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Effect of Ga/(In+Ga) ratio on the Efficiency of $Cu(In_xGa_{1-x})Se_2$ (CIGS) Thin-Film Solar Cells

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ABSTRACT

Copper indium gallium diselenide ($Cu(In_xGa_{1-x})Se_2$, CIGS) continues to attract significant interest as an absorber layer in thin-film solar cells owing to its high absorption coefficient, long carrier diffusion length, and tunable bandgap. A key factor governing its performance is the Ga/(In+Ga) ratio, which directly influences the electronic structure, defect formation, and carrier transport within the absorber. In this study, numerical simulations were carried out using SCAPS-1D to systematically investigate the effect of Ga incorporation across the full compositional range (x = 0–1). Composition-dependent models were employed to account for bandgap variation, electron affinity, acceptor density, defect states, and density of states. The results demonstrate that gallium incorporation significantly modifies device behavior. Increasing Ga content leads to bandgap widening, which enhances the open-circuit voltage (V_{OC}) but reduces the short-circuit current density (J_{SC}) due to diminished absorption in the longer wavelength region. Conversely, indium-rich compositions exhibit stronger photocurrent generation but suffer from lower voltages. The fill factor (FF) exhibits a maximum of ~61% at Ga fraction x = 0.6, while the overall device efficiency follows a bell-shaped dependence, peaking at 11.7% for x = 0.4. These results reveal a trade-off between voltage and current that must be carefully balanced through absorber composition engineering. Overall, this study identifies the optimal Ga/(In+Ga) ratio to lie within the range of 0.3–0.6, where a balance between Jsc, V_{OC} and FF yield the best photovoltaic response. The insights provided here can serve as practical guidelines for tailoring CIGS absorber layers to achieve improved device efficiency.

Keywords:
CIGS solar cells,
Gallium composition,
SCAPS-1D simulation,
Photovoltaic performance.

INTRODUCTION

Copper indium gallium diselenide ($Cu(In_xGa_{1-x})Se_2$ or CIGS) thin-film solar cells have emerged as one of the leading thin-film photovoltaic technologies owing to their high optical absorption coefficient, adjustable electronic properties, and impressive laboratory efficiencies that now exceed 20 % (Stanbery *et al.*, 2021; Thomas *et al.*, 2022). A unique advantage of the CIGS system is its tunable bandgap, which can be engineered by adjusting the Ga/(In+Ga) ratio, often denoted as x, from 0 (pure $CuInSe_2$) to 1 (pure $CuGaSe_2$). This compositional control provides a powerful means of balancing photon absorption with voltage output, thereby enabling optimization of device performance (Lundberg *et al.*, 2005; Machkih *et al.*, 2024) .

Both experimental and theoretical studies have established that increasing the Ga fraction raises the bandgap from approximately 1.04 eV in $CuInSe_2$ up to nearly 1.7 eV in $CuGaSe_2$ (Kong *et al.*, 2005; Thomas *et al.*, 2022). However, this variation is not linear; instead, it exhibits a characteristic “bowing” behavior, necessitating careful parameterization for accurate modeling and device design. From a photovoltaic perspective, a higher Ga/(In+Ga) ratio typically results in an increased open-circuit voltage (Voc), but this benefit comes at the cost of reduced long-wavelength absorption, leading to a decrease in short-circuit current density (Jsc) and a trade-off in overall power conversion efficiency (Gloeckler & Sites, 2005; Machkih *et al.*, 2024).

To address this trade-off, researchers have explored bandgap engineering through Ga grading, where the Ga concentration is varied across the depth of the absorber. A composition profile that increases the Ga fraction towards the back contact has been shown to create a built-in quasi-electric field that aids charge separation, reduces back-surface recombination, and enhances carrier collection (Dullweber *et al.*, 2002; Lundberg *et al.*, 2005) . Nevertheless, despite these advantages, high Ga incorporation can introduce material challenges, including reduced carrier mobility, increased defect density due to compensation mechanisms, poorer crystalline quality, and unfavorable band alignment at the heterointerface with buffer or window layers (Machkih *et al.*, 2024; Thomas *et al.*, 2022).

