

Projected Efficiency of Polarization-Matched p-In_xGa_{1-x}N/i-In_yGa_{1-y}N/n-GaN Double Heterojunction Solar Cells

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Abstract—Traditional p-GaN/i-InGaN/n-GaN double heterojunction solar cells have limited power conversion efficiency due to large polarization charges that accumulate at the heterojunction interfaces, leading to severe band bending that, in turn, hinders the carrier transport. In this study, we proposed the use of a p-type InGaN layer to reduce the polarization field and projected the power conversion efficiencies of p-In_xGa_{1-x}N/i-In_yGa_{1-y}N/n-GaN double heterojunction solar cells that are grown on a c-facet sapphire substrate with various indium components. Numerical simulations predict that a maximal power conversion efficiency that is close to 7% with a short-circuit current density of 4.05 mA/cm² and an open-circuit voltage of 1.94 V can be achieved with a p-In_{0.2}Ga_{0.8}N/i-In_{0.2}Ga_{0.8}N/n-GaN structure due to a polarization-matched p-i interface. Further efficiency enhancement with a higher indium composition over 20% is also possible via the redistribution of the built-in potential with n-GaN doping.

Index Terms—InGaN solar cells, polarization effect.

I. INTRODUCTION

InGaN ALLOYS have been widely used for making high-performance optoelectronic devices, including light-emitting diodes and laser diodes. Recently, InGaN materials have also become attractive for use in heterojunction solar cells for the following reasons. First, the ability to produce widely tunable direct bandgaps, ranging from 0.7 eV with InN to 3.4 eV with GaN, can cover the whole solar spectrum from ultraviolet to visible and infrared wavelengths [1], [2]. Second, the high absorption coefficient ($>10^5$ cm⁻¹) of InGaN-based materials permits strong optical absorption within a relatively thin active

layer, which is desirable for light-weight solar cells [3]. These features may also make InGaN-based solar cells favorable for use in terrestrial applications. Currently, GaN/InGaN-based heterojunction p-i-n solar cells are normally grown on a c-facet sapphire substrate by metal-organic vapor phase epitaxy [4]–[6]. Due to epitaxial strain, the structures are generally composed of an intrinsic InGaN layer as the active region, with an indium content lower than 15%, and a thickness of 60~300 nm, which is sandwiched in-between a n-GaN and p-GaN layer [7]–[9]. However, we note that the critical thickness of In_xGa_{1-x}N that is grown on GaN is less than 10 nm for $x > 0.2$. Thicker growth results in strain relaxation through the formation of misfit dislocations, as well as compositional fluctuations, which adversely affect the electrical properties of the InGaN epilayer [10], [11]. The growth of a thick InGaN layer with a high indium composition is a challenge in real fabrication [12], [13]. Moreover, the i-InGaN epitaxial layer in this structure suffers from both a spontaneous and strain-induced piezoelectric polarization field [14]–[18]. The polarization mismatch effect also gives rise to strong band bending, which may hinder photogenerated carrier separation and transport, and lead to an inadequate power conversion efficiency of InGaN-based solar cells [19]. Previous studies have suggested that the growth of InGaN material on the nitrogen (N) face [20], [21] or insertion of a grading layer at the InGaN/GaN interface [22], [23] will minimize the influence of polarization and help the carrier escape the depletion region. Recently, the experimental implementation of heteroepitaxy and the p-type doping of InGaN are achievable at low indium composition conditions by using molecular beam epitaxy (MBE). However, obtaining high p-type doping in high indium composition is still very challenging [24]. In this study, we assume that the implementation of a p-InGaN layer is achievable. Therefore, we propose the use of a p-type InGaN layer to reduce the polarization field and investigate the projected efficiencies of p-In_xGa_{1-x}N/i-In_yGa_{1-y}N/n-GaN double heterojunction solar cells that are grown on the c-facet with various indium components. The growth of p-type InGaN materials has recently been demonstrated by MBE and metal-organic chemical vapor deposition [4], [5], [25]. Numerical simulations predict that maximal power conversion efficiency that is close to 7% can be achieved with a p-In_{0.2}Ga_{0.8}N/i-In_{0.2}Ga_{0.8}N/n-GaN structure, which is permitted by a polarization-matched p-i interface. Further efficiency enhancement with a higher indium composition over 20% is also possible by lowering the barrier at the n-GaN heterojunction with n-type doping.

