Optoelectronic optimization of graded-bandgap thin-film AlGaAs solar cells

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An optoelectronic optimization was carried out for an Al$_{\xi}$Ga$_{1-\xi}$As (AlGaAs) solar cell containing (i) an $n$-AlGaAs absorber layer with a graded bandgap and (ii) a periodically corrugated Ag backreflector combined with localized ohmic Pd–Ge–Au backcontacts. The bandgap of the absorber layer was varied either sinusoidally or linearly. An efficiency of 33.1% with the 2000-nm-thick $n$-AlGaAs absorber layer is predicted with linearly graded bandgap along with silver backreflector and localized ohmic backcontacts, in comparison to 27.4% efficiency obtained with homogeneous bandgap and a continuous ohmic backcontact. Sinusoidal grading of the bandgap is predicted to enhance the maximum efficiency to 34.5%. Thus, grading the bandgap of the absorber layer, along with a periodically corrugated Ag backreflector and localized ohmic Pd-Ge-Au backcontacts, can help realize ultrathin and high-efficient AlGaAs solar cells for terrestrial applications. © 2020 Optical Society of America

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1. INTRODUCTION

Highly efficient and cost-effective solar cells made ecoresponsibly [1] of Earth-abundant materials with low after-use disposal environmental cost are necessary for sustainability [2]. With crystalline-silicon (Si) delivering about 26% efficiency and multicrystalline-Si about 22% efficiency, Si is the photovoltaic material of choice for solar-photovoltaic modules deployed in solar parks and on rooftops [3,4]. With somewhat higher efficiency and significantly lower weight-to-power ratio [5], gallium arsenide (GaAs) is the current market leader for solar cells deployed for extraterrestrial applications, but it is prohibitively expensive for terrestrial applications [6].

There are two options to reduce the cost of the GaAs solar cell. The first option is the reduction of the thickness of the GaAs absorber layer [7–9]. Not only will that option reduce material usage, but it will also enhance manufacturing throughput. However, a thinner absorber layer will reduce the absorption of incident solar photons. Back-surface modifications such as plasmonic nanostructures [8,10,11], localized ohmic backcontacts [9], and highly reflective backrefectors [9] have been investigated to tackle the problem of low absorption in ultrathin GaAs solar cells, but enhanced photon trapping does not necessarily translate into higher efficiency [12,13].

The second option is to grade the bandgap in the absorber layer by adding aluminum (Al) and controlling the compositional ratio of Al to gallium (Ga) [14,15]. Bandgap grading of the resulting Al$_{\xi}$Ga$_{1-\xi}$As (AlGaAs) absorber layer will allow photon absorption over a wider frequency range. Also, bandgap grading will increase efficiency by creating a drift electric field that will accelerate photogenerated holes towards the $p$–$n$ junction in the solar cell [14]. Linear bandgap grading has been shown experimentally to increase the open-circuit voltage $V_{oc}$ in AlGaAs solar cells [16], which should assist in enhancing the efficiency $\eta$; however, suboptimal bandgap grading can reduce the short-circuit current density $J_{sc}$ to offset the increase in $V_{oc}$.

A recent theoretical study on CIGS solar cells shows that $V_{oc}$ can be enhanced while maintaining or even enhancing $J_{sc}$ [13], by optimally grading the bandgap of the absorber layer. Motivated by these results, we combined both options, i.e., thinning [7–9] and bandgap grading [14–16] of the absorber layer in a coupled optoelectronic model [17] of a thin-film AlGaAs solar cell. We then used the model to determine optimal geometric and bandgap-grading parameters to maximize $\eta$.

The thickness of the AlGaAs absorber layer was allowed to vary from 100 nm to 2000 nm, and the bandgap was allowed to vary either linearly or sinusoidally along the thickness direction. In addition, we incorporated a highly reflective periodically...
corrugated silver (Ag) backreflector and localised ohmic back-
contacts of palladium (Pd), germanium (Ge), and gold (Au) trilayers [9], with the areal ratio ξ ∈ (0, 1) of Pd-Ge-Au and Ag
being a geometric parameter for optimization. When ξ = 1, the
Ag backreflector is absent while a Pd–Ge–Au trilayer extends
across the entire back surface as is typical for a GaAs solar
cell [7,18].

The coupled optoelectronic model has an optical part and
an electrical part. In the optical part, the rigorous coupled-wave
approach (RCWA) [19,20] is used to determine the electron–
hole-pair generation rate in the semiconductor layers of the
solar cell [13,17], assuming normal illumination by unpolarized
polychromatic light endowed with the AM1.5G solar spectrum
[21]. In the electrical part, the electron–hole-pair generation
rate is used as an input to the one-dimensional (1D) drift-
diffusion equations [22,23] applied to the semiconductor layers.

These equations are solved using a hybridizable discontinuous
Galerkin (HDG) scheme [24–28] to determine the current
density Jdev and the electrical power density P = Jdev Vext as
functions of the bias voltage Vext under steady-state conditions.
In turn, the Jdev−Vext and the P−Vext curves yield Jsc, Voc, and
η. Finally, the differential evolution algorithm (DEA) [29]
is used to maximize η as a function of various geometric and
bandgap-grading parameters.

The structure of this paper is as follows. Section 2 contains
the optical and the electrical descriptions of the AlGaAs solar
cell. As implementation details for the optical [12,17] and
the electronic parts [13,17] of the model as well as the DEA
[30,31] for solar-cell problems have been published, we have
not provided them in this paper. Section 3 is divided into four
subsections. The efficiency of the solar cell with a 2000-nm-
 thick GaAs layer as predicted by the model is compared with
experimental results [18] in Section 3.A.1. The effects of the
periodically corrugated Ag backreflector along with localized
ohmic Pd–Ge–Au backcontacts on the performance of the
GaAs solar cells are discussed in Section 3.A.2. Next, optimal
results for solar cells with a homogeneous AlGaAs absorber
layer (Section 3.B), an AlGaAs absorber layer with linearly graded
bandgap (Section 3.C), and an AlGaAs absorber layer with
sinusoidally graded bandgap (Section 3.D) are provided, each
solar cell possessing a periodically corrugated Ag backreflector
along with localized ohmic Pd–Ge–Au backcontacts. The paper
concludes with some remarks in Section 4.

