OPTIMIZATION OF GaN WINDOW LAYER FOR InGaN SOLAR CELLS USING POLARIZATION EFFECT

Omkar Jani[1,2], Balakrishnam Jampana[3], Mohit Mehta[1], Hongbo Yu[2], Ian Ferguson[2], Robert Opila[3], Christiana Honsberg[1]

[1]Department of Electrical and Computer Engineering, University of Delaware, Newark, DE 19716
[2]School of Electrical and Computer Engineering, Georgia Institute of Technology, Atlanta, GA, 30332
[3]Department of Material Science and Engineering, University of Delaware, Newark, DE 19716

ABSTRACT

The III-nitride material system offers substantial potential to develop high-efficiency solar cells. Theoretical modeling of InGaN solar cells indicate strong band bending at the top surface of p-InGaN junction caused due to piezoelectric polarization-induced charge at the strained p-GaN window interface. A counterintuitive strained n-GaN window layer is proposed, modeled and experimentally verified to improve performance of InGaN solar cells. InGaN solar cells with band gap of 2.9 eV are grown using MOCVD with p-type and n-type strained GaN window layers, and fabricated using variable metallization schemes. Fabricated solar cells using n-GaN window layers yield superior V_{OC} and FF compared to those using p-GaN window layers. The V_{OC}'s of InGaN solar cells with n-GaN window layers are further enhanced from 1.5 V to 2 V by replacing the conventional NiO_X top contact metal with Ti/Al, which also verifies the tunneling principle.

INTRODUCTION

While the III-nitride technology is well established for optoelectronic applications such as light-emitting diodes and laser diodes [1], recent developments confirm its substantial potential in photovoltaic applications [2]. With the recent revision of the band gap of InN at 0.65 V [3], [4], [5], the direct band gap of the InGaN material system spans the bulk of the solar spectrum. InGaN is one of the few material systems that provide band gaps greater than 2.4 eV, which are required to achieve practical photovoltaic efficiencies greater than 50% as indicated by detailed-balance modeling [6], [7]. Properties such as high theoretical mobilities, high absorption, high peak and saturation velocities [8], and radiation hardness establish an important role for the III-nitrides for high efficiency photovoltaics.

Among the unique features of III-nitrides are strong spontaneous and piezoelectric (strain-induced) polarization effects [9], [10]. It has been theoretically calculated and confirmed experimentally [11] that the III-nitrides are highly polar molecules due to non-centrosymmetry of charge in the wurtzite structure and the large ionicity of the covalent bonds. Some polarization constants are found to be up to ten times larger than those in conventional III-V and II-VI semiconductor compounds, and comparable to those of ZnO. The net polarization and consequent internal electric fields have been shown to be detrimental to the performance of optoelectronic devices due to polarization-induced potential barriers and band bending [12], [13]; electric fields with values in excess of 6 MV/cm have been reported [11]. Consequently, polarization effects have significant consequences on the performance of InGaN solar cells. However, this phenomenon can be utilized constructively if taken into account during design of the solar cell to improve its collection efficiency.

Previously, we have demonstrated record high single-junction V_{OC}'s at 2.4 V and high IQE's for p-i-n InGaN/GaN solar cells. The present work is a subset of the design optimization process for such solar cells, where we focus on the design of wide-band gap GaN window layers for InGaN solar cells. Window layers serve to passivate the top junction surface [14] and generate a front-surface field [15] to minimize front surface recombination. Due to the relatively high defect and dislocation density on InGaN surfaces [16], high resistivity and highly sensitive Ohmic contacts to the top p-type InGaN junctions [17], it becomes important to fabricate highly efficient and reproducible window layers for InGaN solar cells.

In the present work, we demonstrate the counterintuitive design, fabrication and optimization of the GaN window layer for InGaN solar cells mediated by polarization effects. The experimental results are verified using (1) modified PC1D software [18] enhanced at the source-code level to model polarization [19], and (2) other custom simulation tools.