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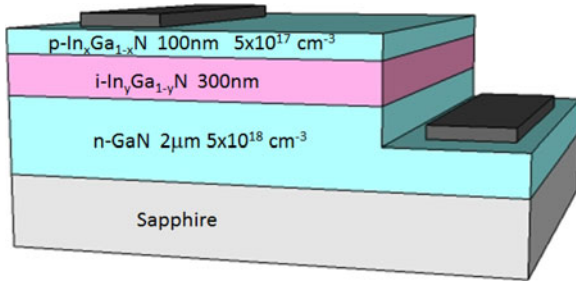


Fig. 1. Schematic layer structure of a p-In_xGa_{1-x}N/i-In_yGa_{1-y}N solar cell.

II. SIMULATION AND METHOD

The band structures and current density–voltage (J – V) characteristics of InGaN-based heterojunction solar cells are investigated numerically by commercially available software, namely, Advanced Physical Models of Semiconductor Devices [26]. The simulated solar cell structure is composed of a 100-nm-thick Mg-doped In_xGa_{1-x}N layer with fully activated p-type doping of $5 \times 10^{17} \text{ cm}^{-3}$, a 300-nm-thick strained intrinsic In_yGa_{1-y}N layer, and a 2- μm -thick Si-doped GaN bottom layer with n-type doping of $5 \times 10^{18} \text{ cm}^{-3}$. To keep the depletion region large, the intrinsic doping density in this study is assumed to be $1 \times 10^{16} \text{ cm}^{-3}$. In our testing, doping density smaller than $1 \times 10^{17} \text{ cm}^{-3}$ in the intrinsic region will give a close result. Fig. 1 illustrates the p-In_xGa_{1-x}N/i-In_yGa_{1-y}N p-i-n double heterojunction solar cell's structure, which is similar to an experimental demonstration [4], [8]. Hereafter, we denote the indium compositions of a p-In_xGa_{1-x}N/i-In_yGa_{1-y}N structure as px-iy, for example, p-In_{0.05}Ga_{0.95}N/i-In_{0.1}Ga_{0.9}N as p0.05-i0.1. The device has an area of $300 \mu\text{m} \times 300 \mu\text{m}$ and assumes ideal ohmic contacts. The unit cell is then discretized into 55 130 mesh points on the 2-D layout to minimize numerical errors and ensure convergence. Optical properties are first calculated based on the surface and internal reflection and the material absorption within each dielectric layer including the sapphire substrate. The distribution of the carrier generation rate under air mass 1.5 global (AM 1.5G) illumination condition is then obtained. Electronic properties are solved using the built-in 2-D self-consistent Poisson and drift-diffusion equations solver for electrons and holes transportation. Moreover, the band offset ratios between the conduction band and valance band are assumed to be 0.67 and 0.33 of the bandgap difference, respectively [27]. We also assume the diffusion length in p-InGaN to be 200 nm [28], which is larger than the layer thickness, and therefore, the additional absorption that occur in p-InGaN is still effective and contributes to the output photocurrent. The actual diffusion length assumption of the p-InGaN layer might be too long under this assumption. Thus, if the actual diffusion is short, we should reduce the p-InGaN/GaN layer thickness as well in order to avoid nonradiative recombination.