2. OPTICAL AND ELECTRICAL DESCRIPTIONS

The solar cell occupies the region \( \mathcal{X} : \{(x, y, z) : -\infty < x < \infty, -\infty < y < \infty, 0 < z < L_x\} \), with the half spaces \( z < 0 \) and
\( z > L_x \) occupied by air. The reference unit cell, identified as \( \mathcal{R} : \{(x, y, z) : -L_x/2 < x < L_x/2, -\infty < y < \infty, 0 < z < L_x\} \), is schematically depicted in Fig. 1.

The region \( 0 < z < L_{\text{MgF}_2} = 110 \text{ nm} \) is occupied by magnesium
fluoride (MgF\(_2\)) [32], and the region \( L_{\text{MgF}_2} < z < L_{\text{ARC}} = 150 \text{ nm} \) is occupied by zinc sulfide (ZnS) [33], the two
layers collectively functioning to reduce light reflection [18].

The region \( L_{\text{ARC}} < z < L_{\text{ARC}} + L_{\text{FSP}} \) is a 20-nm-thick front-
surface passivation (FSP) layer of \( p^+\text{Al}_{0.51}\text{Ga}_{0.49}\text{As} \) (hereafter referred
to as AlInP) [34] to reduce the front-surface recombination rate
and thereby improve \( J_{sc} \) [35]. Next, homogeneous

\[
p^+\text{Al}_{g_1-x}\text{Ga}_{1-x}\text{As} [36] \text{ with fixed } \xi \text{ occupies the 50-nm-thick region } L_{\text{ARC}} + L_{\text{FSP}} < z < L_{\text{ARC}} + L_{\text{FSP}} + L_w \text{ to form a } p-n
\text{ junction with an } n\text{-Al}_{g_1-x}\text{Ga}_{1-x}\text{As} [36] \text{ absorber layer of thickness } L_s \in [100, 2200] \text{ nm}. \text{ The quantity } \xi \text{ is taken to be dependent}
on z in this paper. \text{ With } L_d = L_{\text{ARC}} + L_{\text{FSP}} + L_w + L_s + L_{\text{BSP}}, \text{ the region } L_d - L_{\text{BSP}} < z < L_d \text{ of thickness } L_{\text{BSP}} = 20 \text{ nm}
is a back-surface passivation (BSP) layer of \( n^+\text{-Ga}_{0.49}\text{In}_{0.51}\text{P} \) (hereafter referred to as GaInP) [37] to reduce the back-surface recombination rate and thereby improve \( J_{sc} \) [35,38].

The region \( L_d < z < L_d + L_m \) in \( \mathcal{R} \) has a complicated
morphology. A Pd–Ge–Au triple layer of width \( \xi L_s, \xi \in (0, 1) \),
along the \( x \) axis serves as the localized ohmic backcontact
[9] comprising a Pd layer of thickness \( L_{\text{Pd}} = 20 \text{ nm} \) [39], a
Ge layer of thickness \( L_{\text{Ge}} = 50 \text{ nm} \) [40], and an Au layer of
thickness \( L_{\text{Au}} = 100 \text{ nm} \) [39]. The remainder of the region
\( L_d < z < L_d + L_m \) is occupied by Ag [39] for optical reflection.
Finally, the region \( L_d + L_m < z < L_d + L_m + L_{\text{Ag}} = L_t \),
\( L_{\text{Ag}} = 100 \text{ nm} \), is occupied by Ag serving as an optical
backreflector.

The linear variation of bandgap in the \( n\text{-AlGaAs} \) absorber
layer was modeled as [12,13]

\[
E_g(z) = E_{g,\text{min}} + A \left( E_{g,\text{max}} - E_{g,\text{min}} \right) \frac{z - (L_{\text{ARC}} + L_{\text{FSP}} + L_w)}{L_s},
\]

\[
z \in [L_{\text{ARC}} + L_{\text{FSP}} + L_w, L_{\text{ARC}} + L_{\text{FSP}} + L_w + L_s],
\]

where \( E_{g,\text{min}} \) is the minimum bandgap, \( E_{g,\text{max}} \) is the maximum
bandgap, and \( A \) is an amplitude (with \( A = 0 \) representing a
homogeneous AlGaAs layer). The bandgap is thus minimum
at the front face \( z = L_{\text{ARC}} + L_{\text{FSP}} + L_w \) and maximum at the
back face \( z = L_{\text{ARC}} + L_{\text{FSP}} + L_w + L_s \) of the absorber layer.
The reverse grading (i.e., maximum at \( z = L_{\text{ARC}} + L_{\text{FSP}} + L_w \) and
minimum at \( z = L_{\text{ARC}} + L_{\text{FSP}} + L_w + L_s \)) did not give satisfactory results.
The sinusoidal variation of the bandgap in the $n$-AlGaAs absorber layer was modeled as [12,13,41]

$$E_g(z) = E_{g,min} + A (E_{g,max} - E_{g,min}) \times \left\{ \frac{1}{2} \left[ \sin \left( 2\pi K \frac{z - (L_{ARC} + L_{FSP} + L_w)}{L_s} - 2\pi \psi \right) + 1 \right] \right\} ^n, $$

$z \in [L_{ARC} + L_{FSP} + L_w, L_{ARC} + L_{FSP} + L_w + L_z],$

where $\psi \in [0, 1]$ describes a relative phase shift, $K$ is the number of periods in the AlGaAs layer, and $K > 0$ is a shaping parameter. The parameter $\xi$ for the homogeneous $p$-AlGaAs layer governs the bandgap $E_{g,w}$ in that layer. Optical spectra of the relative permittivities of all materials used in the solar cell are provided in Appendix A.

