

## Simulations of chalcopyrite/c-Si tandem cells using SCAPS-1D



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### ABSTRACT

In this work, we present SCAPS-1D simulations of dual-junction tandem cells with chalcopyrite top subcells with various bandgaps ( $E_g = 1.4, 1.5, 1.6$ , and  $1.7$  eV) and a c-Si bottom subcell. The purpose of these simulations is to assess achievable device performances with a CIGS/c-Si tandem structure when a realistic efficiency of each subcell is applied. The top subcell conditions are simulated based on the state-of-the-art records, and the bottom c-Si cell is designed to have an efficiency of approximately 19%. When the  $E_g$  of the top chalcopyrite cell is below 1.5 eV, the current matching condition between the top cell and bottom cell is not obtained until the top cell's thickness is  $0.2 \mu\text{m}$ . However, with  $E_g$  values of the top chalcopyrite cells at 1.6 eV and 1.7 eV, the current matching conditions could be found. Nevertheless, because the efficiency from the top chalcopyrite cell is approximately 12%, it is predicted that the tandem structure exhibits a similar device performance to the bottom c-Si cell. This result suggests that improving the efficiency of the wide bandgap cell is essential for the tandem cell to overcome the efficiency form a single-junction solar cell.

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### 1. Introduction

The efforts to surpass the efficiency of a solar cell with a single junction have led to numerous trials to fabricate multi-junction cells (tandem cells) comprised of solar cells with different bandgaps (Luque and Marti, 2010; Friedman et al., 2010). This technique provides a potentially higher conversion efficiency because serially connected junctions with different bandgaps absorb a greater range of photons with less energy loss. Theoretically, an infinite stack of junctions can have an efficiency of 65.4% under AM 1.5 illumination, and even further improvement in performance is possible using a concentrated incident spectrum (Martí and Araújo, 1996). In particular, applications of this technique to III-V or a-Si solar cells have been successfully demonstrated for several decades (Dimroth et al., 2014; Chiu et al., 2014; Sasaki et al., 2013; Press release of Fraunhofer-Institut für Solare Energiesysteme, 2014; Ahn et al., 2012).

In contrast to III-V or a-Si solar cells, few studies on chalcopyrite (Cu(In,Ga)Se<sub>2</sub>, CIGS for short)-based tandem solar cells have been performed, despite chalcopyrite materials having tunable bandgaps ranging from 1.0 eV to 1.7 eV (Shafarman et al., 2010; Shafarman and Paulson, 2005). A theoretical calculation predicts an efficiency of 28% from 2 junctions with a controlled combina-

tion of bandgaps (Coutts et al., 2003). However, serial stacking of two chalcopyrite absorber layers is practically difficult because the bottom subcell undergoes a significant degradation in its original device performance due to the high process temperature of the top subcell fabrication (Shafarman and Paulson, 2005). To date, to the best of our knowledge, no monolithically stacked CIGS tandem cell (i.e., not a mechanically stacked multi-junction cell (Nishiwaki et al., 2003) has reported a better device performance compared to an optimized single-junction device. Recently, hybrid multi-junction cells consisting of low-temperature grown top subcells and bottom CIGS solar cells have also been extensively studied because this approach offers a relatively wide process window for the cell stacking (Liska et al., 2006; Bailie et al., 2015; Kosyachenko et al., 2015); nevertheless, the obtained device performance from the hybrid multi-junction cells do not appear to compensate for the effort required to make the multi-junction devices.

Another means to demonstrate a tandem solar cell is to combine a top wide-bandgap CIGS solar cell with a bottom conventional Si-based solar cell (White et al., 2014). This approach has not yet realized an improved device performance compared to an optimized single junction CIGS device, but it appears to be more practical than the all-chalcopyrite tandem cell approach because the conventional Si-based solar cells have not only high efficiencies in excess of 20% (Masuko et al., 2014) but also better thermal stability.

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### Nomenclature

$J_{SC}$  short-circuit current density, mA/cm<sup>2</sup>  
 $V_{OC}$  open-circuit voltage, V  
 FF fill factor, %

$\eta$  conversion efficiency, %  
 $J_{MPP}$  current density at the maximum power point

In this work, we present simulations of (dual-junction) tandem cell with a chalcopyrite top cell ( $E_g \geq 1.4$  eV) and a c-Si bottom cell using the SCAPS-1D (Solar Cell Capacitance Simulator – 1D) simulation tool (Burgelman et al., 2000). First, wide-bandgap CIGS solar cells ( $E_g \geq 1.4$  eV) were simulated to fit the state-of-the-art data reported thus far, and then, a c-Si solar cell was simulated to have an efficiency of 18–19%. With the thinning of the absorber layer of the top subcells (i.e., wide-bandgap CIGS solar cells), the current matching conditions were determined to enable both the top and bottom subcells to have the same  $J_{MPP}$  or  $J_{SC}$  values. The obtained results suggested that the  $E_g$  of the top subcell must be greater than or equal to 1.6 eV (among the sample set in the present study) to obtain the current matching condition while ensuring a practical top-subcell layer thickness. Nevertheless, the simulation indicated that the tandem solar cell does not provide a substantial benefit in

terms of the device performance. The relatively lower efficiencies from the top CIGS subcells limit the device performances of the tandem solar cells. Thus, improvement of efficiencies of wide-bandgap CIGS solar cells must be undertaken beforehand to demonstrate a CIGS/c-Si tandem solar cell that exceeds the device performance from an optimized single-junction device.