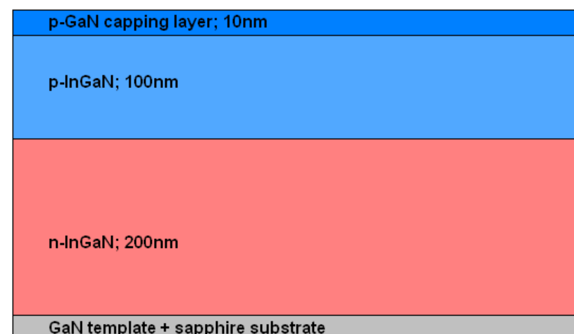
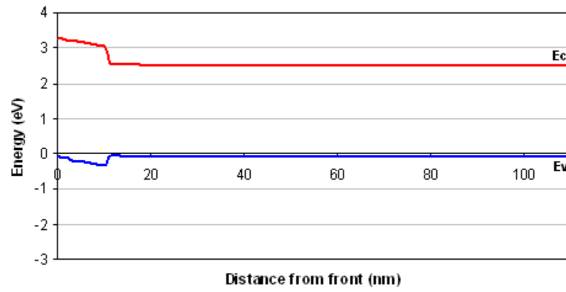
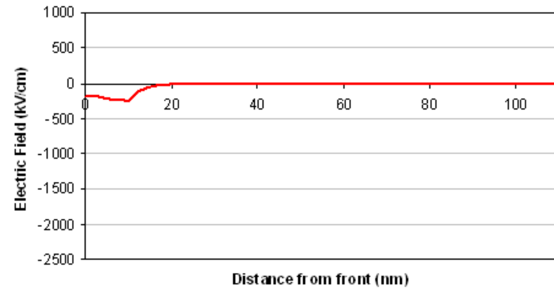


Fig.1. Typical p-GaN window layer for InGaN solar cell.



P-cap without polarization: (a)



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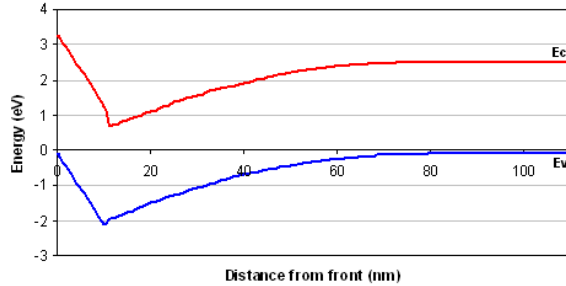
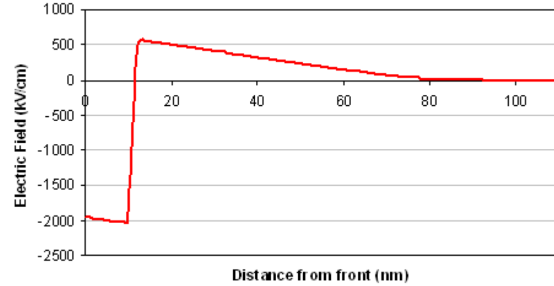


P-cap with polarization: (c)



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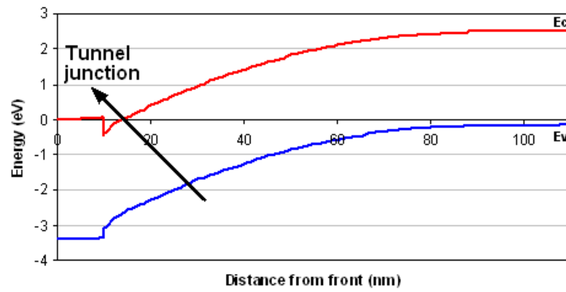
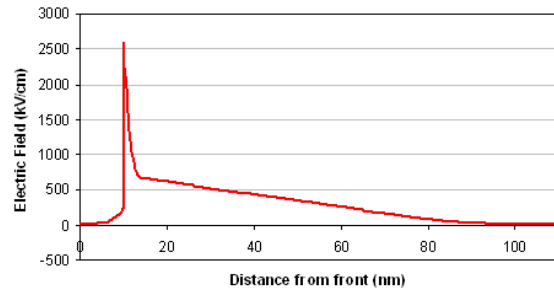


N-cap with polarization: (e)



(f)