The polarization charges at the surfaces and interfaces with various indium compositions are calculated based on an ab initio model, which was developed by Fiorentini and coworkers [14], [18]. Equations (1)–(4), shown below, calculate the polarization charges of a ternary alloy layer, including spontaneous and

piezoelectric polarization, P^{SP} and P^{Pz} , respectively, using the relationship between composition x , bandgap, lattice constant a , and strain ε

$$p_{\text{In}_x\text{Ga}_{1-x}\text{N}}^{\text{SP}} = -0.042x - 0.034(1-x) + 0.038x(1-x) \quad (1)$$

$$p_{\text{InN}}^{\text{Pz}} = -1.373\varepsilon + 7.559\varepsilon^2 \quad (2)$$

$$p_{\text{GaN}}^{\text{Pz}} = -0.918\varepsilon + 9.541\varepsilon^2 \quad (3)$$

$$\varepsilon(x) = [a_{\text{subs}} - a(x)]/a(x). \quad (4)$$

The piezoelectric polarization can be expressed by Vegard's law as

$$p_{\text{In}_x\text{Ga}_{1-x}\text{N}}^{\text{Pz}} = xp_{\text{InN}}^{\text{Pz}}[\varepsilon(x)] + (1-x)p_{\text{GaN}}^{\text{Pz}}[\varepsilon(x)]. \quad (5)$$

We note that the strain is defined from the lattice constant of GaN, and other material parameters that are used in the calculation can be found in [22]. The nonlinear wavelength-dependent absorption coefficient of InGaN alloys was taken, as shown in [22]

$$\alpha(E) = 10^5 \sqrt{a \cdot (E - E_g) + b \cdot (E - E_g)^2} \quad (6)$$

where E is the incident photon energy given in eV, and a and b are dimensionless fitting parameters. The parameters a and b are 3.52517 and -0.6571 when the indium composition equals 0%, and become 0.51672 and 0.468836, respectively, when the indium composition equals 50%; the fitting parameters of InGaN for indium compositions between 0% and 50% are obtained by linear interpolation.

In addition, we assume that the InGaN is ideally epitaxially grown without strain relaxation. Therefore, the ratio of polarization equals unity. Although a screening ratio between 0.4 and 0.6 is commonly used to fit the empirical data for InGaN-based light-emitting devices [29], we have calculated and found that the polarization charge induced at the interface under strain relaxation is still close to the unrelaxed case. This is because if the InGaN lattice is totally relaxed, the InGaN and GaN top layer would be still under tensile strain. However, if the top GaN layer experiences strain relaxation, the piezoelectric field is also reduced. Therefore, at the end of this paper, we discuss the dependence of the device characteristics on the ratio of polarization at the GaN/InGaN interface induced by strain relaxation.

III. RESULTS AND DISCUSSION

To relieve the polarization effects using a p-doped InGaN layer, the current density–voltage curves of InGaN heterojunction solar cells with an intrinsic In_{0.1}Ga_{0.9}N layer are first simulated for p-layers with different indium compositions, ranging from 0% to 10%, as shown in Fig. 2(a). The corresponding short-circuit current density J_{sc} , open-circuit voltage V_{oc} , fill factor (FF), and efficiency are plotted in Fig. 2(b)–(e), respectively. The cell, which is denoted as p0-i0.1, represents the reference cell with p-GaN, which has been experimentally demonstrated. With a slight indium composition in the p-layer, the photovoltaic characteristics are significantly improved over the reference counterpart. The J_{sc} increases and V_{oc} decreases with the

