Numerical Study of (0001) Face GaN/InGaN p-i-n Solar Cell With Compositional Grading Configuration

Yen-Kuang Kuo, Bing-Cheng Lin, Jih-Yuan Chang, Fang-Ming Chen, and Hao-Chung Kuo

***Abstract*— The advantages of a (0001) face GaN/InGaN p-i-n solar cell with compositional grading configuration between i-InGaN/p-GaN layers are studied numerically. With the use of the grading layer, the conversion efficiency is markedly promoted due to the reduction of potential barrier height for holes and due to the decrease of polarization. Optimized conversion efficiency is obtained when the thickness of the grading layer increases to a critical value. This critical thickness is strongly influenced by the polarization charges and doping concentration of the grading layer. When the density of the polarization charges is high or the doping concentration is low, a thick grading layer is required to achieve high efficiency.**

***Index Terms*— Grading layer, InGaN, solar cell.**

I. Introduction

INDIUM gallium nitride (InGaN) alloys have favorable photovoltaic properties such as high absorption coefficient, high carrier mobility, and high radiation resistance [1], [2]. Besides, the InGaN alloy is direct bandgap material whose characteristic wavelength ranges from infrared to ultraviolet region, which can cover most of the solar spectrum by tuning the alloy composition [3], [4]. Under this circumstance, current matching can be easily achieved [5]. As a result, it has the potential in realizing high-efficiency multijunction solar cell based solely on the III-nitride material system.

The spontaneous and piezoelectric polarization may lead to significant interface charges in nitride-based devices grown on c-plane sapphire substrate. In light-emitting diodes (LEDs), the effect of polarization might deteriorate the electron overflow, retard the hole injection, decrease the overlap of electron and hole wavefunctions in the quantum wells (QWs), and thus degrade the LED performance [6]. As for the solar cells, it was reported recently that the carrier collection efficiency could be seriously reduced due to polarization-induced electric field, whose direction is opposite to that of the built-in electric field [7], [8], in the p-i-n structures. The J-V curve shows abrupt current drop and has quite low fill factor (FF) when the density of interface charges is high.

Since the polarization effect is harmful to the device performance of solar cells, it is important to mitigate this effect. Several methods can be employed to overcome this issue, such as the usage of N-face template, p-side down structure, AlGaInN quaternary polarization-matched material, and compositional grading configuration in the heterojunction. The first three methods can be used to fully solve the detrimental influence of polarization effect. However, they suffer from the problems in fabrication, i.e., the difficulty in crystal growth and the unfavorable property for current spreading. As for the last method, even though it can only diminish the polarization effect, the solar cell can be fabricated easily under this situation. Moreover, when a compositional grading configuration is employed, the discontinuity of energy band in the heterojunction is reduced, which is beneficial for carriers to transport across the heterojunction and thus can enhance the carrier collection efficiency [9].

II. Device Structure and Parameters

In this letter, the effect of the usage of InGaN grading layer between the intrinsic InGaN layer and p-GaN layer is studied. The electrical properties of the conventional GaN/InGaN p-i-n solar cell structures with and without a grading layer are investigated numerically with the APSYS program [10]. The original structure used for reference is based on the solar cell fabricated by Horng *et al* [11]. The solar cell was grown on a c-plane sapphire substrate, followed by a 2.0-μm-thick undoped GaN layer and a p-i-n structure, which consists of a 1.0-μm-thick n-GaN layer (n-doping $= 5\times10^{18}$ cm^{-3}), a 0.15-μm-thick undoped InGaN absorption layer, and a 0.15-μm-thick p-GaN top layer (p-doping $= 8\times10^{17}$ cm^{-3}). The indium composition of the InGaN layer is 10%. Most of the material parameters utilized in the simulation are based on the recommended values in [12] and [13]. The polarization-induced surface charges at the interfaces are calculated by the methods developed by Fiorentini *et al* [14]. In the simulation, the degree of piezoelectric polarization in the GaN/InGaN interfaces is controlled by modifying the parameter "degree of relaxation," which is denoted by "R" in the following study. When the value of R increases, the piezoelectric polarization reduces proportionally while the spontaneous polarization remains unchanged. In order to focus on the exploration of polarization effect, the Shockley-Read-Hall

Manuscript received November 1, 2011; revised February 22, 2012; accepted March 20, 2012. Date of publication April 3, 2012; date of current version May 10, 2012. This work was supported in part by the National Science Council, Taiwan, under Grant NSC-99-2119-M-018-002-MY3.

Y.-K. Kuo, J.-Y. Chang, and F.-M. Chen are with the Department of Physics, National Changhua University of Education, Changhua 500, Taiwan (e-mail: ykuo@cc.ncue.edu.tw; jihyuan67@gmail.com; peter321567@hotmail.com).