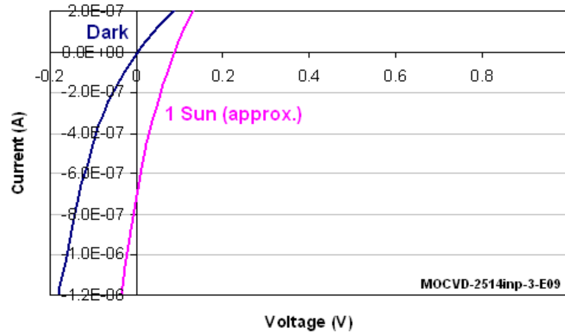
Fig. 2. PC1D simulated band diagram and electric field for (a) and (b) p-GaN/p-InGaN heterointerface without polarization effects, (c) and (d) p-GaN/p-InGaN heterointerface with polarization effects 100% strain, and (e) and (f) n-GaN/p-InGaN heterointerface with polarization effects 100% strain.

DESIGN

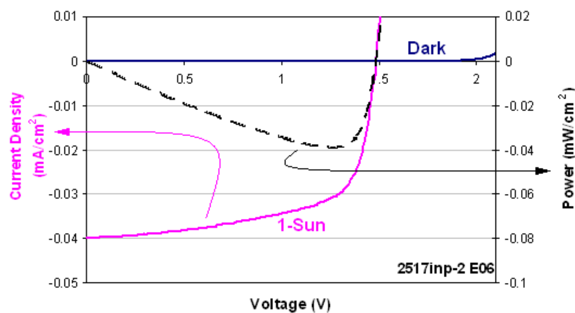
For a p-n $In_{0.2}Ga_{0.8}N$ solar cell with a p-type $In_{0.2}Ga_{0.8}N$ junction at the top, it is intuitive to use a thin p-type GaN window layer as shown in Figure 1. The expected band diagram and electric field at the p-GaN/p-InGaN heterointerface, without considering any polarization effects, are simulated in PC1D and shown in Figure 2(a) and 2(b), respectively.

However, thin GaN window layers, designed in a 2 – 10 nm thickness range, are typically strained due to lattice mismatch with the underlying InGaN layer and hence, generate substantial piezoelectric polarization. The simulated band diagram and electric field for this structure with a completely pseudomorphic p-GaN window layer are shown in Figure 2(c) and 2(d), respectively. It is seen that the downward bending of bands at the strained-p-GaN/p-InGaN heterointerface tends to develop a potential well that accumulates a 2-Dimensional Electron Gas (2DEG). Moreover, electric field developed at the p-InGaN side of the heterointerface opposes the collection of the holes from p-InGaN bulk to the p-GaN window layer. Hence, alternate methods to cap the p-InGaN layer are investigated.

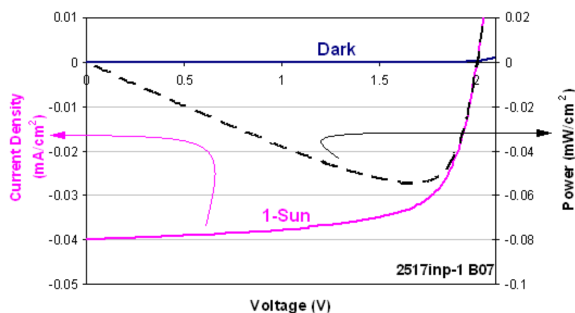
PC1D simulations as well as literature [20], [21] indicate that tunneling contacts using n-type material can potentially provide superior Ohmic characteristics to p-type GaN or InGaN contacts. Such tunneling contacts are evident from simulated band diagram of n-GaN/p-InGaN heterointerface as shown in Figure 2(e). The strong band bending and 2DEG at the interface aids to the tunneling of holes from p-InGaN to n-GaN window and enhance collection of the solar cell. The 2DEG also aids lateral current spreading, which redueces the grid spacing



(a)



(b)



(c)

Fig. 3. Measured I-V curves for $In_{0.12}Ga_{0.88}N$ p-n solar cells with (a) p-GaN window, (b) n-GaN window using NiOX contact, and (c) n-GaN window using Ti/Al/Ti/Au contact.

constraints at the top surface of the solar cell. Moreover, due to the lower resistivity and ease of forming Ohmic contacts to n-GaN compared to p-GaN, this tunneling contact using n-type material indicates a viable alternative.