## 2. Methods

First, we assumed that the CIGS/c-Si tandem solar cells have an ideal tunnel junction, having neither electrical resistance nor optical loss, between the top and bottom subcells. The current matching conditions were examined by adjusting the thickness of the CIGS solar cells (i.e., the top subcell). We also assumed that the optical loss in each interface is negligible. Because the SCAPS-1D simulation tool does not fully support a solar cell with a multi-junction structure, by simulating top and bottom subcells separately, the current matching conditions were obtained.

The simulations of the top CIGS ( $E_g = 1.4, 1.5, 1.6$ , and  $1.7$  eV) subcells are mostly based on the NUMOS model (Burgelman et al., 2007; Decock et al., 2011), which is one of the default models in the SCAPS-1D simulation package; the structure of the CIGS solar cell is shown in Fig. 1(a). The absorption coefficients of the CIGS absorber layers ( $E_g = 1.4, 1.5, 1.6$ , and  $1.7$  eV) were calculated from interpolation of measured optical constants reported by P. D. Paulson and coworkers (Paulson et al., 2003). In addition, to adjust the calculated absorption coefficients realistically, the absorption coefficients corresponding the sub-bandgap range were also corrected. Table 1 lists the basic input values for the top CIGS subcells' simulations. We also assumed that the CIGS solar cells do not have an internal bandgap gradient. To simulate a c-Si subcell for the bottom subcell, in-house data were used (Jeong et al., 2014; Do et al., 2014). The simulations were performed to generate a c-Si solar cell with efficiency of 18–19%. The schematic diagram and input values of the c-Si solar cells are also given in Fig. 1(b) and Table 1.

Finding the current matching point between the two subcells is straightforward. With thinning of the top cell's absorber layer, the  $J_{MPP}$  and  $J_{SC}$  of the top CIGS subcell and the transmitted light through the top CIGS subcell were calculated. The transmitted light spectrum,  $S(\lambda)$ , is given by

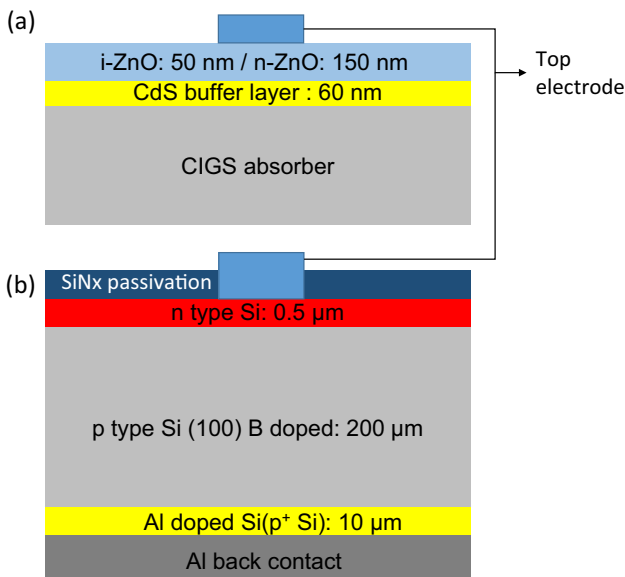


Fig. 1. Schematic diagrams of a CIGS solar cell and a c-Si solar cell.

Table 1  
Input parameters for SCAPS-1D simulation.