The RCWA [19,20] was used to calculate the electric field phasor $E(x, z, \lambda_0)$ everywhere inside the solar cell as a result of illumination by a monochromatic plane wave normally incident on the plane $z = 0$ from the half space $z < 0$, $\lambda_0$ being the free-space wavelength. The electric field phasor of the incident plane wave was taken as $E_{inc}(z, \lambda_0) = E_0 \frac{\hat{z}}{\sqrt{\epsilon_0}} \exp(i k_0 z)$ with $E_0 = 4\sqrt{\epsilon_0} \lambda_0 V \text{ m}^{-1}$. With the assumption that every absorbed photon excites an electron–hole pair, the $x$-averaged electron–hole-pair generation rate was calculated as [13]

$$G(z) = \frac{\eta_0}{h E_0} \frac{1}{2} \int_{L_z/2}^{L_z/2} \int_{0,\max}^{\lambda_0,\max} \text{Im}\{\varepsilon(x, z, \lambda_0)\} \times |E(x, z, \lambda_0)|^2 S(\lambda_0) d\lambda_0 dx,$$

for $z \in [L_{ARC}, L_{Ag}]$, where $h$ is the reduced Planck constant, $\eta_0 = 120\pi$ $\Omega$ is the intrinsic impedance of free space, $S(\lambda_0)$ is the AM1.5G solar spectrum [21], $\lambda_0,\max = 300 \text{ nm}$, and $\lambda_{0,\max} = (1240/E_{g,min}) \text{ nm}$ with $E_{g,min}$ in eV. For use in the electrical part of the model, $G(z)$ contains the effects of highly reflective Ag, the localized ohmic Pd–Ge–Au back contacts, and the MgF$_2$/ZnS double-layer antireflection coating. The $x$-averaging is justified since the charge carriers generally flow along the $z$ axis because the solar cell operates under the influence of a bias voltage $V_{oc}$, applied along the same axis; furthermore, $L_z \sim 500 \text{ nm}$ is miniscule in comparison to the lateral dimensions of the solar cell.

The region $L_{ARC} < z < L_{Ag}$ contains four semiconductor layers: the $p^+$-AllnP FSP layer, the $p$-AlGaAs layer, the $n$-AlGaAs absorber layer, and the $n^+$-GaInP BSP layer. All four were incorporated in the electrical part [13,17] of the model, as all four contribute to charge-carrier generation. Electrical parameters used for all four semiconductor layers [42–46] are provided in Appendix A.

The thermal speed $\bar{v}(\lambda_0)$, the hole thermal speed $\bar{v}_{th,h}(\lambda_0)$, and the electron neutral mobility $\mu_e(\lambda_0)$ are the $x$-averaged values of $\bar{v}(\lambda_0)$, $\bar{v}_{th,h}(\lambda_0)$, and the electron mobility $\mu_e(\lambda_0)$, respectively. In the solar cell, the hole mobility $\mu_p(\lambda_0)$, and the DC relative permittivity $\varepsilon_{rel}(\lambda_0)$ were incorporated in the electrical calculations. Also, we incorporated all three recombination processes: radiative, Shockley–Read–Hall, and Auger [22,23]. The Shockley–Read–Hall recombination rate was taken to depend on $E_g(\lambda_0)$ as the trap/defect density $N_v$, the electron thermal speed $\bar{v}_{th,e}(\lambda_0)$, and the hole thermal speed $\bar{v}_{th,h}(\lambda_0)$ are $\xi$ dependent in both $Al_xGa_{1-x}As$ layers. However, the radiative recombination and Auger recombination rates were considered independent of the bandgap due to lack of available data. The electrical part yields values of $J_{sc}$, $V_{oc}$, the fill factor $FF$ [23], and $\eta$.

The DEA [29] was used to maximize $\eta$ with respect to certain geometric and bandgap parameters, using a custom algorithm implemented with MATLAB version R2019a.

### 3. NUMERICAL RESULTS AND DISCUSSION

#### A. GaAs Solar Cell

1. **Model Validation**

First, we validated our coupled optoelectronic model by comparison with the experimental results for the MgF$_2$/ZnS/AllnP/$p$-GaAs/n-GaAs/GaInP/Pd–Ge–Au solar cell containing a $L_s = 2000$-nm-thick homogeneous GaAs layer [18]; i.e., without Ag ($L_{Ag} = 0$ and $\xi = 1$ in reference to Fig. 1), $\bar{v}(\lambda_0) = 0$, and $\bar{v}(\lambda_0) \equiv 0 \forall \lambda_0 \in [L_{ARC} + L_{FSP} + L_w, L_{ARC} + L_{FSP} + L_w + L_z]$. Table 1 provides a comparison of $J_{sc}$, $V_{oc}$, $FF$, and $\eta$ obtained from our model and experimental data for GaAs cells containing a $p$-GaAs absorber layer.

| $L_{Ag}$ (nm) | $\xi$ | $J_{sc}$ ($mA cm^{-2}$) | $V_{oc}$ (V) | $FF$ (%) | $\eta$ (%) |
|---------------|-------|------------------------|--------------|-----------|-----------|
| $0$           | $1$   | $29.8$                 | $1.081$      | $85.1$    | $27.4$    |
| $300$         | $0.75$| $29.5$                 | $1.045$      | $84.6$    | $26.1$    |

For $L_{Ag} = 0$ and $\xi = 1$, the model-predicted efficiency of 27.4% is close to the highest efficiency (27.6%) reported [7] for GaAs solar cells, but geometric data is not available in Ref. [7] for a proper comparison with the model predictions.