In this paper, we systematically explore how the Ga/(In+Ga) ratio in the absorber affects key material parameters; bandgap, electron affinity, defect levels, effective densities of states, carrier mobilities, and doping density and then assess their combined impact on simulated solar cell performance using the SCAPS-1D simulation tool (Burgelman *et al.*, 2000). By parameterizing the CIGS absorber as a function of composition (x = 0.2, 0.4, 0.6, 0.8, and 1.0), constructing SCAPS .def files for each composition, and running standard JV and quantum-efficiency simulations, we aim to identify the optimal Ga fraction that maximizes conversion efficiency while balancing Voc and Jsc tradeoffs.

Parameterization of $Cu(In_xGa_{1-x})Se_2$ Absorber Layer *Equations*

The material parameters (see Table 1) of the CIGS absorber were varied as a function of indium fraction x (0.2–1.0) using composition-dependent models established in chalcopyrite literature. The bandgap was modeled using the bowing relation (Rau & Schock, 1999; Shafarman *et al.*, 2011). The electron affinity was linearly interpolated between $CuInSe_2$ $(\chi = 4.58\,eV)$ and $CuGaSe_2$ $(\chi = 4.20\,\text{eV})$ based on reported band alignments (Wei *et al.*, 1998); (Minemoto *et al.*, 2003). Hole mobility and net acceptor density were modeled empirically, decreasing with gallium incorporation due to enhanced compensation by donor-like GaCu defects (Sites & Mauk, 1989); (Gloeckler & Sites, 2005). A single deep defect level was introduced 0.6 eV above the valence band edge, consistent with reported selenium vacancy and antisite defect levels (Zhu *et al.*, 2008).

The effective density of states in the conduction and valence bands was adjusted consistently with changes in the bandgap energy. A reference value of $2.0 \times 10^{24}\ \text{m}^{-3}$ was used at a bandgap of 1.2 eV, and values were scaled using the effective mass approximation so that they varied smoothly with the Ga/(In+Ga) composition ratio. This approach follows the treatment outlined by Sze & Ng (2007), ensuring physically consistent material parameters across the full compositional range.

Table 1: Parameters and equations

Parameter	Equation / Value	Reference(s)
Bandgap $E_g(x)$	$E_g(x) = xE_g^{\text{CIS}} + (1-x)E_g^{\text{CGS}} - b\,x(1-x)$ with $E_g^{\text{CIS}} = 1.04\,\text{eV}, E_g^{\text{CGS}} = 1.68\,\text{eV}, b = 0.20\,\text{eV}$	(Rau & Schock, 1999; Shafarman *et al.*, 2011)
Electron affinity $\chi(x)$	Linear interpolation: $\chi(x) = x\chi^{\text{CIS}} + (1-x)\chi^{\text{CGS}}$ with $\chi^{\text{CIS}} = 4.58\,eV, \chi^{\text{CGS}} = 4.20\,eV$	(Minemoto *et al.*, 2003; Wei *et al.*, 1998)
Hole mobility $\mu_p(x)$	Empirical trend (decreasing with Ga): $5.0 \times 10^{-4}\ (x = 0.2) \rightarrow 2.0 \times 10^{-3}\ (x = 1.0)\ m^2/V \cdot s$	(Gloeckler & Sites, 2005; Sites & Mauk, 1989)
Acceptor density $N_a(x)$	Empirical reduction with Ga: $1.0 \times 10^{21}(x = 0.2) \rightarrow 5.5 \times 10^{21}(x = 1.0) m^{-3}$, due to Ga_{Cu} donor compensation	(Gloeckler & Sites, 2005; Sites & Mauk, 1989)
Defect energy level $E_t(x)$	$E_t = E_g(x) - 0.6$ (≈0.6 eV above V_B)	(Zhu *et al.*, 2008)