B.-C. Lin and H.-C. Kuo are with the Department of Photonics, Institute of Electro-Optical Engineering, National Chiao Tung University, Hsinchu 300, Taiwan (e-mail: jasonlin0723@hotmail.com; hckuo@faculty.nctu.edu.tw).

Color versions of one or more of the figures in this letter are available online at http://ieeexplore.ieee.org.

Digital Object Identifier 10.1109/LPT.2012.2192723

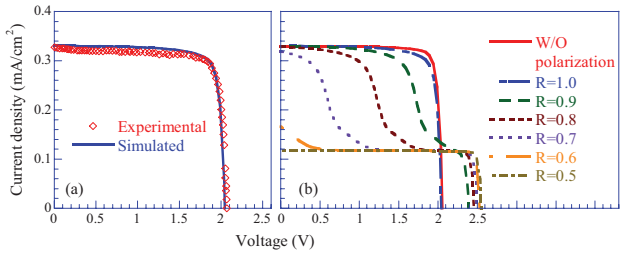

Fig. 1. (a) Experimental and simulated J-V curves of the original GaN/InGaN p-i-n solar cell. (b) J-V curves of different situations of polarization.

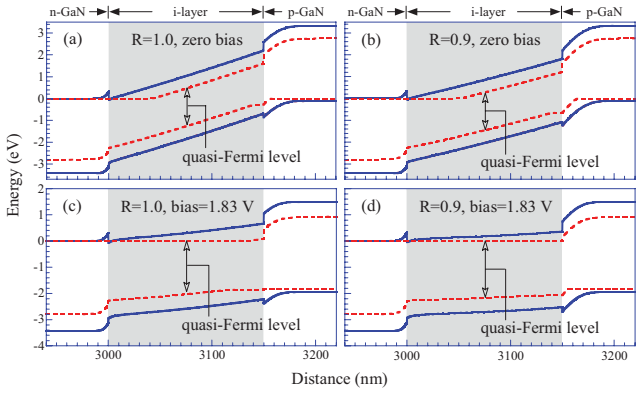

Fig. 2. Energy band diagrams of GaN/InGaN p-i-n solar cell in the situations of (a) R = 1.0 and (b) R = 0.9 at zero bias, and (c) R = 1.0 and (d) R = 0.9 at 1.83 V.

(SRH) recombination lifetime of InGaN layer is assumed to have the same value of 0.3 ns for all the situations under study.

III. Analysis and Discussion

The experimental and simulated current-voltage (J-V) curves of the original GaN/InGaN p-i-n solar cell under AM1.5G illumination are plotted in Fig. 1(a), which shows good agreement between these two curves. The value of R is set to be one for the original structure. Fig. 1(b) shows the J-V curves of different situations of polarization. The device performance degrades with the decrease of R or, accordingly, with the increase of polarization. The major factor responsible for the degradation in device performance is presumably the abrupt current drop shown in Fig. 1(b), which results in the reduction of fill factor. The conditions of maximum power in the situation of R = 1.0 are 1.83 V, 0.30 mA/cm^2, and 0.55 mW/cm^2, respectively. The current density drops abruptly to 0.16 mA/cm^2 with the same forward bias in the situation of R = 0.9.

Fig. 2 shows the energy band diagrams of the GaN/InGaN p-i-n solar cell under a forward bias of zero and 1.83 V with different situations of polarization. When the forward bias is zero, as shown in Figs. 2(a) and (b), the degree of tilting in energy band of the major absorption region, i.e., the InGaN layer, indicates that the total internal electric field is diminished with the decrease of R, which is due to the increase of polarization-induced surface charges and electric field, whose direction is opposite to that of the built-in electric field. The energy band on the p-side should be pulled down the same amount for both

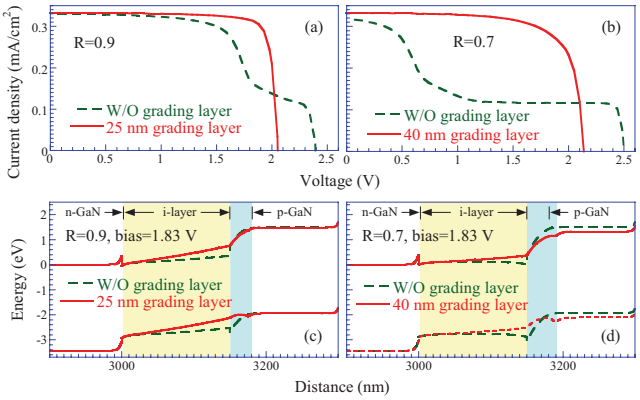

Fig. 3. J-V curves in the situations of (a) R = 0.9 and (b) R = 0.7, and energy band diagrams in the situations of (c) R = 0.9 and (d) R = 0.7 of original and new proposed structures.