Parenthetically, no interface defects were taken into consideration in the model, suggesting that all the experimentally observed characteristics can be accounted for by the bulk properties of MgF$_2$, ZnS, AllnP, $p$-GaAs, n-GaAs, GaInP, Pd, Ge, and Au.

2. **Effect of Localized Ohmic Backcontacts**

Typically, the Ag backreflector is absent while a Pd–Ge–Au trilayer extends across the entire back surface of a GaAs solar cell, i.e., $\xi = [7,18]$. Therefore, next we considered the effect of the localization of ohmic backcontacts by including Ag for better optical backreflection [9]. We maximized

Table 1. Comparison of $J_{sc}$, $V_{oc}$, $FF$, and $\eta$ Predicted by the Coupled Optoelectronic Model for a GaAs Solar Cell with a Homogeneous GaAs Absorber Layer ($L_{Ag} = 0$) with Experimental Data [18] for $L_{Ag} = 0$, $\xi = 1$, $L_s = 2000$ nm, and $\xi = 0$.
Table 2. $J_{sc}$, $V_{oc}$, FF, and $\eta$ Predicted by the Coupled Optoelectronic Model for a GaAs Solar Cell with a Homogeneous GaAs Absorber Layer (i.e., $A = 0$), When Ag Is Either Absent ($\zeta = 1$) or Not ($\zeta < 1$) and $L_s \in [200, 1000, 2000]$ nm

| $L_s$ (nm) | $L_x$ (nm) | $L_{Ag}$ (nm) | $J_{sc}$ (mA cm$^{-2}$) | $V_{oc}$ (V) | FF (%) | $\eta$ (%) |
|------------|------------|---------------|------------------------|--------------|--------|----------|
| 100        | -          | 0             | 17.3                   | 1.132        | 84.2   | 16.5     |
| 100        | 510        | 0.05          | 19.7                   | 1.093        | 85.1   | 18.3     |
| 1000       | -          | 0             | 28.3                   | 1.089        | 85.1   | 26.3     |
| 1000       | 510        | 0.05          | 29.4                   | 1.090        | 85.0   | 27.3     |
| 2000       | -          | 0             | 29.8                   | 1.081        | 85.1   | 28.0     |
| 2000       | 510        | 0.05          | 30.4                   | 1.081        | 85.1   | 28.0     |

$\eta$ as a function of $L_s \in [100, 1000]$ nm and $\zeta \in [0.05, 1]$, for $L_x \in [100, 1000, 2000]$ nm, $\xi = 0$, and $\xi(\zeta) \equiv 0 \forall \zeta \in [L_{ARC} + L_{FSP} + L_w, L_{ARC} + L_{FSP} + L_{Ag} + L_x]$. For all three values of $L_s$, the efficiency was found to be maximum for $L_x = 510$ nm and $\zeta = 0.05$. Values of $J_{sc}$, $V_{oc}$, FF, and $\eta$ obtained from the coupled optoelectronic model are provided in Table 2. The effect of the inclusion of the Ag backreflector to localize the ohmic Pd–Ge–Au backcontacts is to increase $J_{sc}$. However, that increase is more for smaller $L_x$. At the same time, $V_{oc}$ decreases significantly for $L_x = 100$ nm, but it does not change for the two higher values of $L_x$. As a result, the efficiency is enhanced from 16.5% to 18.3% (a relative enhancement of 10.9%) for $L_x = 100$ nm, but from 27.4% to just 28.0% (a relative enhancement of 2.1%) for $L_x = 2000$ nm. In other words, the effect of localized ohmic backcontacts on $\eta$ is significant for thin absorber layers but less pronounced for thick absorber layers.

The value of $\zeta = 0.05$ is in accord with the experimental and theoretical findings of Vandamme et al. [9]. Hence, we ensured that $\zeta \geq 0.05$ for optimization of AlGaAs solar cells.

B. Optimal AlGaAs Solar Cell: Homogeneous Bandgap

Next, we considered the optoelectronic optimization of the solar cell with a homogeneous $n$-AlGaAs absorber layer (i.e., $A = 0$), a periodically corrugated Ag backreflector, and localized ohmic Pd–Ge–Au backcontacts. Whereas $L_{Ag} = 100$ nm was fixed, the parameter space for optimizing $\eta$ was chosen as $E_{g,w} \in [1.424, 2.09]$ eV, $E_{g,\text{min}} \in [1.424, 2.09]$ eV, $L_x \in [100, 1000]$ nm, and $\zeta \in [0.05, 1]$. The common allowed range of $E_{g,w}$ and $E_{g,\text{min}}$ is consistent with $\xi \in [0, 0.8]$. Optimization was done for several discrete values of $L_x$, ranging from 100 nm to 2000 nm.

Values of $J_{sc}$, $V_{oc}$, FF, and $\eta$ predicted by the coupled optoelectronic model are presented in Table 3 for seven different values of $L_x$. The values of $E_{g,w}$, $E_{g,\text{min}}$, $L_x$, and $\zeta$ for the optimal designs are also provided in the same table.

For the thinnest $n$-AlGaAs absorber layer ($L_x = 100$ nm), the maximum efficiency predicted is 18.5% with $E_{g,w} = 2.09$ eV ($\xi = 0.8$), $E_{g,\text{min}} = 1.424$ eV ($\xi = 0$), and $L_x = 500$ nm. The values of $J_{sc}$, $V_{oc}$, and FF corresponding to this optimal design are 18.9 mA cm$^{-2}$, 1.149 V, and 85.1%, respectively. For this design, the $n$-AlGaAs layer is really a $p$-GaAs layer, but the $p$-AlGaAs layer is different from a $p$-GaAs layer. If $\xi = 0$ were to be fixed (i.e., the $p$-AlGaAs layer were to be replaced by a $p$-GaAs layer), the efficiency would be slightly less at $\sim 18.3\%$ (Table 2).