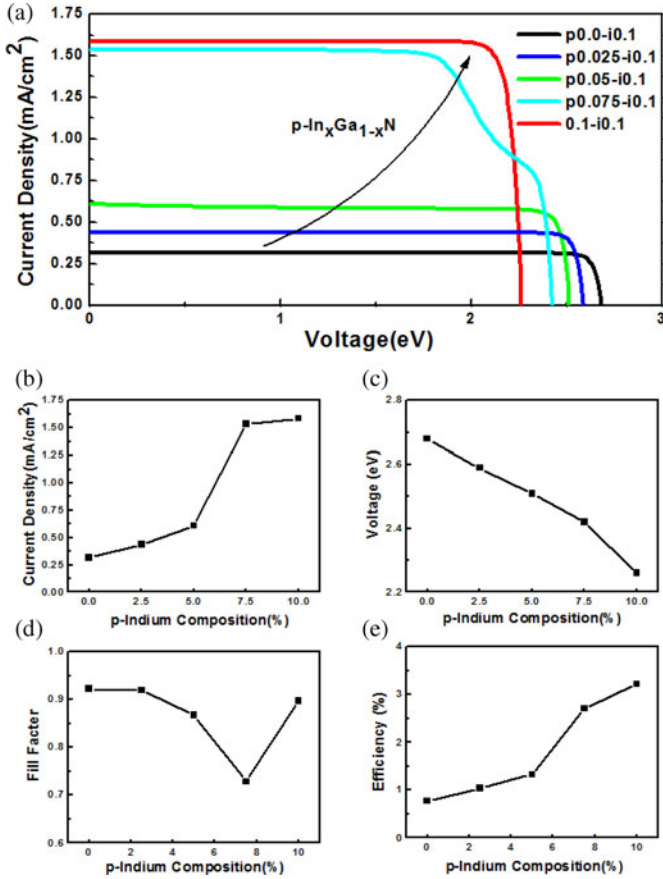


Fig. 2. (a) Current density–voltage characteristics for p-In_xGa_{1-x}N/i-In_{0.1}Ga_{0.9}N/n-GaN solar cells with varying indium compositions. The corresponding parameters are plotted as a function of the p-type indium composition: (b) Short-circuit current density J_{sc} , (c) open-circuit voltage V_{oc} , (d) FF, and (e) efficiency.

indium composition in the p-type layer monotonically due to decreased interface polarization charges. However, there is also a sudden increase in J_{sc} and decrease in FF with an indium composition of 0.075, due to a redistribution of the built-in field on the intrinsic layer, which will be further discussed later. The conversion efficiency of the p0.1-i0.1 cell is significantly enhanced by 4.14 times over the reference cell. The maximal conversion efficiency of p0.1-i0.1 achieves 3.22% with a V_{oc} , J_{sc} , and FF of 2.26 V, 1.59 mA/cm², and 89.8%, respectively. Results shown in Fig. 2(a)–(e) conclude that a p-InGaN layer can effectively mitigate the degradation of the conversion efficiencies due to polarization mismatch.

As we know, for an InGaN double heterojunction solar cell, three fields are applied in the system. One is a field due to the p-n-diode junction built-in potential, another is the polarization-induced field caused by fixed sheet charges at the heterointerface, and the final one is due to an applied voltage, which are denoted as the built-in field, polarization field, and applied field, respectively. Following the previous discussion, the increased indium content of the p-InGaN layer lowers the polarization charges at the p-i heterojunction interface, reducing the polarization field in the intrinsic layer and maintaining a depletion region for charge separation.

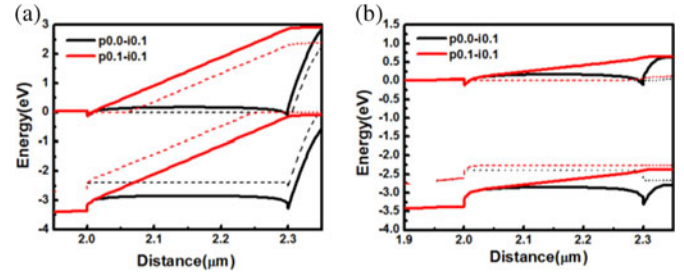


Fig. 3. Energy band diagrams of p0.0-i0.1 and p0.1-i0.1 structures under 1-sun solar radiation at near (a) short-circuit-current and (b) open-circuit-voltage conditions. The colored solid lines represent the positions of conduction and valence bands, and dashed lines denote the quasi-Fermi levels.