Conduction band DOS $N_c(x)$	$N_c(x) = N_c(0)\left(\frac{E_g(x)}{E_g(0)}\right)^{3/2}$, with $N_c^0 = 2.0 \times 10^{24}\ \mathrm{m}^{-3}$ at $E_g(0) = 1.2\ eV$	(Sze *et al.*, 2021)
Valence band DOS $N_v(x)$	$N_v(x) = N_v(0)\left(\frac{E_g(x)}{E_g(0)}\right)^{3/2}$ with $N_v^0 = 2.0 \times 10^{24}\ \mathrm{m}^{-3}$ at $E_g(0) = 1.2\ eV$	(Sze *et al.*, 2021)

Computed parameter values

Table 2 presents the composition-dependent material parameters for ($Cu(In_xGa_{1-x})Se_2$ absorber layers, computed using the semi-empirical models described in Section 2.1. These values including bandgap, electron affinity, hole mobility, net acceptor density, trap energy level, and effective density of states; were derived for Ga fractions x = 0.2, 0.4, 0.6, 0.8, and 1.0, and serve as input for SCAPS-1D device simulations.

Table 2: Computed parameter values

x	$E_g(x)$ [eV]	chi(x) [eV]	Hole Mobility μ [m^2/V·s]	Donor N(x) [m^{-3}]	Et [eV]	$N_c(x)$ [m^{-3}]	$N_v(x)$ [m^{-3}]
0.2	1.52	4.276	0.0005	1.00×10^{21}	0.92	2.85×10^{24}	2.85×10^{24}
0.4	1.376	4.352	0.000875	2.13×10^{21}	0.776	2.46×10^{24}	2.46×10^{24}
0.6	1.248	4.428	0.00125	3.25×10^{21}	0.648	2.12×10^{24}	2.12×10^{24}
0.8	1.136	4.504	0.001625	4.38×10^{21}	0.536	1.84×10^{24}	1.84×10^{24}
1	1.04	4.58	0.002	5.50×10^{21}	0.44	1.61×10^{24}	1.61×10^{24}

MATERIALS AND METHODS

In this work, the effect of the Ga/(In+Ga) ratio on the performance of $Cu(In_xGa_{1-x})Se_2$ (CIGS) thin-film solar cells was investigated using the one-dimensional device simulator SCAPS-1D (Burgelman *et al.*, 2000). The material parameters of CIGS were determined as a function of composition (x = 0.2, 0.4, 0.6, 0.8, and 1.0) based on empirical equations and literature values. The bandgap $E_g(x)$ was calculated using a quadratic interpolation between $CuInSe_2$ (CIS) and $CuGaSe_2$ (CGS), including a bowing parameter. Electron affinity $\chi(x)$ was obtained through linear interpolation between CIS and CGS. Hole mobility and acceptor density were assigned according to experimentally observed Ga-dependent trends, while the defect energy level $E_t(x)$ was defined at approximately 0.6 eV above the valence band. The conduction band effective density of states $N_c(x)$ and the valence band effective density of states $N_v(x)$ were scaled with the bandgap according to a $\left(\frac{E_g(x)}{E_g(0)}\right)^{3/2}$ dependence. All equations and reference values were taken from the literature to ensure realistic modeling.

The calculated parameters were compiled for each composition and used to generate the Solar Cell Capacitance Simulator (SCAPS-1D) (Burgelman *et al.*, 2000) definition (.def) files representing CIGS absorber layers with varying Ga/(In+Ga) ratios. Device structures were constructed following the typical configuration: glass / ZnO:Al / i-ZnO / CdS buffer / CIGS absorber / Mo back contact. The .def files were then employed in SCAPS to simulate current–voltage (J–V) characteristics under standard AM1.5G illumination conditions (1000 W/m², 300 K). From these SCAPS-1D simulations, photovoltaic parameters including open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and conversion efficiency (η) were extracted and analyzed as a function of Ga content.

