled with the following auxiliary equations, these are solved for the electrostatic potential, \( V \), and the hole and electron concentrations, \( p \) and \( n \), on a domain defined by the device structure subject to boundary conditions (at the contacts, for one-dimensional simulations) and the device operating conditions (the applied bias, operating temperature, and incident light flux).

\[ D = \varepsilon \nabla V \]  \hspace{1cm} (4)

\[ J_p = -q \mu_p \nabla (V - V_p) - k T \mu_p \nabla p \]  \hspace{1cm} (5)

\[ J_n = -q \mu_n \nabla (V + V_n) + k T \mu_n \nabla n \]  \hspace{1cm} (6)

It is here, in the transport equations (5) and (6), that a significant assumption is made. Carrier transport within the device is assumed to be based on drift-diffusion mechanisms only. Tunneling and thermionic emission are neglected. This is not a severe restriction and further
discussion of this issue is beyond the scope of this paper, but is addressed elsewhere in these proceedings [3]. Tuning and thermionic emission at the contacts is modeled using effective carrier recombination velocities for the boundary conditions.

As can be seen by examining equations (1) through (6), there are only a modest number of parameters to be set in order model any device constructed from any semiconductor material, so long as the assumptions regarding transport are not violated. These parameters are: \( N \), the trapped charge density; \( G \), the optical generation rate; \( R \), the net recombination rate; \( \varepsilon \), the electric permittivity; \( \mu_e \) and \( \mu_h \), the carrier mobilities; and \( V_e \) and \( V_h \), the band parameters. While this is a convenient way to express the model equations, it is a somewhat misleadingly simple representation. All the information regarding device structure and material characterization is contained in these terms.

MODELING ISSUES

All the information relating to the device structure and material parameters of a graded band gap solar cell are contained in the eight parameters mentioned above. Accurate modeling of any device depends on detailed knowledge of these parameters. Even for a relatively simple CdS/CIS structure, there is debate about the exact structure of the device (i.e. presence of an OVC layer, interface states, contact characteristics, etc.) and the correct material characteristics (i.e. absorption coefficients, mobilities, trap/recombination centers, etc.). In a graded band gap structure, these difficulties are compounded. These issues are discussed below.

Absorption Coefficients

Even in CIS, there is presumably some variation in absorption coefficient with position within the CIS layer since the ratios of copper to indium to selenium tend vary (i.e. Cu-poor near the CdS interface). The addition of gallium would, of course, change the optical band gap as some function of gallium content. Any other material (such as sulfur) would have a similar effect. Characterization of the absorption coefficient as a function of gallium content is needed in order to produce accurate simulations.

Trapping/Recombination

The effective doping and carrier lifetimes in CIS cells are thought to be a result of native defects in the material. Detailed modeling of trapping and recombination can be quite complicated. However, reasonable modeling results have been obtained by assuming a fixed trapped charge density (effective doping) and by modeling recombination as a mid gap single level trap. Improved models are needed for a full understanding of trapping and recombination. ADEPT can be used to examine proposed models, but even a simple model presents a challenge in a graded band gap CIGS solar cell. How do the effective doping and lifetimes depend on band gap (gallium content)? How sensitive is device performance to these parameters?

Mobility

As with the other parameters, carrier mobility is sure to be a function of gallium content and represents another area of material characterization that must be addressed.

Band Parameters

The most explicit effect of band gap grading appears in the band parameters [4].

\[
qV_p = -(\chi - \chi_{ext}) - (E_g - E_{g,ref}) + kT \ln \frac{N_v}{N_{v,ref}} + kT \ln \frac{F_{\chi}(hv)}{eN_v}
\]

\[
qV_n = -(\chi - \chi_{ext}) + kT \ln \frac{N_c}{N_{c,ref}} + kT \ln \frac{F_{\chi}(hv)}{eN_c}
\]

Here, \( \chi \) is the electron affinity, \( E_g \) is the band gap, and \( N_v \) and \( N_c \) are valence and conduction band densities of state. The last term in each band parameter expression accounts for degenerate (Fermi-Dirac) statistics. The 'ref' subscript refers to an arbitrary reference material. Note that we have assumed parabolic bands.

The band parameters are what allow the modeling of heterostructures and, specifically, graded band gap structures. The electron affinity, band gap, and densities of state can all vary with gallium content. The precise relationship must be determined experimentally.

Examination of equations (7) and (8) can give some insight into the effect the grading of gallium content may have on cell performance. Note that, neglecting degeneracy, the band parameters are constant with position in a uniform material and hence have no effect on carrier transport. In a graded structure, however, the effect is significant and can sometimes lead to nonintuitive results.