At the optimized conversion efficiency, the p-In_{0.1}Ga_{0.9}N layer is polarization-matched to the i-In_{0.1}Ga_{0.9}N layer when the polarization charges at the p-i interface are zero. To elaborate on the efficiency restrained by the polarization effect, Fig. 3 shows a comparison of the energy band diagrams of the p0-i0.1 and p0.1-i0.1 structures under 1-sun solar irradiance at near (a) short-circuit-current and (b) open-circuit-voltage conditions. As shown in Fig. 3(a), a large band bending in the p-GaN region caused by the fixed net polarization charges leads to a large dead layer in the intrinsic region. Moreover, the valence band discontinuity across the p-i heterojunction interface (at 2.3- μ m distance) also gives rise to a small barrier for hole transport in the valence band. Both factors are responsible for the small photocurrent output. On the other hand, the p-In_{0.1}Ga_{0.9}N is polarization-matched to the intrinsic layer, which ameliorates the distribution of the built-in field across the intrinsic region, and improves the photogenerated carrier separation and collection. Fig. 3(b) shows the activation energy under illumination and forward bias conditions, where the cell with p-In_{0.1}Ga_{0.9}N obtains a lower V_{oc} than that with p-GaN. Since the V_{oc} is depicted by the separation of quasi-Fermi levels, it is therefore slightly limited by the difference in bandgaps between the n-GaN and p-In_{0.1}Ga_{0.9}N layers. However, the increase in photocurrent output is sufficient to overcome the degradation of V_{oc} in order to observe a clear improvement in the power conversion efficiency.

Next, we calculate the efficiency map of ternary p-In_xGa_{1-x}N/i-In_yGa_{1-y}N/n-GaN solar cells with various indium compositions for both p-type and intrinsic layers. The projected efficiencies are plotted in Fig. 4 for $x = 0.00$ – 0.25 , and $y = 0.10$ – 0.25 . It is observed that the efficiencies of solar cells with a p-GaN layer are quite low due to the largely accumulated polarization charges at the p-i heterojunction interface. The electrons are generated near the p-i interface close to the surface, while holes easily accumulate at the p-i interface as a result of band discontinuity. Therefore, the situation leads to a very large recombination rate in the active region that lowers the carrier collection. By using the polarization match concept, the heterojunction solar cells with a p-In_xGa_{1-x}N layer could considerably improve the power conversion efficiency. This is because the reduced interface polarization charges suppressed the band bending, which improved the distribution of the built-in field, as well as the hole transport. Therefore, when the indium

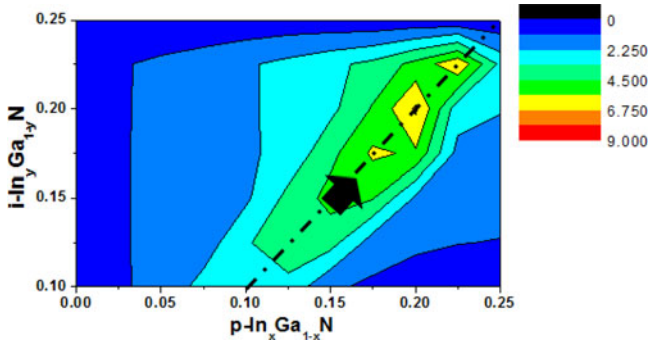


Fig. 4. Power conversion efficiency map of InGaN heterojunction solar cells consisting of p-In_xGa_{1-x}N and i-In_yGa_{1-y}N with various indium compositions. The dot-dashed line and arrow represent the polarization-matched combinations.

composition of the p-layer is higher than that of the intrinsic layer, polarization mismatch would also reduce the efficiency.