	CIGS $E_g = 1.4$ eV	CIGS $E_g = 1.5$ eV	CIGS $E_g = 1.6$ eV	CIGS $E_g = 1.7$ eV	n + Si	p-Si	p + Si
Thickness ( $\mu\text{m}$ )	Variable	Variable	Variable	Variable	0.5	200	10
$E_g$ (eV)	1.4	1.5	1.6	1.7	1.12	1.12	1.12
$n$ ( $\text{cm}^{-3}$ )	$1.0\text{E}+00$	$1.0\text{E}+00$	$1.0\text{E}+00$	$1.0\text{E}+00$	$1.0\text{E}+20$	$1.0\text{E}+16$	$5.0\text{E}+18$
$p$ ( $\text{cm}^{-3}$ )	$5.0\text{E}+15$	$1.0\text{E}+16$	$5.0\text{E}+15$	$5.0\text{E}+15$	$1.0\text{E}+01$	$1.0\text{E}+01$	$1.0\text{E}+01$
Bulk defect type	Neutral	Neutral	Neutral	Neutral	Neutral	Neutral	Neutral
Bulk defect ( $\text{cm}^{-3}$ , above $E_{V,\text{CIGS}}$ )	$2.0\text{E}14$ at 0.3 eV $1.0\text{E}14$ at 0.8 eV	$1.0\text{E}15$ at 0.8 eV	$1.0\text{E}15$ at 0.8 eV	$1.0\text{E}15$ at 0.8 eV	$5.0\text{E}14$ at 0.6 eV	$4.0\text{E}12$ at 0.6 eV	$4.0\text{E}14$ at 0.6 eV
Interface defect	N/A	CdS/CIGS (neutral)	CdS/CIGS (neutral)	CdS/CIGS (neutral)	N/A	N/A	N/A
Interface defect ( $\text{cm}^{-2}$ , above $E_{V,\text{CIGS}}$ )	N/A	$1.0\text{E}11$ at 0.6 eV	$1.0\text{E}11$ at 0.6 eV	$1.0\text{E}10$ at 0.6 eV	N/A	N/A	N/A

$$S(\lambda) = S_o(\lambda) \cdot \exp(-\alpha_{ZnO}(\lambda) \cdot d_{ZnO}) \cdot \exp(-\alpha_{CdS}(\lambda) \cdot d_{CdS}) \cdot \exp(-\alpha_{CIGS}(\lambda) \cdot d_{CIGS}), \quad (1)$$

where  $S_o$  is the incident light spectrum,  $\alpha$  is the absorption coefficient of a material, and  $d$  is the thickness of a material. The reflection losses from each interface were not taken into account.

Next, the transmitted light spectra were used as the input light spectra of the bottom c-Si subcell. Finally, the  $J_{MPP}$  and  $J_{SC}$  values of the c-Si subcell were calculated. The absorber thickness of the top CIGS subcell was limited to 0.2  $\mu\text{m}$  in the simulation, given that it is practically difficult to maintain the device properties of a thin absorber layer with thickness less than 0.2  $\mu\text{m}$  (Lundberg et al., 2003; Kim et al., 2013).

### 3. Results and discussion

#### 3.1. Top-subcell simulations

The simulations of CIGS solar cells were performed mostly based on the NUMOS model. Only the absorption profiles were obtained from P. D. Paulson's study (Paulson et al., 2003). Fig. 2 shows the J-V curves of CIGS solar cells for the top-subcells, and their J-V characteristics are given in Table 2. The CIGS solar cells with  $E_g = 1.4, 1.5$  and  $1.6$  eV do not exhibit large differences in the  $V_{OC}$ , which reflects the real data obtained to date (Contreras et al., 2012). In addition, the simulated  $V_{OC}$  of the CIGS solar cells are slightly smaller than the real data because we assumed the CIGS absorber layers do not have internal bandgap gradients (Hanket et al., 2009; Kim et al., 2015). If a CIGS solar cell has a wider bandgap near the CdS/CIGS interface, then a higher  $V_{OC}$  is expected (Kim et al., 2015). However, to induce the current matching condition between the top subcell and bottom subcell, the top CIGS solar cells should be thinner than the normal absorber layer (i.e., 2  $\mu\text{m}$ ). In such a case, the internal bandgap gradients make the simulation complicated; furthermore, when the CIGS absorber

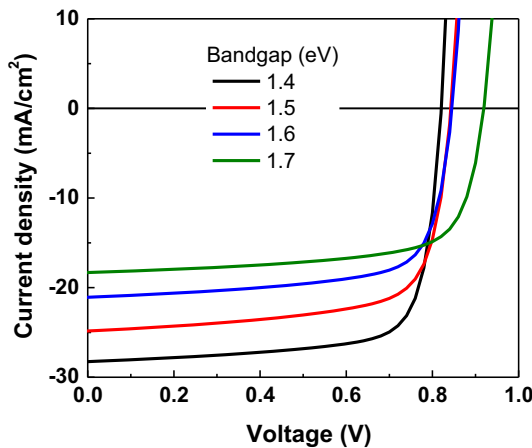


Fig. 2. Simulated J-V curves of the CIGS subcells.

layers are thin, it becomes ambiguous to choose the representative bandgaps of the CIGS absorber layers.