For the thickest $n$-AlGaAs absorber layer ($L_x = 2000$ nm), the maximum efficiency predicted is 28.8% with $E_{g,w} = 2.09$ eV ($\xi = 0.8$), $E_{g,\text{min}} = 1.424$ eV, and $L_x = 500$ nm. The values of $J_{sc}$, $V_{oc}$, and FF corresponding to this optimal design are 30.2 mA cm$^{-2}$, 1.090 V, and 87.3%, respectively. Again, for this optimal design, the $n$-AlGaAs layer is really a $n$-GaAs layer, but the $p$-AlGaAs layer is different from a $p$-GaAs layer. If the $p$-AlGaAs layer were to be replaced by a $p$-GaAs layer, the efficiency would decrease somewhat to $\sim 28\%$ (Table 2).

Regardless of the value of $L_x$, the optimal design in Table 3 has $L_x = 505 \pm 5$ nm and $\zeta = 0.05$, similar to the optimal design for its GaAs counterpart (Table 2). Even lower values of $\zeta$ would give higher efficiencies, but the localized ohmic Pd–Ge–Au backcontacts are necessary because of superior electron-collection capability [9]. Also, both $E_{g,\text{min}}$ and $E_{g,w}$ are independent of $L_x$ in Table 3, $E_{g,\text{min}}$ being at its minimum allowed value and $E_{g,w}$ at its maximum allowed value.

C. Optimal AlGaAs Solar Cell: Linearly Graded Bandgap

1. Optimal Designs

Next, we considered the maximization of $\eta$ when the bandgap of the $n$-AlGaAs absorber layer is linearly graded according to Eq. (1), $L_{Ag} = 100$ nm, and $\zeta \neq 1$. The parameter space used for optimizing $\eta$ was chosen as $E_{g,w} \in [1.424, 2.09]$ eV, $E_{g,\text{min}} \in [1.424, 2.09]$ eV, $L_x \in [100, 1000]$ nm, and $\zeta \in [0.05, 1.0]$. The common allowed range of $E_{g,w}$, $E_{g,\text{min}}$, and $E_{g,\text{max}}$ is consistent with $\xi \in [0, 0.8]$. Values of $J_{sc}$, $V_{oc}$, FF, and $\eta$ for the optimal designs are presented in Table 4 for seven different values of $L_x$. The corresponding values of $E_{g,w}$, $E_{g,\text{min}}$, $E_{g,\text{max}}$, $A$, $L_x$, and $\zeta$ are also provided in the same table.

For the thinnest $n$-AlGaAs absorber layer ($L_x = 100$ nm), the maximum efficiency predicted is 21.0% with $E_{g,w} = 1.424$ eV ($\xi = 0$), $E_{g,\text{min}} = 1.424$ eV ($\xi = 0$), $E_{g,\text{max}} = 1.98$ eV ($\xi = 0.45$), $A = 0.99$, and $L_x = 500$ nm. A relative enhancement of 13.5% over the maximum efficiency 18.5% in Table 3 for the homogeneous absorber layer of the same thickness is predicted. The values of $J_{sc}$, $V_{oc}$, and FF corresponding to
the optimal design are 16.8 mA cm$^{-2}$, 1.399 V, and 89.3%, respectively.

For the thickest $n$-AlGaAs absorber layer ($L_z = 2000$ nm), the maximum efficiency predicted is 33.1% with $E_{g,w} = 1.424$ eV ($\xi = 0$), $E_{g,min} = 1.424$ eV ($\xi = 0$), $E_{g,max} = 1.98$ eV ($\xi = 0.45$), $A = 1$, and $L_z = 500$ nm. The values of $J_{sc}$, $V_{oc}$, and FF corresponding to this optimal design are 24.7 mA cm$^{-2}$, 1.507 V, and 88.8%, respectively. A relative enhancement of 14.9% is predicted with linear bandgap grading of the $n$-AlGaAs absorber layer over the optimal efficiency of 28.8% with the homogeneous $n$-AlGaAs absorber layer in Table 3. For this optimal design, the $p$-AlGaAs layer is really a $p$-GaAs layer, but the $n$-AlGaAs absorber layer is different from a $n$-GaAs absorber layer. Although $V_{oc}$ is significantly higher with the linearly graded bandgap compared with the homogeneous bandgap (Table 3), $J_{sc}$ is lower with the linearly graded bandgap.

Similar to the data for the homogeneous absorber layer provided in Table 3, the optimal designs in Table 4 have $L_z = 505 \pm 5$ nm and $\xi = 0.05$, regardless of the value of $L_z$. Also, both $E_{g,min}$ and $E_{g,w}$ are independent of $L_z$ in Table 4, just as in Table 3. For both homogeneous and linearly graded absorber layers, $E_{g,min}$ is at its minimum allowed value; however, the value of $E_{g,w}$ is at its minimum allowed value for the linearly graded absorber layer (Table 4) but at its maximum allowed value for the homogeneous absorber layer (Table 3). The values of $A \sim 1$ and $E_{g,max} = 1.98$ eV are independent of $L_z$ for the linearly graded absorber layer (Table 4), the latter being significantly lower than its maximum allowed value.