The polarization-matched structures are marked along the dashed line, as indicated in Fig. 4. The corresponding J - V curves on the dashed line are shown in Fig. 5(a), where the indium compositions of both p-type and intrinsic layers are the same. It appears that the efficiencies are enhanced with increasing indium content. Maximal power conversion efficiency occurs with approximately 20% indium composition. A peak efficiency of 6.93% is achieved with the p0.2-i0.2 structures, where J_{sc} is 4.05 mA/cm², and V_{oc} is 1.94 V. This indicates that the reduced polarization interface charges can boost the characteristics of InGaN solar cells. However, the efficiency of the p0.25-i0.25 cell structure is lower than that of p0.2-i0.2, which is not so intuitive. The energy band diagrams of p0.2-i0.2 and p0.25-i0.25 cells under illumination and without external bias are plotted in Fig. 5(b). Compared with the p0.2-i0.2 cell, which is shown in Fig. 5(c), the p0.25-i0.25 cell has a larger fixed negative polarization charge and larger band offset at the i-In_{0.25}Ga_{0.75}N/n-GaN interface. This results in a larger potential drop in the n-GaN layer instead of the intrinsic layer, which increases the recombination at the intrinsic layer. Therefore, as shown in Fig. 5(d), the electron and hole current output from the p and i layers are limited. From this viewpoint, increasing n-type doping can redistribute the built-in field for further efficiency enhancement [5]. These results suggest that p-type and intrinsic InGaN layers with an optimized indium composition of approximately 20% are desirable for monolithic growth on a GaN template.

Finally, we investigate the dependence of the device characteristics on the ratio of piezoelectric polarization at the GaN/InGaN interface by introducing a parameter “degree of relaxation” for the cap In_xGa_{1-x}N layer, which is denoted by “ R_{relax} .” By definition, R_{relax} equal to unity means 100% strain relaxation, corresponding to the case of no piezoelectric charges at the p-i interface. As the value of R_{relax} reduces, the piezoelectric polarization increases proportionally, while the spontaneous polarization remains unchanged. Therefore, Fig. 4 represents the case where $R_{relax} = 0.0$. We further calculate the projected efficiency map for $R_{relax} = 0.5$ and $R_{relax} = 1.0$, as plotted

