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Nonlinear effects in modeling thin-film graded-bandgap solar cells

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ABSTRACT

We model the effect of concentrated sunlight on CIGS thin-film graded-bandgap solar cells using an optoelectronic numerical model. For this purpose it is necessary first to solve the time-harmonic Maxwell equations to compute the electric field in the device due to sunlight and so obtain the electron-hole-pair generation rate. The generation rate is then used as input to a drift-diffusion model governing the flow of electrons and holes in the semiconductor components that predicts the current generated. The optical submodel is linear; however, the electrical submodel is nonlinear. Because the Shockley–Read–Hall contribution to the electron-hole recombination rate increases almost linearly at high electron/hole densities, the efficiency of the solar cell can improve with sunlight concentration. This is illustrated via a numerical study.

Keywords: Sunlight concentration, CIGS thin film solar cells, Optoelectronic optimization

1. INTRODUCTION

Thin-film photovoltaic solar cells (PVSCs) could play an essential part in providing eco-responsible energy sources to help tackle the climate emergency.[1] But to fully realize their potential, the efficiency of thin-film PVSCs needs to be improved.[2] In a previous paper,[3] we had examined the effects of concentrated solar radiation on the efficiency of CIGS solar cells in which we allow bandgap grading of the CIGS layer via compositional grading. By this, we mean that the semiconductor is $CuIn_{1-\xi}Ga_{\xi}Se_2$, where $\xi \in [0, 1]$ is a compositional parameter that can be varied during manufacture to obtain a graded bandgap. We showed that bandgap grading could enhance efficiency and that concentrated solar illumination further improves efficiency. This is also predicted for other types of thin-film solar cells.[2,3]

Our predictions were based on an optoelectronic model that predicts the efficiency η of the solar cell using two submodels. In the optical submodel, the standard transfer-matrix method[4] is used to determine the electron-hole-pair (EHP) generation rate $G(z)$ as a function of the thickness coordinate z inside the solar cell, assuming normal illumination by unpolarized polychromatic light endowed with the AM1.5G solar spectrum. Then $G(z)$ is used as an input to the drift-diffusion model to obtain the charge-carrier fluxes in the electrical submodel, and hence the current $J_{\rm dev}$ generated by the solar cell and the electrical power density $P = J_{\rm dev}V_{\rm ext}$ as functions of the bias voltage $V_{\rm ext}$ under steady-state conditions. In turn, the $J_{\rm dev}$–$V_{\rm ext}$ and the P–$V_{\rm ext}$ curves yield the efficiency of the device along with the short-circuit current density $J_{\rm sc}$, open-circuit voltage $V_{\rm oc}$, and the fill factor FF. We then choose parameters of the cell (such as ξ as a function of z in the CIGS layer as well as the thickness of that layer) that can be varied and use a genetic algorithm to optimize the design of the cell to improve the value of η. A complete description of the optoelectronic model and the optimization procedure can be found in Ref. 2.

Unfortunately, while developing a new solver for the electrical submodel in our original code. This means that the detailed results from the code in the cases when the bandgap is graded are incorrect. We describe this issue together with the new numerical model in more detail in Ref. 5. The current paper is devoted to

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reexamining the case of a CIGS solar cell using either a homogeneous or a graded-bandgap CIGS layer. For each bandgap profile, we optimize the design of the device. In particular, we give new results for linearly and nonlinearly graded-bandgap CIGS layers. We confirm that, as noted in Ref. 3, bandgap grading can markedly improve the device's efficiency. In addition, concentrated sunlight also increases the efficiency of all the designs. We discuss this in relation to nonlinearities occurring in the drift-diffusion equations.

2. THE MODEL

We use the same model for the solar cell as in Ref. 3. In particular, we assume the multilayered structure consisting of MgF_2/AZO/od-ZnO/CdS/CIGS/Al_2O_3/Mo shown in Fig. 2. The MgF_2 layer acts as an anti-reflection coating. Electrons are collected in the aluminum-doped zinc oxide (AZO) layer, while oxygen-deficient zinc oxide (od-ZnO) and cadmium sulfide (CdS) form an n-type semiconductor. Then CIGS is the p-type photon-absorbing layer of thickness $L_s = L_2 - L_1$, Al_2O_3 is a passivation layer, and molybdenum (Mo) is the back-contact and optical reflector. Further details on this design, including the thickness of the layers and the optical and electrical parameters for the various materials, are given in Ref. 3.