cases of solar cells when they are with the same forward bias of 1.83 V. In this case, as shown in Figs. 2(c) and (d), the tilting of the energy band of InGaN layer in the situation of R = 0.9 is further decreased and is still smaller than that in the situation of R = 1.0. It is noteworthy that, in this kind of double-heterojunction structure, the band offset between the InGaN and GaN layers might retard the carriers from being collected. As a result, if the internal electric field is not large enough, the carriers can not transport across this energy barrier effectively. This is the reason why the solar cell in the situation of R = 0.9 shows an abrupt current drop when the forward bias increases while the R = 1.0 one does not have this kind of tendency. Note that, in real-fabricated devices, even the more-relaxed structure could benefit from the reduced polarization field, the increased structural defects would degrade the minority carrier lifetime and hurt efficiencies. Thus, the ultimate goal is to seek for the solution which can efficiently eliminate the detrimental polarization effect while the crystalline quality can be maintained.

Fig. 3 shows the J-V curves and energy band diagrams of the original GaN/InGaN p-i-n solar cell without grading layer and the new proposed structure with InGaN compositional grading layer. For the grading layer, the doping concentration is the same as that of the p-GaN layer (8×10^{17} cm^{-3}) and the thickness is 25 nm in the situation of R = 0.9 and 40 nm in the situation of R = 0.7. In the new proposed structure, the abrupt current drop is eliminated until the applied bias equals to the open-circuit voltage (V_{oc}) for both situations of R. The conversion efficiency is enhanced due to the improvement of fill factor. The reduction of V_{oc} is presumably due to the decrease of polarization charges [7]. The improvement of fill factor can be ascribed to the following two factors. The first one is that the potential barrier height in the valence band between the InGaN layer and p-GaN layer decreases with the use of grading layer. The hole collection efficiency is thus enhanced. The second influencing factor is the reduced polarization effect. When the grading layer is employed, the density of polarization charges in the i-InGaN/p-GaN interface decreases and the tilting of energy band increases when

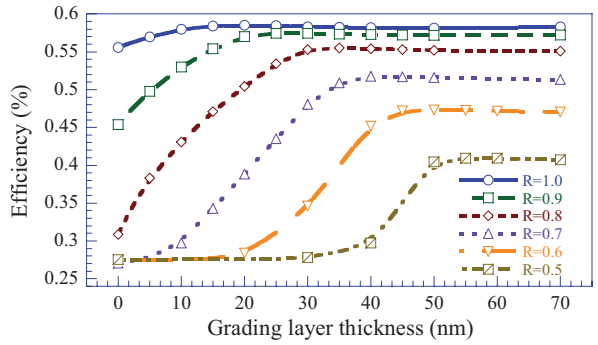

Fig. 4. Conversion efficiencies of the GaN/InGaN p-i-n solar cell as a function of the thickness of the grading layer with different situations of polarization.

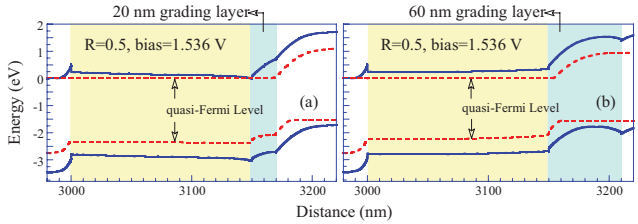

Fig. 5. Energy band diagrams of GaN/InGaN p-i-n solar cells with (a) 20-nm and (b) 60-nm grading layers in the situation of $R = 0.5$.

compared to the original structure, which is beneficial for carrier collection.

Fig. 4 shows the conversion efficiencies of GaN/InGaN p-i-n solar cell as a function of the thickness of grading layer with different situations of polarization. It is evident that the conversion efficiency is improved with the use of grading layer in all situations of R. When the thickness of grading layer increases to a critical value, the efficiency reaches to the maximum and then saturates due to the decrease of polarization-induced surface charges. Fig. 5 shows the energy band diagrams of GaN/InGaN p-i-n solar cells with 20 and 60-nm grading layers in the situation of R = 0.5. For the structure with 20-nm grading layer, the titling of energy band in InGaN layer is still in the direction detrimental for carrier collection. However, when a thicker grading layer, i.e. the 60-nm grading layer, is employed, the tilting is reversed. It indicates that the polarization charges accumulated in the i-InGaN/p-GaN interface can be effectively reduced with the use of an appropriate grading layer. Fig. 6(a) shows the conversion efficiencies as a function of the thickness of grading layer with different p-type doping concentrations in the situation of R = 0.9. For the structure with lower p-type doping concentration grading layer, the efficiency is inferior in all thicknesses of grading layer under study. The reason is that the lightly p-doped grading layer introduces a potential barrier in the valence band which prevents the photogenerated holes from being collected, as shown in Fig. 6(b). In addition, with the decrease of p-type doping concentration, it requires a thicker grading layer to achieve high efficiency due to the more serious polarization effect.