2. Detailed Study for Highest Efficiency

The highest efficiency of 33.1% for the solar cell whose $n$-AlGaAs absorber layer has a linearly graded bandgap is delivered in Table 4 by the optimal design for $L_z = 2000$ nm. We determined the spatial profiles of the bandgap $E_g$, electron affinity $\chi(z)$, conduction-band energy $E_c(z)$, valence-band energy $E_v(z)$, intrinsic energy $E_i(z)$, electron density $n(z)$, hole density $p(z)$, intrinsic charge-carrier density $n_i(z)$, recombination rate $R(z)$, and generation rate $G(z)$ in the absorber layer of this solar cell. Furthermore, we determined the total device current density $J_{dev}$ delivered to an external circuit as well as the electrical power density $P$ as functions of the bias voltage $V_{ext}$.

Spatial profiles of $E_g(z)$ and $\chi(z)$ for the optimal solar cell with $n$-AlGaAs absorber layer of thickness $L_z = 2000$ nm are provided in Fig. 2(a), whereas Fig. 3(a) presents the spatial profiles of $E_c(z)$, $E_v(z)$, and $E_i(z)$. The spatial variations of $E_c$ and $E_v$ are similar to that of $E_g$ [Fig. 2(a)]. Figure 3(b) presents the spatial profile of $n(z)$, $p(z)$, and $n_i(z)$ in steady-state condition. The intrinsic carrier density varies linearly such that it is small, where $E_g$ is large and vice versa.

Spatial profiles of $G(z)$ and $R(z)$ are given in Fig. 4(a). The generation rate is higher near the front face and lower near the back face of the $n$-AlGaAs absorber layer, which is in accord [22] with higher electron–hole-pair generation, where $E_g$ is lower and vice versa. Finally, the $J_{dev}$-$V_{ext}$ characteristics of the solar cell shown in Fig. 4(b) deliver $J_{dev} = 23.9$ mA cm$^{-2}$ and $V_{ext} = 1.375$ V for best performance (i.e., for maximum $P$).

D. Optimal AlGaAs Solar Cell: Sinusoidally Graded Bandgap

1. Optimal Designs

Finally, we considered the maximization of $\eta$ when the bandgap of the $n$-AlGaAs absorber layer is sinusoidally graded according to Eq. (2), $L_{Ag} = 100$ nm, and $\xi \neq 1$. The parameter space used for optimizing $\eta$ was chosen as $E_{g,w} \in [1.424, 2.09]$ eV, $E_{g,min} \in [1.424, 2.09]$ eV, $E_{g,max} \in [1.424, 2.09]$ eV, $A \in [0, 1]$, $\alpha \in [0, 8]$, $K \in [0, 8]$, $\psi \in [0, 1]$, $L_z \in [100, 10000]$ nm, and $\xi \in [0.05, 1]$.
Values of $J_{sc}$, $V_{oc}$, $FF$, and $\eta$ predicted by our model presented in Table 5 for seven different values of $L_z$. The values of $E_{g,w}$, $E_{g,\text{min}}$, $E_{g,\text{max}}$, $A$, $\alpha$, $K$, $\psi$, $L_z$, and $\zeta$ for the optimal designs are also provided in the same table. For the thinnest $n$-AlGaAs absorber layer ($L_z = 100$ nm), the maximum efficiency predicted is 21.2% with $E_{g,w} = 2.09$ eV ($\xi = 0.8$), $E_{g,\text{min}} = 1.424$ eV ($\xi = 0$), $E_{g,\text{max}} = 1.98$ eV ($\xi = 0.45$), $A = 1$, $\alpha = 6$, $K = 3$, $\psi = 0.75$, and $L_z = 510$ nm. The values of $J_{sc}$, $V_{oc}$, and $FF$ corresponding to this optimal design are 16.1 mA cm$^{-2}$, 1.455 V, and 90.3%, respectively. A relative enhancement of 14.5% over the optimal efficiency 18.5% for the homogeneous $n$-AlGaAs absorber layer (Table 3) is predicted.

For the thickest $n$-AlGaAs absorber layer ($L_z = 2000$ nm), the maximum efficiency predicted is 34.5% with $E_{g,w} = 2.09$ eV ($\xi = 0.8$), $E_{g,\text{min}} = 1.424$ eV ($\xi = 0$), $E_{g,\text{max}} = 1.98$ eV ($\xi = 0.45$), $A = 0.99$, $\alpha = 6$, $K = 3$, $\psi = 0.75$, and $L_z = 550$ nm. The corresponding values of $J_{sc}$, $V_{oc}$, and $FF$ are 24.8 mA cm$^{-2}$, 1.556 V, and 89.2%, respectively. A relative enhancement of 19.8% is predicted with sinusoidal grading of $n$-AlGaAs absorber layer over the optimal efficiency of 28.8% with homogeneous $n$-AlGaAs absorber layer (Table 3). Just as in Section 3.C.1, although $V_{oc}$ is significantly higher with the sinusoidally graded bandgap compared to the homogeneous bandgap (Table 3), $J_{sc}$ is lower with the sinusoidally graded bandgap. The optimal designs in Table 5 have $L_z = 525 \pm 25$ nm and $\zeta = 0.05$. The values of $E_{g,\text{min}}, E_{g,\text{max}}, A, \alpha$, and $\psi$ are the same.