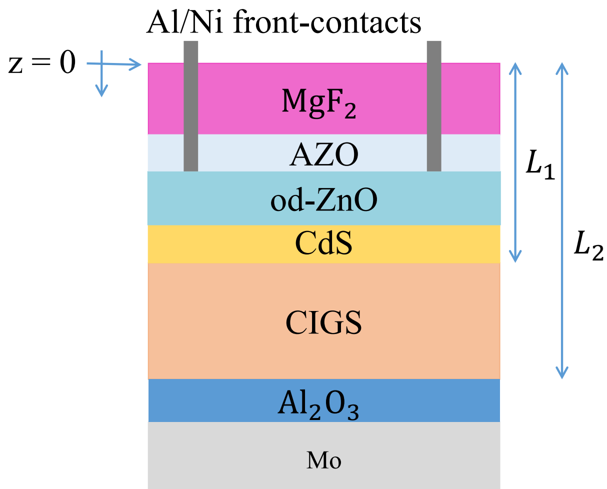

Figure 1. Schematic of the reference unit cell of the CIGS thin-film solar cell,[6] the thickness of the CIGS layer being $L_s = L_2 - L_1$.

All the layers in the notional cell are homogeneous and isotropic except for the CIGS layer in which the bandgap energy $\mathsf{E}_g(z)$ is taken to be one of the following:

1. The bandgap energy $\mathsf{E}_g = \mathsf{E}_a$ is homogeneous in the CIGS absorber layer.
2. The bandgap energy varies linearly with depth z as

$$\mathsf{E}_g(z) = \mathsf{E}_a + (\mathsf{E}_b - \mathsf{E}_a)\left[\frac{z - L_1}{L_s}\right],\ z \in (L_1, L_2), \tag{1}$$

   with E_a and E_b the minimum and maximum possible bandgap energy, respectively, while $0 \le A \le 1$ is the perturbation amplitude.

3. A nonlinear (sinusoidal) bandgap profile is modeled as[3]

$$\mathsf{E}_g(z) = \mathsf{E}_a + A(\mathsf{E}_b - \mathsf{E}_a)\left[\frac{1}{2}\left(\sin\left\{2\pi\left[K\frac{z - L_1}{L_s} - \nu\right]\right\} + 1\right)\right]^\alpha,\ z \in (L_1, L_2). \tag{2}$$

   The parameters ν, K and α are the relative-phase-shift parameter, the cycle number, and the shaping parameter of the nonlinear bandgap grading in the CIGS layer.

Table 1. Predicted optimal parameters to achieve the maximum η for $c_{\rm sun} = 1$ in the three bandgap-grading profiles. See Eqs. (1) and (2) for the definition of the parameters.

Parameter	Homogeneous	Linear	Nonlinear
E_a (eV)	1.19	0.96	0.95
L_s (nm)	2200	2000	2000
A		0.99	0.98
E_b (eV)		1.62	1.62
α			4
K			0.39
ν			0.15
η (%)	18.4	24.2	28.3

3. RESULTS AND DISCUSSION

The solar cell was illuminated from above by sunlight from $c_{\rm sun} \in \{1, 10, 100\}$ suns, the solar irradiance from each having the standard AM1.5G spectrum. For the three different bandgap-grading profiles mentioned in the previous section, we first optimized the design to obtain maximum efficiency for one sun ($c_{\rm sun} = 1$) using our new optoelectronic model. The parameter space for optimizing η for a homogeneous-bandgap CIGS layer was set to: $\mathsf{E}_{\rm a} \in [0.947, 1.626]$ eV. The parameter space for optimizing η for a linear-bandgap CIGS layer was set to: $\mathsf{E}_{\rm a} \in [0.947, 1.626]$ eV, $\mathsf{E}_{\rm b} \in [0.947, 1.626]$ eV, and A$\in [0, 1]$. Finally, the parameter space for optimizing η for nonlinear-bandgap CIGS layer was set to: $\mathsf{E}_{\rm a} \in [0.947, 1.626]$ eV, A$\in [0, 1]$, $\alpha \in [0, 8]$, $\kappa \in [0, 8]$ eV, and $\nu \in [0, 1]$.

The predicted optimal efficiencies for solar cells with homogeneous, linearly graded, and nonlinearly graded CIGS layers are 18.4%, 24.2%, and 28.3%, respectively. Note that these efficiencies exceed the values reported by us in Ref. 2 except for the homogeneous case for which it remains almost unchanged. The corresponding optimal parameters for each case are reported in Table 1.