Fig. 3 presents the external quantum efficiency (EQE) curves (a) of the CIGS solar cells shown in Fig. 2 and their first derivative with respect to wavelength (b). The obtained simulations reveal that the CIGS solar cells with various bandgaps do not exhibit any significant difference in the short wavelength region (i.e., <500 nm). Only the cutoffs of the EQE curves of each bandgap move toward the short wavelength in accordance with their bandgaps. Fig. 3(b) shows the first derivatives of the EQE curves with respect to wavelength, where the local minima provide approximations of the bandgaps. The CIGS solar cells with nominal bandgaps = 1.4, 1.5, 1.6 and 1.7 eV are estimated to have bandgaps of 1.38, 1.48, 1.59, and 1.69 eV, respectively, suggesting that the absorption profiles approximated from P. D. Paulson's study (Paulson et al., 2003) fit properly.

Chalcopyrite materials are known to have quite a high absorption coefficient, and thus, the top subcell thinning process is

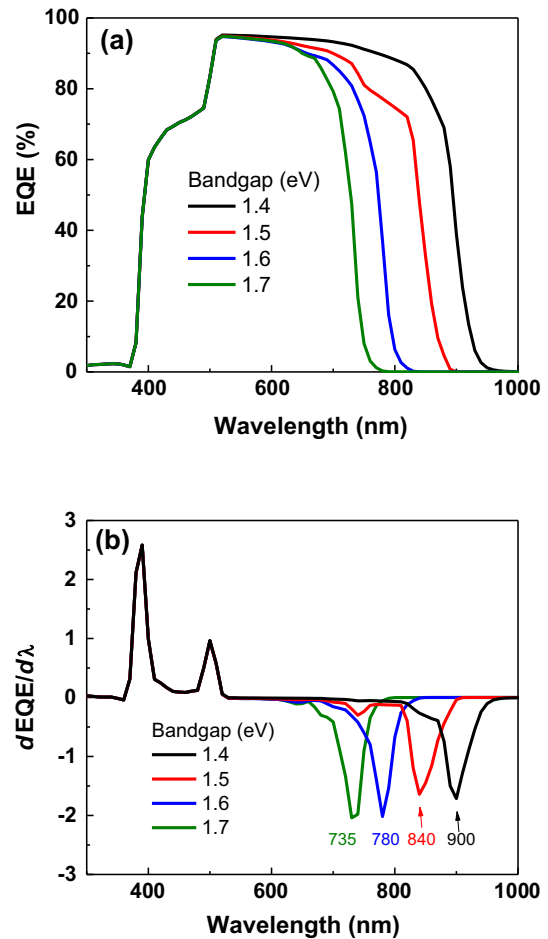


Fig. 3. (a) EQE curves of simulated CIGS subcells and (b) their first derivatives with respect to wavelength.

Table 2  
Light J-V characteristics of the CIGS solar cells shown in Fig. 2.

Top cell bandgap (eV)	V <sub>oc</sub> (V)	J <sub>sc</sub> (mA/cm <sup>2</sup> )	FF (%)	η (%)	V <sub>MPP</sub> (V)	J <sub>MPP</sub> (mA/cm <sup>2</sup> )
1.4	0.831	28.2	76.9	18.0	0.723	24.9
1.5	0.843	24.6	71.3	14.8	0.722	20.5
1.6	0.845	20.9	71.5	12.6	0.725	17.4
1.7	0.917	18.0	69.1	11.4	0.783	14.5

indispensable to ensure the current matching condition with the bottom c-Si solar cell. Fig. 4 shows illuminated J-V characteristics with respect to the thickness of the top CIGS solar cell. First, the efficiencies of the CIGS solar cells remain almost constant until a thickness of 0.5  $\mu\text{m}$  (see Fig. 4(a)). However, beyond this point (i.e., less than 0.5  $\mu\text{m}$ ), the efficiencies begin to decline, mostly due to the decrease in  $J_{\text{SC}}$  (see Fig. 4(b)). In fact, incomplete light absorption occurs even when the CIGS thickness is less than 1  $\mu\text{m}$ . However, the fill factor improvement with the CIGS absorber thinning compensates the loss from the incomplete light absorption (see Fig. 4(d)). Thus, the decline of the efficiencies is only evident for absorber layers thinner than 0.5  $\mu\text{m}$ . The reason for the fill factor improvement is based on the reduction of SRH recombination. For example, a CIGS solar cell ( $E_g = 1.7$  eV) with a thickness of 1.0  $\mu\text{m}$  have approximately 35% greater SRH recombination current than that with a thickness of 0.25  $\mu\text{m}$  at  $V = 0$  V. Basically, the SRH recombination reduction is attributed to the decrease of the device volume. Consequently, it helps to maintain  $V_{\text{OC}}$  even when the absorber thickness is considerably thinner than a normal thickness (i.e.,  $\geq 1$   $\mu\text{m}$ ). The fill factor improvement (or maintaining  $V_{\text{OC}}$ ) seems to be uncommonly observed; however, there are several previous works reporting solar cells with a thin absorber that maintain a similar (even improved) fill factor and/or  $V_{\text{OC}}$  (Lundberg et al., 2003; Kim et al., 2013; Kim and Shafarman, 2016; Smestad and Ries, 1992). Nevertheless, these simulation results are built on the assumption that the thickness of a CIGS absorber does not affect any of shunting, recombination mechanisms, or interfaces. As a result, the CIGS solar cells with thin absorber layers (i.e.,

$< 1$   $\mu\text{m}$ ) preserve their device behaviors compared to cells with normal absorber layer thicknesses (i.e.,  $\geq 1$   $\mu\text{m}$ ).