RESULTS AND DISCUSSION

Table 3 presents the photovoltaic performance parameters of $Cu(In_xGa_{1-x})Se_2$ (CIGS) solar cells as a function of the indium mole fraction (x). The results highlight how changes in composition influence the open-circuit voltage (Voc), short-circuit current density (Jsc), fill factor (FF), and overall efficiency of the devices.

Table 3 Photovoltaic Performance Parameters of CIGS Solar Cells at different Indium Compositions

$Cu\ (In_xGa_{1-x})\ Se_2$	Voc (V)	Jsc (mA/cm²)	FF (%)	Efficiency (%)
$x = 0$	1.7973	16.907024	34.17	10.38
$x = 0.2$	1.0542	21.253893	51.16	11.46
$x = 0.4$	0.7340	26.211581	60.66	11.67
$x = 0.6$	0.5858	30.359989	61.26	10.90
$x = 0.8$	0.4818	34.017530	60.30	9.88
$x = 1.0$	0.4098	36.681919	57.19	8.60

Figures (1-4) shows the variation of photovoltaic performance parameters of CIGS solar cells as a function of the indium mole fraction (x). The results show how the open-circuit voltage **(**Voc**)** [Figure 1], short-circuit current density (Jsc) [Figure 2], fill factor (FF) [Figure 3], and overall efficiency [Figure 4] respond to compositional changes between the two end members, $CuGaSe_2$ (x = 0) and $CuInSe_2$ (x = 1).