GROWTH AND FABRICATION

Epitaxy similar to that shown in Figure 1 is performed in an Emcore MOCVD D125 rotating disk reactor with a short jar configuration. The epitaxial solar cell is grown on a 2 µm GaN template, which in turn is grown on a 2-inch single-side-polished sapphire substrate. The epitaxial solar cell consists of a 100 nm p-InGaN/200 nm n-InGaN homojunction capped by a 10 nm p-GaN layer. Indium composition of 12% is used for InGaN, which translates into a band gap of 2.9 eV. The epitaxial structure is fabricated into a solar cell, where Ohmic contact to n-InGaN is formed using an e-beam-evaporated 10 nm Ti/30 nm Al/10 nm Ti//50 nm Au metal. A low resistivity contact to the top p-GaN window layer is achieved using a 10 nm NiO_X layer formed by e-beam deposition of 5 nm Ni/5 nm Au followed by an oxidation anneal at 500 °C for 1 minute. The contact pad used for p-GaN consists of 50 nm Ni/50 nm Au.

A second set of epitaxy is performed, with the structure similar to that shown in Figure 1, except that the 10 nm p-GaN window layer is replaced by a 10 nm n-GaN window layer. An additional fabrication scheme is also applied, where Ohmic contacts to both, n-InGaN as well as n-GaN window, are achieved using e-beam-evaporated 10 nm Ti/30 nm Al/10 nm Ti//50 nm Au metal.

RESULTS AND DISCUSSION

The epitaxial material quality is confirmed using X-ray diffraction and photoluminescence, while the fabricated devices are tested for Current-Voltage (I-V) characteristics and internal quantum efficiency (IQE).

Typical I-V curves for the InGaN solar cells with p-GaN and n-GaN window are shown in Figure 3. As seen in Figure 3(a), InGaN solar cells with p-GaN window layers demonstrate very low Open-Circuit Voltages (V_{OC}) and Fill Factors (FF). Figure 3(b) shows a typical I-V curve for InGaN solar cells with n-GaN window layers employing a NiO_X top contact. These devices demonstrate a V_{OC} around 1.5 V and FF of 66%. However, the highest V_{OC}'s are measured at 2 V and FF at 68% for InGaN solar cells with n-GaN window and Ti/Al/Ti/Au contacts as seen in Figure 3(c).

These results are in agreement with the tunneling-model based on calculations presented in the 'design' section of this paper. The combination of strong polarization charge at the p-GaN/p-InGaN interface with a non-ideal NiO_X/p-GaN contact substantially reduces the V_{OC} and FF of the solar cell. It is also speculated that the p-InGaN layer is completely depleted of charge and hence, the resultant solar cell demonstrates linear characteristics rather than a diode-like behavior. On the other hand, solar cells with n-GaN window layers demonstrate high V_{OC}'s due to a simplified tunneling process at the n-GaN/p-InGaN heterojunction. Moreover, this tunneling is further enhanced using Ti/Al top-contacts due to their low work-functions and ability to form low resistance Ohmic contacts to n-type III-nitrides.

While this counterintuitive principle of using n-GaN window layers for p-InGaN junctions is demonstrated, it is essential to further verify this principle and optimize the recipe of the n-type window layer.

CONCLUSION

The counterintuitive principle of using n-GaN window layer for a top p-InGaN junction is theoretically, as well as experimentally demonstrated for InGaN solar cells. Strained n-GaN window layers enhance tunneling of holes from the p-InGaN junction due to the piezoelectrically induced sheet charge and strong band bending at the heterointerface. Fabricated InGaN solar cells with band gap of 2.9 eV and n-GaN window layer demonstrate a superior performance compared to those with p-GaN window layers. The V_{OC}'s of InGaN solar cells with n-GaN window layers are enhanced from 1.5 V to 2 V by replacing the conventional NiO_X top contact metal to Ti/Al. While the principle of tunneling is experimentally demonstrated, future work focuses on optimizing the contacting scheme.

ACKNOWLEDGEMENTS

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