### 3.2. Bottom-subcell simulations

In this work, a c-Si solar cell with a typical performance was employed as the bottom-subcell in the tandem solar cell. More specifically, this simulation of the c-Si solar cell is modeled after an in-house c-Si solar cell, which exhibits an efficiency of 18.7% with  $V_{\text{OC}} = 637$  mV,  $J_{\text{SC}} = 37.2$   $\text{mA}/\text{cm}^2$ , and fill factor = 78.9% (Jeong et al., 2014). The structure and device fabrication procedure are described in detailed in elsewhere (Do et al., 2014; Lee et al., 2015). Basically, the simulation of the c-Si solar cells is mostly based on the default parameters provided with the SCAPS-1D; the charge carrier densities of each layer are measured values. However, to account for optical loss from the  $\text{SiN}_x$  passivation layer, a measured absorption profile was incorporated into the simulation. Fig. 5 presents the simulated J-V curve of the c-Si solar cell. The simulated device exhibits an efficiency of 18.7% with  $V_{\text{OC}} = 639$  mV,  $J_{\text{SC}} = 36.9$   $\text{mA}/\text{cm}^2$ , and fill factor = 79.4%, indicating that the difference between the real and simulated results is insignificant.

### 3.3. Tandem cell simulations

A straightforward strategy was used to simulate CIGS/c-Si tandem solar cells. First, light transmission through the top CIGS sub-cells were calculated using each layer's absorption profiles, and