Consider the band structure of a hypothetical heterostructure as shown in Figure 1. If this were a uniform material, the local vacuum energy would be parallel to both the valence and conduction band edges. That is clearly not the case in a heterostructure. We see that the gradients of the band edges can be opposite in sign to the electric field. It is this gradient, or effective field, that represents the true 'quasi-drift' force acting on the carriers. This effective field is, in general, different for holes and electrons.

Even this can lead to an incorrect interpretation if the electron affinities and/or densities of state change significantly with band gap. It is the gradients of \( V_n \) and \( V_p \) that contribute to the effective fields acting on the carriers.
states was varied with position in such a way as to exactly cancel the effect of the graded band gap. This is shown in Figure 3. In fact, this device has a somewhat lower efficiency than a comparable CdS/CIS cell (14.1% versus 14.8% simulated efficiencies).

We see in equations (7) and (8) that changes in the electron affinity and the densities of state with position can also contribute significantly to the effective fields. In fact, counter-intuitive predictions of performance can result. More useful in interpreting performance is the use of an effective band diagram, where the variations of electron affinity, band gap, and densities of state with position are all lumped into an effective band gap and effective electron affinity. Examination of this diagram correctly shows the influence of the effective fields on carrier transport. This is illustrated in Figures 2 and 3.

SIMULATION RESULTS

It should be apparent that to gain a complete understanding of how gallium affects cell performance requires detailed characterization of CIGS material as a function of gallium content. In addition, the spatial variation of the gallium content must be known as well. A parameter study of how performance is affected over reasonable bounds on each parameter would require a very large number of simulations, and is beyond the scope of this paper. However, by limiting the parameters to be varied to a small set, some insight into graded band gap cell performance can be achieved.

We will limit ourselves to the simple cell structure for which the conventional energy band diagram is shown in Figure 2. It consists of a 0.05 μ n-type CdS layer on top of a 1.95 μ CIGS absorber layer. All parameters dependent on gallium content are assumed to vary linearly with position. The point of minimum gallium content is taken to be 0.5 μ into the CIGS layer. A simple CdS/CIS equivalent structure is used for comparison purposes (Case 0). Reasonable materials parameters are used in the simulations and are assumed to be independent of gallium content. Only the band gap and absorption coefficients are allowed to vary with gallium content. It should be noted that simplified models were used and no attempt was made to match experimental data. The purpose here is to show trends in performance.
Several variations of the band gap grading were simulated. First, in Case 1 the CIGS layer is assumed to have a constant band gap for the first 0.5 microns and then a linearly graded band gap up to the back contact. In Case 2 only the first 0.5 microns of the CIGS layer is graded, and finally, in Case 3 the entire CIGS layer is graded, similar to the situation depicted in Figure 2. The maximum band gap in Cases 1 to 3 was 1.2 eV. The performance characteristics are summarized in Table 1.

### Table 1. Computed performance characteristics for four examples of graded band gap CIGS cells.

<table>
<thead>
<tr>
<th></th>
<th>Case 0</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V_{oc} ) mV</td>
<td>515</td>
<td>519</td>
<td>590</td>
<td>595</td>
</tr>
<tr>
<td>( J_{sc} ) mA/cm²^2</td>
<td>41.1</td>
<td>41.7</td>
<td>39.0</td>
<td>39.6</td>
</tr>
<tr>
<td>FF</td>
<td>71.9</td>
<td>72.0</td>
<td>69.4</td>
<td>71.0</td>
</tr>
<tr>
<td>( \eta )</td>
<td>15.8</td>
<td>16.0</td>
<td>16.5</td>
<td>17.3</td>
</tr>
</tbody>
</table>

Case 1 basically corresponds to the addition of a back surface field. The (small) improvement in efficiency is due primarily to an increase in the collection efficiency. In Case 2, there is no BSF and the somewhat larger increase in performance is due to the bigger band gap in the junction region. However, the collection efficiency is reduced since the effective field tends to hinder collection. The collection efficiency can be recovered by now including a BSF, as in Case 3. There is an improvement in cell efficiency of 1.5 points.

It must be noted that the effect of band gap grading on cell performance is sensitive to many of the parameters that were not varied in this example. A comprehensive parameter study is needed if a good understanding of graded band gap solar cells is to be achieved.

### SUMMARY

In this paper, the issues involved in modeling graded band gap CIGS solar cells were addressed. Experimental characterization of CIGS material is needed in order to improve our understanding of the performance of these devices. The value of detailed numerical device simulation programs as an analysis tool was demonstrated. Future work will involve a comprehensive examination of the sensitivity of the performance characteristics to parameters that might possibly vary with band gap.

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### REFERENCES


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