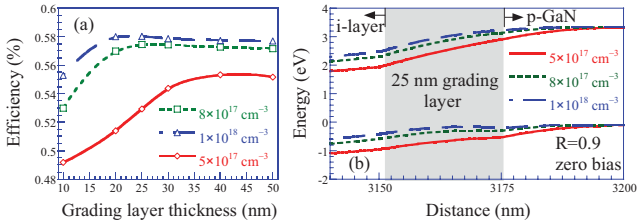

Fig. 6. (a) Conversion efficiencies as a function of the thickness of the grading layer and (b) energy band diagrams near the 25-nm grading layer with different p-type doping concentrations in the situation of $R = 0.9$.

IV. Conclusion

The (0001) face GaN/InGaN p-i-n solar cell with compositional grading configuration between i-InGaN/p-GaN layers is numerically investigated. The simulation results show that the solar cell can benefit from the employment of grading layer due to the elimination of potential barrier for holes in the valence band and the mitigation of polarization effect. The use of a thick grading layer is required to efficiently release the detrimental polarization effect if the density of polarization charges is high or the doping concentration is low.

References

[1] W. Walukiewicz, *et al.*, "Structure and electronic properties of InN and In-rich group III-nitride alloys," *J. Phys. D*, vol. 39, no. 5, pp. R83–R99, Feb. 2006.

[2] O. Jani, I. Ferguson, C. Honsberg, and S. Kurtz, "Design and characterization of GaN/InGaN solar cells," *Appl. Phys. Lett.*, vol. 42, pp. 132117-1–132117-2, Sep. 2007.

[3] J. Wu, *et al.*, "Unusual properties of the fundamental band gap of InN," *Appl. Phys. Lett.*, vol. 80, no. 21, pp. 3967–3969, May 2002.

[4] I. Vurgaftman and J. R. Meyer, "Band parameters for nitrogen-containing semiconductors," *J. Appl. Phys.*, vol. 94, pp. 3675–3696, Sep. 2003.

[5] A. Yamamoto, M. R. Islam, T.-T. Kang, and A. Hashimoto, "Recent advances in InN-based solar cells: Status and challenges in InGaN and InAlN solar cells," *Phys. Status Solidi C*, vol. 7, no. 5, pp. 1309–1316, May 2010.

[6] Y.-K. Kuo, J.-Y. Chang, M.-C. Tasi, and S.-H. Yen, "Advantages of blue InGaN multiple-quantum well light-emitting diodes with InGaN barriers," *Appl. Phys. Lett.*, vol. 95, no. 1, p. 011116-1, Jul. 2009.

[7] Z. Q. Li, M. Lestradet, Y. G. Xiao, and S. Li, "Effects of polarization charge on the photovoltaic properties of InGaN solar cells," *Phys. Status Solidi A*, vol. 208, pp. 928–931, Apr. 2011.

[8] J.-Y. Chang and Y.-K. Kuo, "Numerical study on the influence of piezoelectric polarization on the performance of p-on-n (0001)-face GaN/InGaN p-i-n solar cells," *IEEE Electron Device Lett.*, vol. 32, no. 7, pp. 937–939, Jul. 2011.

[9] Y.-K. Kuo, B.-C. Lin, J.-Y. Chang, and Y.-A. Chang, "Numerical simulation of single-junction $In_{0.5}Ga_{0.5}P$ solar cell with compositional grading configuration," *IEEE Photon. Technol. Lett.*, vol. 23, no. 12, pp. 822–824, Jun. 15, 2011.

[10] *APSYS by Crosslight Software Inc.*, Burnaby, Canada [Online]. Available: http://www.crosslight.com

[11] R.-H. Horng, *et al.*, "Improved conversion efficiency of GaN/InGaN thin-film solar cells," *IEEE Electron Device Lett.*, vol. 30, no. 7, pp. 724–726, Jul. 2009.

[12] I. Vurgaftman and J. R. Meyer, "Band parameters for III-V compound semiconductors and their alloys," *J. Appl. Phys.*, vol. 89, pp. 5815–5875, Jun. 2001.

[13] L. Hsu, R. E. Jones, S. X. Li, K. M. Yu, and W. Walukiewicz, "Electron mobility in InN and III-N alloys," *J. Appl. Phys.*, vol. 102, pp. 073705-1–073705-6, Oct. 2007.

[14] V. Fiorentini, F. Bernardini, and O. Ambacher, "Evidence for nonlinear macroscopic polarization in III-V nitride alloy heterostructures," *Appl. Phys. Lett.*, vol. 80, pp. 1204–1206, Feb. 2002.