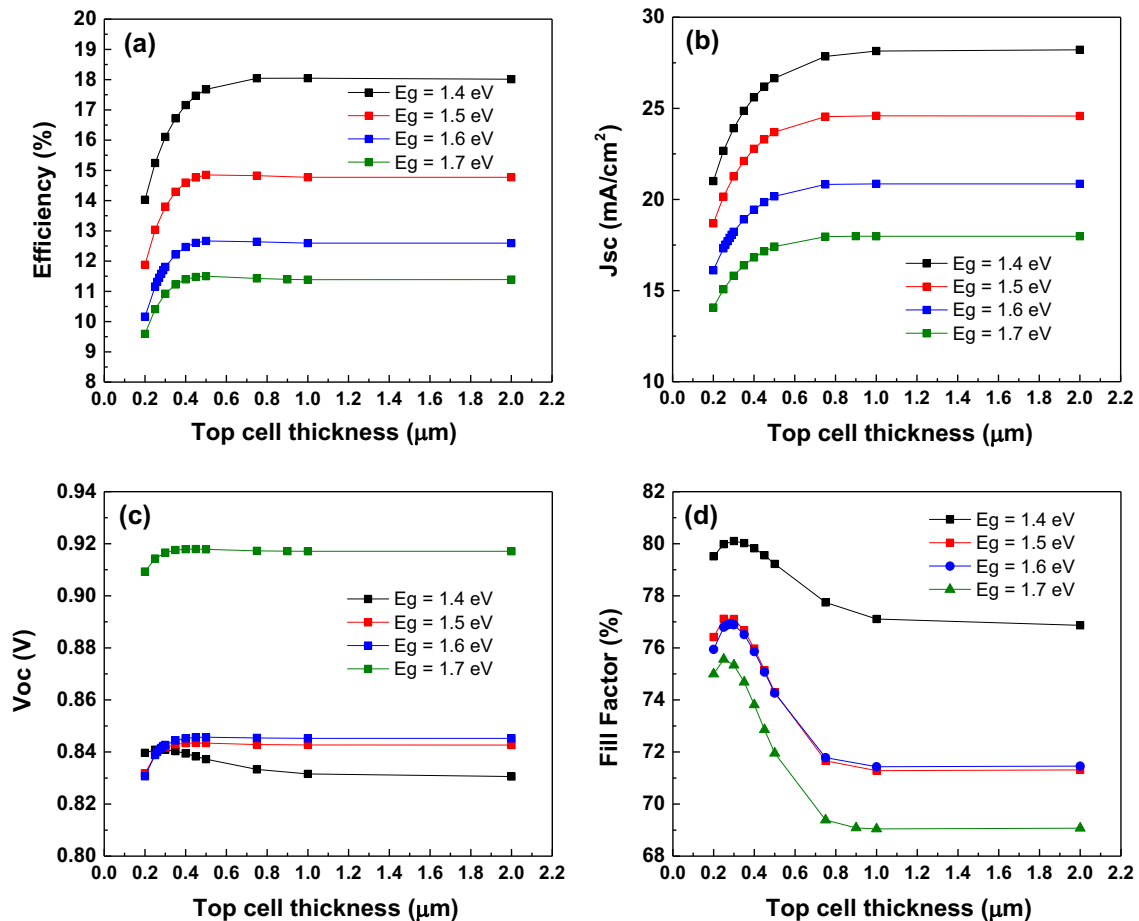


Fig. 4. Simulated light J-V characteristics with respect to the absorber thickness: (a) efficiency, (b)  $J_{\text{SC}}$ , (c)  $V_{\text{OC}}$ , and (d) FF.

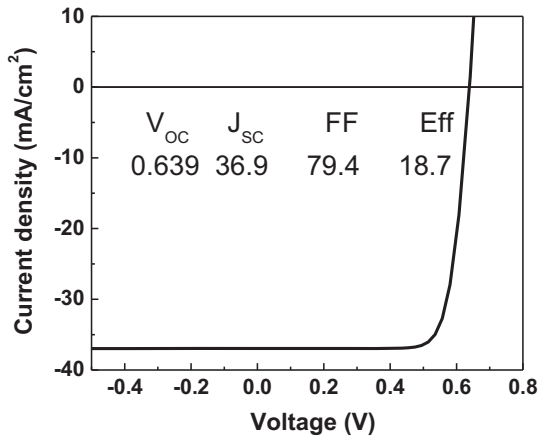


Fig. 5. Simulated J-V curve of a c-Si solar cell.

then the transmitted light spectra were used as the incident light of the bottom c-Si subcells.

In the present study, the current matching condition is defined as the condition where the top and bottom subcells have either the same  $J_{MPP}$  or  $J_{SC}$  value. In other words, each combination of CIGS/c-Si tandem cells can achieve up to two current matching conditions. Some previous studies only defined the current matching condition using the  $J_{SC}$  (Elbar et al., 2015; Ho Song et al., 2015). However, using  $J_{MPP}$  can be more advantageous in the present study because the bottom c-Si solar cell has a significantly greater fill factor than

the top CIGS subcells. By allowing the currents of the two subcells to have the same  $J_{MPP}$ , a greater fill factor from the tandem solar cell can be obtained in this study (Friedman et al., 2010). In addition, further top-subcell-thinning should be performed to match the same  $J_{SC}$  from the top and bottom subcells. If the top and bottom subcells have similar fill factors (e.g., III-V tandem cells), then both approaches (i.e., matching  $J_{SC}$  vs. matching  $J_{MPP}$ ) should provide similar results. Thus, both the cases should be examined.

Fig. 6 displays the  $J_{MPP}$  and  $J_{SC}$  values of the top and bottom subcells with respect to the thicknesses of the CIGS absorber in the top subcells. First, the CIGS solar cells with  $E_g = 1.4$  and  $1.5$  eV failed to meet the current matching condition until the CIGS absorber thickness =  $0.2 \mu\text{m}$ . However, the  $1.6$ -eV-CIGS solar cells with absorber thickness =  $0.27$  and  $0.24 \mu\text{m}$  were found to have both of the  $J_{MPP}$  and  $J_{SC}$  current matching conditions with the bottom c-Si solar cells, respectively. Not surprisingly, the  $1.7$ -eV-CIGS solar cell was also found to have two current matching points with the bottom c-Si solar cell at  $J_{MPP} = 14.5 \text{ mA/cm}^2$  (thickness =  $1.0 \mu\text{m}$ ) and  $J_{SC} = 17.1 \text{ mA/cm}^2$  (thickness =  $0.44 \mu\text{m}$ ).

With the current matching conditions above, CIGS/c-Si tandem solar cells were simulated; their J-V characteristics are given in Fig. 7 and Table 3. The construction of J-V curves of the tandem solar cells is based on the assumption that the lower-current subcell dominates the JV characteristic of a tandem solar cell (Kurtz et al., 1994). The simulated results revealed all of the combinations (i.e., Fig. 7(a)–(d)) exhibit similar conversion efficiencies of approximately 19–20%, indicating that the tandem devices do not significantly exceed the device performance of an optimized single-junction CIGS solar cell. Considering practical issues, the