### Table 5. Predicted Parameters of the Optimal AlGaAs Solar Cell with a Specified Value of $L_z \in [100, 2000]$ nm, When the $n$-AlGaAs Absorber Layer Is Sinusoidally Graded According to Eq. (2), $L_{Ag} = 100$ nm, and $\zeta < 1$

| $L_z$ (nm) | $E_{g,w}$ (eV) | $E_{g,\text{min}}$ (eV) | $E_{g,\text{max}}$ (eV) | $A$ | $\alpha$ | $K$ | $\psi$ | $L_z$ (nm) | $\zeta$ | $J_{sc}$ (mA cm$^{-2}$) | $V_{oc}$ (V) | $FF$ (%) | $\eta$ (%) |
|-----------|---------------|-----------------|-----------------|-----|-----|-----|-----|-----------|-------|-----------------|---------|--------|---------|
| 100       | 2.09          | 1.424           | 1.98            | 1.0 | 6   | 3   | 0.75| 510       | 0.05  | 16.1             | 1.455   | 90.3   | 21.2    |
| 200       | 2.09          | 1.424           | 1.98            | 1.0 | 6   | 1   | 0.75| 520       | 0.05  | 19.2             | 1.471   | 80.2   | 22.6    |
| 300       | 2.06          | 1.424           | 1.98            | 1.0 | 6   | 1   | 0.74| 512       | 0.05  | 19.7             | 1.486   | 80.2   | 23.5    |
| 400       | 2.09          | 1.424           | 1.98            | 1.0 | 6   | 1   | 0.75| 509       | 0.05  | 20.2             | 1.497   | 82.0   | 24.8    |
| 500       | 2.08          | 1.424           | 1.98            | 1.0 | 6   | 1   | 0.75| 524       | 0.05  | 20.8             | 1.505   | 83.0   | 26.0    |
| 1000      | 2.09          | 1.424           | 1.98            | 1.0 | 6   | 2   | 0.75| 516       | 0.05  | 22.5             | 1.533   | 87.8   | 30.4    |
| 2000      | 2.09          | 1.424           | 1.98            | 0.99| 6   | 3   | 0.75| 550       | 0.05  | 24.8             | 1.556   | 89.2   | 34.5    |
for all values of \( L_z \); however, \( K \in \{1, 2, 3\} \) does vary with \( L_z \). The values of \( A \sim 1 \) and \( E_{g, \text{max}} = 1.98 \text{ eV} \) are independent of \( L_z \) for the sinusoidally graded absorber layer (Table 5), the latter being significantly lower than its maximum allowed value.

The highest possible efficiency (34.5%) with a sinusoidally graded \( n \)-AlGaAs absorber layer is 4.2% higher than the highest possible efficiency (33.1%) with a linearly graded \( n \)-AlGaAs absorber layer (Table 4). The short-circuit current density is almost the same for both linearly and sinusoidally graded \( n \)-AlGaAs absorber layers; however, the open-circuit voltage is somewhat higher for a sinusoidally graded \( n \)-AlGaAs absorber layer. By comparing Tables 4 and 5, we conclude that sinusoidally graded \( n \)-AlGaAs absorber layer leads to significantly higher efficiency than the linearly graded \( n \)-AlGaAs absorber layer for \( L_z \geq 1000 \text{ nm} \), but both types of graded-bandgap absorber layers deliver practically the same efficiency for \( L_z \leq 500 \text{ nm} \).

## 2. Detailed Study for Highest Efficiency

We performed a detailed study for the solar cell with thickest \( L_z = 2000 \text{ nm} \) sinusoidally graded \( n \)-AlGaAs absorber layer, because it delivers the highest efficiency. The variations of \( E_g \) and \( \chi \) with \( z \) in the semiconductor region are provided in Fig. 2(b). The magnitude of \( E_g \) is large near both faces of the \( n \)-AlGaAs absorber layer, whose features elevate \( V_{ac} \) [13]. The regions in which \( E_g \) is small are of substantial thickness, these regions being responsible for elevating \( G(z) \) [22].

Figure 5(a) shows the variations of \( E_z \), \( E_i \), and \( E_v \) with respect to \( z \). The spatial profiles of \( E_z \) and \( E_i \) are similar to that of \( E_g \). Figure 5(b) shows the spatial variations of the electron, hole, and intrinsic carrier densities in steady-state condition. The intrinsic carrier density varies sinusoidally such that \( n_i \) is small where \( E_g \) is large and vice versa. Profiles of \( G(z) \) and \( R(z) \) are shown in Fig. 5(a). The generation rate is higher in regions with lower bandgap and vice versa. The \( J_{dev}-V_{ext} \) characteristics of the solar cell are shown in Fig. 6(b). Our optoelectronic model predicts \( J_{dev} = 23.8 \text{ mA cm}^{-2} \) and \( V_{ext} = 1.45 \text{ V} \) for best performance.

## 4. CONCLUSION

A coupled optoelectronic model along with the DEA was implemented to evaluate the effectiveness of grading the bandgap of the \( n \)-AlGaAs absorber layer for improving the power conversion efficiency of thin-film AlGaAs solar cells. Both linearly and sinusoidally graded bandgaps were studied, with the semiconductor region of the solar cell backed by a periodically corrugated Ag backreflector combined with the localized ohmic Pd–Ge–Au backcontacts.

A 2000-nm-thick \( n \)-AlGaAs absorber layer that is sinusoidally graded can deliver 34.5% efficiency, 24.8 mA cm\(^{-2}\) short-circuit current density, 1.556 V open-circuit voltage, and 89.2% fill factor. In comparison, the efficiency is 28.8%, the short-circuit current density is 30.2 mA cm\(^{-2}\), the open-circuit
Voltage is 1.090 V, and the fill factor is 87.3% when the bandgap of the absorber layer is homogeneous. Efficiency enhancement can also be achieved by linearly grading the bandgap of the n-AlGaAs absorber layer, but the gain is significantly smaller compared with sinusoidal graded bandgaps can when the absorber layer is at least 1000 nm thick. However, for thinner n-AlGaAs absorber layers, both linearly graded bandgaps and sinusoidally bandgap grading provide almost equal efficiency gains over the homogenous bandgap.

When the bandgap is sinusoidally graded in the n-AlGaAs absorber layer, the electron–hole-pair generation rate is higher in the broad small-bandgap regions than elsewhere in the n-AlGaAs absorber layer [22]. The open-circuit voltage is elevated in the optimal designs [13], because the bandgap is high in the vicinity of both faces of the n-AlGaAs absorber layer. Both of these characteristics help to increase the efficiency.