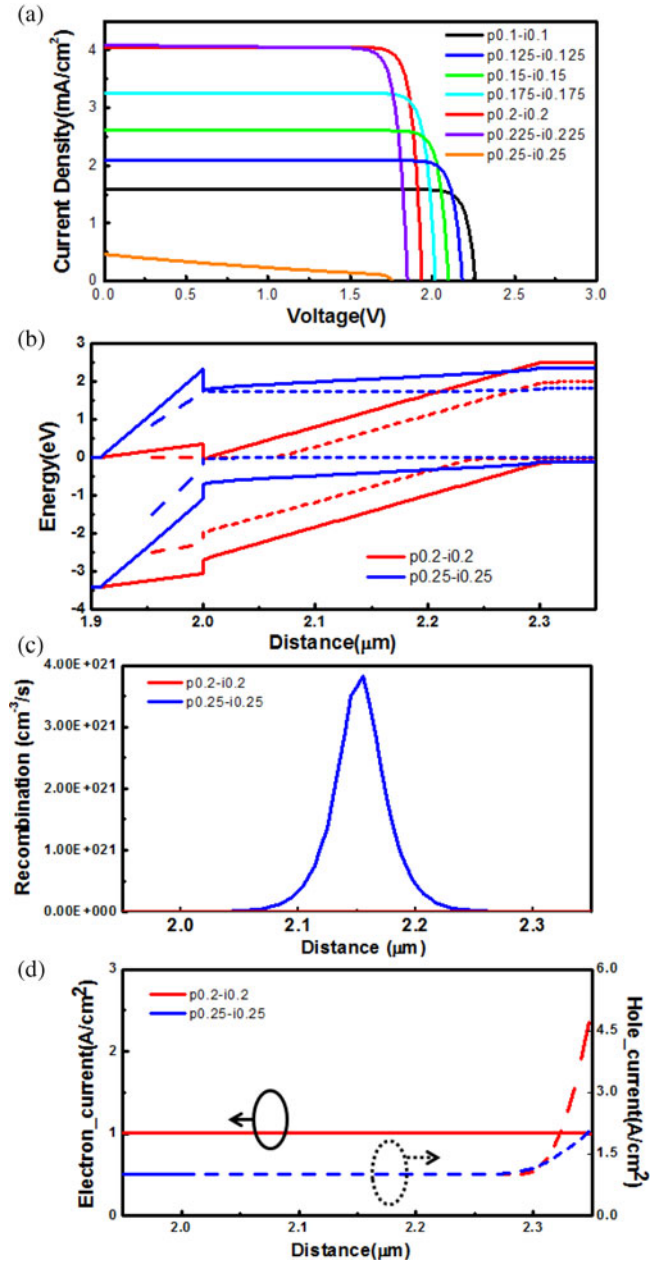


Fig. 5. (a) Current density–voltage characteristics of p-i polarization-matched InGaN heterojunction solar cells with various indium compositions. (b) Energy band diagrams. Colored solid lines represent the conduction and valence band, and dashed lines represent the quasi-Fermi levels. (c) Total recombination rates and (d) the electron and hole current density distribution of the p0.2-i0.2 and p0.25-i0.25 cell structures under illumination and without an external bias.

in Fig. 6(a) and (b), respectively. It can be seen that maximal efficiencies for $R_{relax} = 0.5$ and $R_{relax} = 1.0$ of 9.10% and 9.12%, respectively, occurred in the p0.25-i0.25 structure. As the polarization charges at the p-i interface are reduced, we can expect a much-improved efficiency. However, we note that strain relaxation is often associated with the severe degradation of material quality. Therefore, the maximal efficiency with 100% strain relaxation is probably much worse than that without strain relaxation.

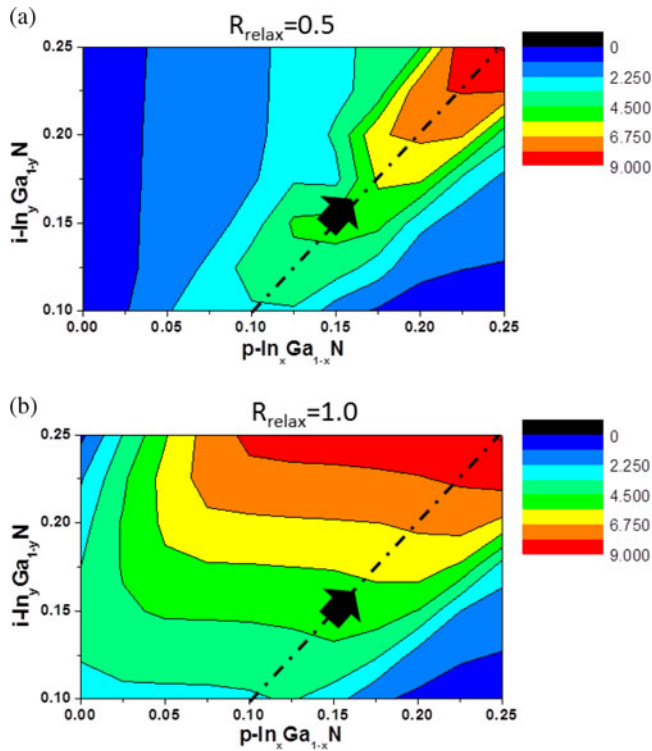


Fig. 6. Power conversion efficiency map of InGaN heterojunction solar cells consisting of p-In_xGa_{1-x}N and i-In_yGa_{1-y}N with various indium compositions for (a) $R_{\text{relax}} = 0.5$ and (b) $R_{\text{relax}} = 1.0$. The dot-dashed line and arrow represent the polarization-matched combinations.

IV. CONCLUSION

In summary, we have investigated the projected efficiencies of p-In_xGa_{1-x}N/i-In_yGa_{1-y}N/n-GaN double heterojunction solar cells with various indium compositions for monolithic growth on a c-facet sapphire substrate. The proposed p-type InGaN layer reduces the polarization charges at the p-i heterojunction interface, leading to a redistribution of the built-in potential and facilitating charge transport. We observe that an In content of 20% for a polarization-matched p-i interface is optimal and leads to a maximum power conversion efficiency that is close to 7% under the assumption of no strain relaxation. Further efficiency enhancement with a higher indium composition over 20% is also possible via the redistribution of the built-in field with n-GaN doping.

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