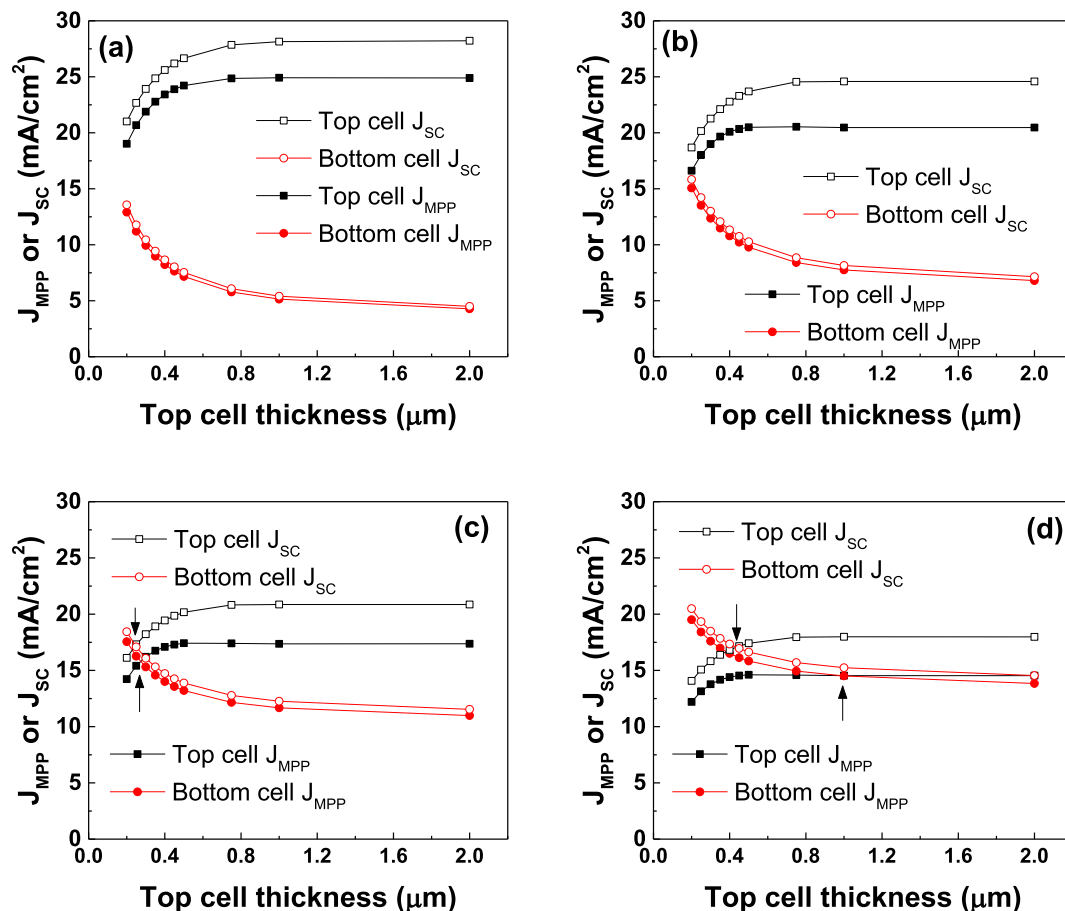
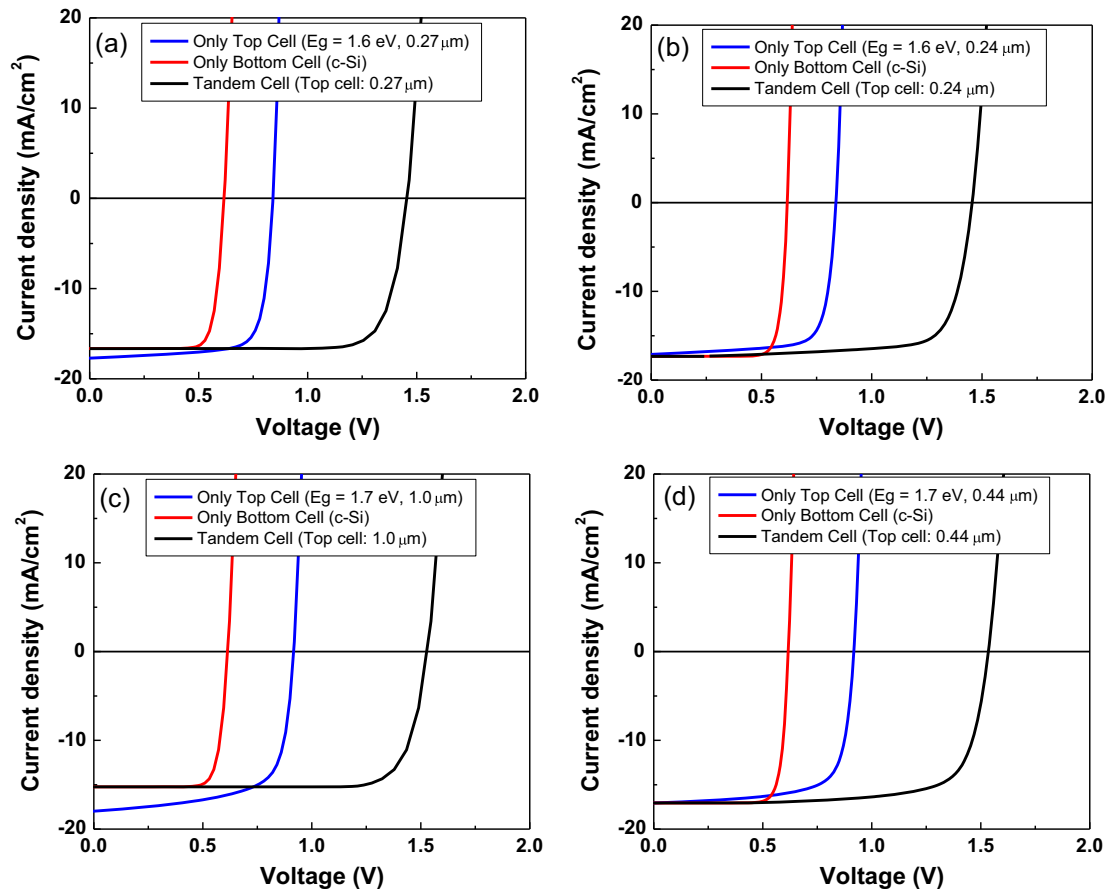