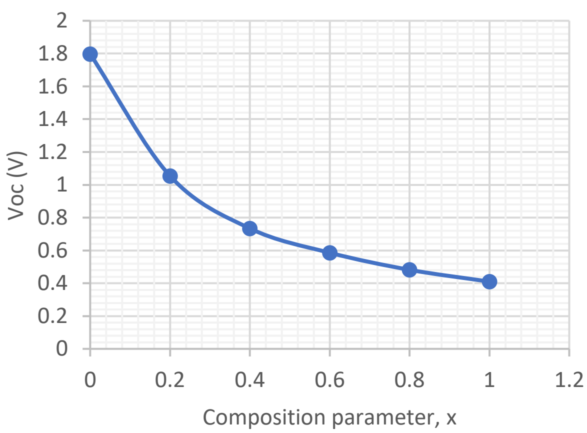

Figure 1: Graph of Voc against Composition parameter

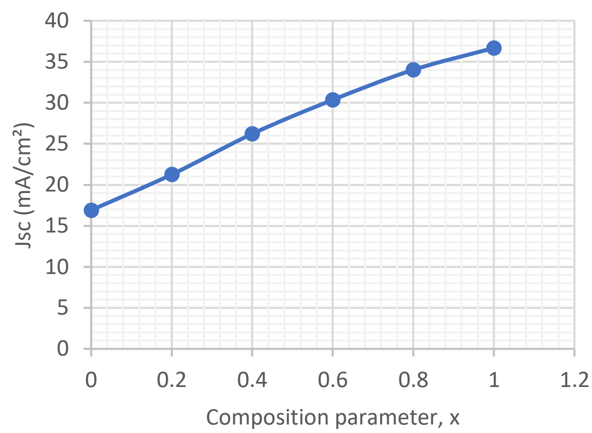

Figure 2: Graph of Jsc against Composition parameter

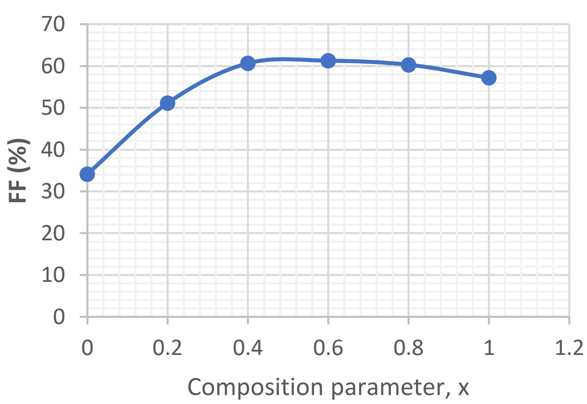

Figure 3: Graph of FF against Composition parameter

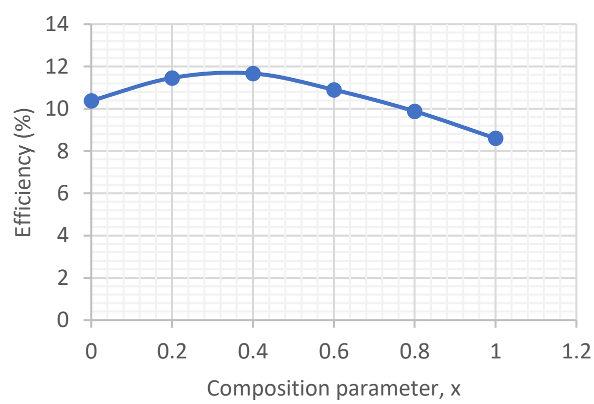

Figure 4: Graph of Efficiency against Composition parameter

The performance data obtained in this work highlight the classic trade-off in CIGS absorbers: increasing indium content reduces the bandgap (from ~1.80 eV at $x = 0$ to ~0.41 eV $at\ x = 1$), leading to a significant rise in short-circuit current density J_{sc} from 16.9 to 36.7 mA/cm^2. This increase reflects the broader spectral absorption of narrower-bandgap materials. The obtained values are consistent with literature, where $CuInSe_2$ devices routinely exceed 35 mA/cm² under AM1.5G illumination, while Ga-rich alloys typically show Jsc<20 mA/cm^2 due to their wide bandgaps (Repins *et al.*, 2008). In contrast, the open-circuit voltage Voc decreases monotonically with higher indium content, from ~1.80 V for $CuGaSe_2$ to ~0.41 V for $CuInSe_2$. This trend follows the Shockley–Queisser detailed balance model, where $V_{oc} \approx E_g/q - (kT/q)\ln(J_0/J_{sc})$ (Shockley & Queisser, 2018). The reduction in Voc with indium incorporation is further exacerbated by higher defect densities and shorter minority carrier lifetimes in $CuInSe_2$ compared to Ga-rich films. The near-ideal Voc of $CuGaSe_2$ indicates very low nonradiative recombination losses at the Ga-rich end. The fill factor (FF) exhibits a non-linear trend, improving from 34% at $x = 0$ to a peak of ~61% at $x = 0.6$, before declining slightly at $x = 1$. This suggests that intermediate compositions benefit from improved charge transport and reduced series resistance, while In-rich alloys suffer from increased recombination or interface defects. Consequently, efficiency follows a bell-shaped dependence on composition, peaking at 11.7% for $x = 0.4$. This result is in line with long-standing observations that optimal Ga/(Ga+In) ratios lie between 0.3 and 0.6 for single-junction CIGS cells (Rau & Schock, 1999). Although the reported peak efficiency is below the current record (~23.6%), it captures the intrinsic absorber performance prior to advanced interface and alkali optimizations.

CONCLUSION

This study demonstrates that the Ga/(In+Ga) ratio exerts a decisive influence on the photovoltaic performance of CIGS absorbers. Increasing gallium widens the bandgap and enhances open-circuit voltage, but reduces long-wavelength absorption and limits current generation. Conversely, indium-rich compositions maximize photocurrent but suffer severe voltage losses. The balance between these opposing trends results in an optimal composition window ($x = 0.3 - 0.6$), where efficiency peaks at ~11.7%. This efficiency, though below record values, reflects intrinsic absorber behavior in the absence of advanced interface engineering, alkali treatments, or graded bandgap profiles. The results reaffirm the centrality of bandgap engineering in CIGS technology and highlight the need for complementary strategies such as defect passivation, interface band alignment control, and tandem integration to overcome the open-circuit voltage deficit and push device performance beyond current limits.

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