Optoelectronic optimization thus indicates that 34.5% efficiency (Table 5) can be achieved for AlGaAs solar cell with a 2000-nm-thick sinusoidally graded n-AlGaAs absorber layer. This efficiency is significantly higher compared with 27.4% efficiency demonstrated with the homogeneous n-AlGaAs absorber layer with a continuous ohmic Pd–Ge–Au backcontact (Table 1). Efficiency improvements of equivalent magnitude—e.g., from 22% to 27.7%—have been predicted by bandgap grading of the CIGS absorber layer in thin-film CIGS solar cells [13]. Thus, bandgap grading can provide a way to realize more efficient thin-film solar cells for ubiquitous harnessing of solar energy at low wattage levels.

**APPENDIX A: OPTICAL AND ELECTRICAL PARAMETERS**

The optical permittivity $\varepsilon$ of any material is, in general, a function of $\lambda_0$. The optical relative permittivities of MgF$_2$ [32], ZnS [33], AlInP [34], GaInP [37], Pd [39], Ge [40], Au [39], and Ag [39] are provided in Fig. 7 for $\lambda_0 \in [300, 950]$ nm. The real and imaginary parts of the optical relative permittivity of AlGaAs are provided in Fig. 8 as functions of any material is, in general, a function of $\lambda_0$.

### Table 6. Electrical Properties of AlInP \([42, 43]\), GaInP \([42, 43, 46]\), and Al$_{1-x}$Ga$_x$As \([44–46]\)

| Parameter                        | Symbol (unit) | AlInP \([42, 43]\) | GaInP \([42, 43, 46]\) | Al$_{1-x}$Ga$_x$As \([44–46]\) |
|----------------------------------|---------------|---------------------|-------------------------|----------------------------------|
| Bandgap                          | $E_g$ (eV)    | 2.35                | 1.9                     | $1.424 + 1.247\xi$, $0 \leq \xi < 0.45$; $1.9 + 0.125\xi + 0.143\xi^2$, $0.45 \leq \xi \leq 1$ |
| Electron affinity                | $\chi$ (eV)  | 3.78                | 4.1                     | $4.07 - 1.1\xi$, $0 \leq \xi < 0.45$; $3.64 - 0.14\xi$, $0.45 \leq \xi \leq 1$ |
| Doping density                   | $N_d$ (cm$^{-3}$) | $2 \times 10^{18}$ (acceptor) | $2 \times 10^{18}$ (donor) | $1 \times 10^{19}$ (acceptor and donor) |
| Conduction-band                  | $N_c$ (cm$^{-3}$) | $2.5 \times 10^{18}$ | $6.5 \times 10^{17}$ | $2.5 \times 10^{33}$ $(0.063 + 0.083\xi)^{3/2}$, $0 \leq \xi < 0.45$; $2.5 \times 10^{33}$ $(0.85 - 0.14\xi)^{3/2}$, $0.45 \leq \xi < 1$ |
| Density of states                | $N_s$ (cm$^{-3}$) | $7 \times 10^{18}$ | $1.5 \times 10^{19}$ | $2.5 \times 10^{33}$ $(0.51 + 0.25\xi)^{3/2}$, $0 \leq \xi < 0.45$; $-255 + 1160\xi - 720\xi^2$, $0.45 \leq \xi \leq 1$ |
| Valence-band density of states   | $\mu_n$ (cm$^2$V$^{-1}$s$^{-1}$) | 100                | 500                     | $370 - 970\xi + 740\xi^2$, $0 \leq \xi < 0.45$; $1 + 9\xi$, $0 \leq \xi \leq 1$ |
| Hole mobility                    | $\mu_p$ (cm$^2$V$^{-1}$s$^{-1}$) | 30                  | 10                      | $10^{-10}$                     |
| DC relative permittivity         | $\varepsilon_{dc}$ | 11.8                | 11.8                    | 13.18 - 3.12\xi                 |
| Defect/trap density              | $N_i$ (cm$^{-3}$) | $10^{17}$           | $10^{17}$               | $(1 + 9\xi) \times 10^{15}$, $0 \leq \xi < 0.45$; $10^{-16}$ |
| Defect/trap level                | $E_i$ (eV)     | midgap              | midgap                  | $0.75$ eV below conduction-band energy, $10^{-16}$ |
| Electron capture cross section   | $\sigma_n$ (cm$^2$) | $10^{-14}$          | $10^{-14}$              | $10^{-10}$                     |
| Hole capture cross section       | $\sigma_p$ (cm$^2$) | $10^{-14}$          | $10^{-14}$              | $10^{-10}$                     |
| Radiative recombination coefficient | $R_B$ (cm$^{-3}$s$^{-1}$) | $10^{-10}$         | $10^{-10}$              | $1.8 \times 10^{-10}$          |
| Electron thermal speed           | $v_{th,n}$ (cm s$^{-1}$) | $10^7$             | $10^7$                  | $(4.4 - 2.1\xi) \times 10^7$ |
| Hole thermal speed               | $v_{th,p}$ (cm s$^{-1}$) | $10^7$             | $10^7$                  | $(1.8 - 0.5\xi) \times 10^7$ |
| Auger electron recombination coefficient | $C_{nu}$ (cm$^3$s$^{-1}$) | $10^{-30}$        | $10^{-30}$              | $10^{-30}$                     |
| Auger hole recombination coefficient | $C_{pu}$ (cm$^3$s$^{-1}$) | $10^{-30}$        | $10^{-30}$              | $10^{-30}$                     |
of $\lambda_0 \in [300, 950]$ nm and $\xi \in [0, 0.8]$ [36], data being unavailable for $\xi \in (0.8, 1)$.

Table 6 provides the values of electrical parameters used for all four semiconductors [43–46].

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