Fig. 6.  $J_{MPP}$  and  $J_{SC}$  Comparisons between the top- and bottom-subcells. Top CIGS subcell bandgap: (a)  $1.4 \text{ eV}$ ; (b)  $1.5 \text{ eV}$ ; (c)  $1.6 \text{ eV}$ ; and (d)  $1.7 \text{ eV}$ . The current matching points are indicated with arrows.



**Fig. 7.** Light J-V curves of tandem CIGS/c-Si solar cells. Bandgap of the top CIGS subcell = 1.6 eV: (a)  $J_{MPP}$ - and (b)  $J_{SC}$ -matching conditions; Bandgap of the top CIGS subcell = 1.7 eV: (c)  $J_{MPP}$ - and (d)  $J_{SC}$ -matching conditions.

**Table 3**

Light J-V characteristics of the CIGS/c-Si tandem solar cells shown in Fig. 7.

Top cell condition	Voc (V)	Jsc (mA/cm <sup>2</sup> )	FF (%)	$\eta$ (%)	V <sub>MPP</sub> (V)	J <sub>MPP</sub> (mA/cm <sup>2</sup> )
(a) 1.6 eV (t = 0.27 $\mu$ m)	1.454	16.7	81.5	19.8	1.253	15.8
(b) 1.6 eV (t = 0.24 $\mu$ m)	1.455	17.3	77.1	19.4	1.258	15.4
(c) 1.7 eV (t = 1.0 $\mu$ m)	1.526	15.2	81.9	19.0	1.310	14.5
(d) 1.7 eV (t = 0.44 $\mu$ m)	1.535	17.1	74.7	19.6	1.323	14.8

engineering window must be far narrower than that expected from the present study. One of the major concerns not discussed here is the optical losses that inevitably occur at each interface and layer. In the present study, only absorption in each layer is taken into account; however, other optical loss factors, such as reflection and haze, must deteriorate light transmission, suggesting the optical design of tandem solar cells should be more sophisticated. Nevertheless, to guarantee the appropriateness for the pursuit of CIGS/c-Si tandem solar cells, improving the top-cell efficiencies should be addressed. To obtain a 25% efficient CIGS/c-Si tandem solar cell (without improving the bottom cell's efficiency), a  $\geq 17\%$ -efficient wide bandgap CIGS solar cell ( $E_g \geq 1.6$  eV), should first be demonstrated.

#### 4. Conclusions

Tandem solar cells consisting of top CIGS and bottom c-Si subcells were computationally examined using the SCAPS-1D simulation tool. First, CIGS solar cells (top subcell) of various bandgaps (i.e., 1.4, 1.5, 1.6, and 1.7 eV) having state-of-the-art efficiencies and a conventional c-Si solar cell (bottom subcell) were simulated

separately. Next, with CIGS absorber thinning, the current matching condition with the bottom c-Si subcell was examined. The CIGS subcells with  $E_g = 1.4$  and  $1.5$  eV were found to not achieve the current matching condition until thickness =  $0.2 \mu\text{m}$ . Tandem devices with top CIGS subcells having  $E_g = 1.6$  and  $1.7$  eV exhibited the current matching conditions before the absorber thickness reached  $0.2 \mu\text{m}$ ; nevertheless, these tandem devices were found to have similar device performances compared to the bottom c-Si solar cell. These results indicated that improving the efficiency from the top CIGS subcell is essential to ensure a benefit from the tandem device.

#### Conflict of interest

The authors declare no competing financial interests.

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