Next, using the fixed predicted optimal parameters, we reran the optoelectronic model with $c_{\rm sun} = 10$ and $c_{\rm sun} = 100$ representing two different concentration ratios. The predicted values of efficiencies are presented in Table 2. Two conclusions are obvious from this table. The first, from the column of the table corresponding to $c_{\rm sun} = 1$, is that bandgap grading allows the creation of a more efficient solar cell in keeping with our general conclusions discussed in Ref. 2. The second is that concentrating the solar illumination also increases efficiency, although not in direct proportion to the concentration ratio $c_{\rm sun}$.

Table 2. Efficiencies for the three bandgap-grading profiles and three sunlight concentrations. The first column (1 Sun) reports the efficiency predicted by optimization. The remaining columns report efficiencies only changing the sunlight concentration ratios $c_{\rm sun}$.

Grading type	η (%)		
	$c_{\rm sun} = 1$	$c_{\rm sun} = 10$	$c_{\rm sun} = 100$
Homogeneous	18.4	20.2	22.2
Linear	24.2	26.9	31.7
Nonlinear	28.3	32.8	37.0

We note that the Maxwell system (represented by the Helmholtz equations for s- and p-polarized waves and solved by the transfer-matrix method) in the optical submodel is linear. Thus the electric-field strength for $c_{\rm sun} > 1$ is a direct multiple of the electric-field strength for $c_{\rm sun} = 1$. Since the EHP generation rate in turn depends on the square of the magnitude of the electric field in the semiconductor layers normalized by the input magnitude, we know that if $G_{c_{\rm sun}}(z)$ denotes the generation rate for $c_{\rm sun}$, we have

$$G_{c_{\rm sun}}(z) = c_{\rm sun}\, G_1(z)\,. \tag{3}$$

Thus solar concentration enhances the generation rate and introduces the potential for a higher density of electrons and holes in the device.

However, the effect of the higher generation rate is not simple to predict because the drift-diffusion system in the electrical submodel is nonlinear due to the nonlinearity of the electron-hole recombination rate, as well as the transport term. In our model of CIGS, we included the radiative recombination rate$R_{\rm rad}$ and the Shockley–Read–Hall (SRH) recombination rate $R_{\rm SRH}$.[2] Therefore, if $R_{c_{\rm sun}}(z)$ denotes the total recombination rate in relation to $c_{\rm sun}$, then $R_{c_{\rm sun}}(z) \neq c_{\rm sun}\, R_1(z)$ in general.

We determined the values of the net generation rate $\gamma_{c_{\rm sun}}$ and the net recombination rate $\rho_{c_{\rm sun}}$ (which are the integrals of $G_{c_{\rm sun}}(z)$ and $R_{c_{\rm sun}}(z)$, respectively, over the semiconductor region of each solar cell) to understand the role of sunlight concentration on the net generation and recombination rates. Values of the per-sun generation rate and the per-sun recombination rate in relation to the number of suns are presented in Table 3. From this table, we conclude that Eq. (3) holds for all three cases of bandgap variations. The net recombination rate $\rho_{100} \leq \rho_{10} \leq c_{\rm sun}\rho_1$ for all three cases shows that the reduced per-sun recombination rate is one of the reasons for efficiency enhancement in the CIGS solar cell on exposure to concentrated sunlight. The other effect that plays an important role in efficiency enhancement is the higher open-circuit voltage with the higher device current density due to sunlight concentration, $V_{\rm oc}$ being proportional to $\ln{(1 + J_{\rm sc}/J_{\rm dark})}$ for ideal photodiodes.

Table 3. Per-sun generation rate and per-sun recombination rate in relation to the number of suns. Both rates are in units of 10^{22} cm^{-2} s^{-1}.

Grading type	$\gamma_{c_{\rm sun}}/c_{\rm sun}$			$\rho_{c_{\rm sun}}/c_{\rm sun}$		
	$c_{\rm sun} = 1$	$c_{\rm sun} = 10$	$c_{\rm sun} = 100$	$c_{\rm sun} = 1$	$c_{\rm sun} = 10$	$c_{\rm sun} = 100$
Homogeneous	220.4	220.4	220.4	8.397	8.185	7.098
Linear	232.3	232.3	232.3	5.174	5.172	5.153
Nonlinear	251.8	251.8	251.8	4.838	4.835	4.830

4. CONCLUSION

We studied the effect of concentrated sunlight on a CIGS thin-film graded-bandgap solar cell using an optoelectronic model. The numerical study shows that reduction in the per-sun recombination rate is one of the reasons for efficiency enhancement in the CIGS solar cell on exposure to concentrated sunlight. The other nonlinear effect that plays an important role in efficiency enhancement is the higher open-circuit voltage with the higher device current density due to sunlight concentration. The numerical results presented here supersede the ones in Refs. 3 and 6.

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