Modeling of N-i-P Vs. P-i-N InGaN Solar Cells with Ultrathin GaN Interlayers for Improved Performance

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Abstract- **P-i-N structure solar cells often provide improved performance over N-i-P devices because acceptors are easier to activate when the p-type layer is close to the surface. However, for strained InGaN solar cells on GaN, the polarization-induced electric field creates a barrier for photocurrent that impedes device performance. In this paper we show that for Ga-face growth, N-i-P structures can provide improved performance because the electric field from the junction is parallel to that formed from polarization induced sheet charges. Thus the fields complement each other to assist in creating photocurrent in N-i-P devices. Additionally we simulate an N-i-P cell using the recently demonstrated insertion of ultra-thin GaN interlayers to achieve thick strained layers with high material quality.**

INTRODUCTION

The $In_xGa_{1-x}N$ system has been researched extensively for photovoltaic use after the bandgap of InN was discovered to be 0.64 eV. Furthermore this system has several beneficial qualities. It has a direct bandgap over the entire compositional range, possesses high carrier mobility and drift velocity, is highly resistant to radiation deterioration, and exhibits high optical absorption ($> 10^5$ cm^{-1}) near the bandgap.

Unfortunately this system has proven difficult to grow at high indium concentration because of phase separation [1], indium clustering [2], and cracking due to low critical thicknesses [3]. These effects quickly degrade device performance to unacceptable levels. Several groups have made significant advances despite these challenges. Both Molecular Beam Epitaxy (MBE) and Metalorganic Chemical Vapor Deposition (MOCVD) growth have resulted in single phase $In_xGa_{1-x}N$ with In content up to 40% [4-7].

Theoretical investigations on the spontaneous and piezoelectric polarization effects in the III-nitride material system has matured substantially with only around 20% difference between experiments and ab-initio predictions [8]. Despite the well-known, commercial application of these effects in high-electron mobility transistors and other devices, only a few papers mention these strong effects in solar cell devices [9, 10]. For solar cells, it beneficial to have coherently strained InGaN layers as this reduces dislocations and improves device quality. But strained InGaN on GaN substrate creates large polarization electric fields. For instance one group found the electric field to be around 2.45 MV/cm with just 18% indium [11] . As material quality and modeling are improved, it will become possible to optimize the use of polarization effects. In this paper we propose the modification of traditional P-i-N designs, showing that the recommended N-i-P configuration solar cell is a superior design over P-i-N designs for InGaN. Additionally we report simulations of solar cells including the periodic insertion of ultrathin GaN interlayers in the InGaN absorbing region. This design has recently been shown to eliminate phase-separation in >120 nm-thick InGaN [12].

DEVICE DESIGN

The piezoelectric parameters used are listed in Table 1. The doping in p-type regions was 5e17/cm^3 while the doping in n-type regions was 1e18/cm^3. The i-region was simulated with either a 126 nm bulk $In_{0.1}Ga_{0.9}N$ layer or with 6 regions of 21 nm $In_{0.1}Ga_{0.9}N$ with 1.5 nm GaN interlayers.

RESULTS

The polarization-induced electric fields naturally formed on strained InGaN layers oppose the junction field created in typical P-i-N junctions. This effect has been noted in [9, 10] and is reproduced here in Fig. 1. The use of only 30% of the theoretical polarization sheet charge has drastic effects on the band diagram, reversing direction of the photo-generated current. It is hard to predict the exact value of the polarization field as defects, phase separation, indium clustering, doping and free carriers can screen the polarization induced sheet charges [13, 14]. Regardless, as material quality improves the effect is likely to become more substantial and could severely lower the efficiency of solar cells used in the P-i-N configuration. However, as shown in Fig. 2, switching to an N-i-P device alleviates this effect as the junction and polarization field are now in the same direction. The band diagram is only slightly modified for up to 100% of the theoretically predicted polarization. This indicates that with improved material quality, the natural polarization of the InGaN layer will assist rather then detract from the photo-generated current.

Finally, as mentioned above, the use of ultrathin GaN interlayers has been shown to prevent indium phase separation, while allowing for thicker strained InGaN layers. Fig. 3 and 4 show again that the N-i-P configuration is a superior design. Further simulations will show that for high polarization fields the predicted external quantum efficiency (EQE) of N-i-P designs should not vary substantially while the EQE of P-i-N devices is expected to approach zero.

TABLE 1
MATERIAL PARAMETERS

Parameter	Symbol	Units	GaN	$In_{0.1}Ga_{0.9}N$
Lattice Constant	A	Nm	0.3189	0.3225
Elastic Constants	c13	Gpa	106	104.6
Elastic Constants	c33	Gpa	398	380.6
Piezoelectric Tensor	e13	C/m^2	-0.527	-0.523
Piezoelectric Tensor	e33	C/m^2	0.895	0.911
Spontaneous Polarization	Psp	C/m^2	-0.034	-0.031

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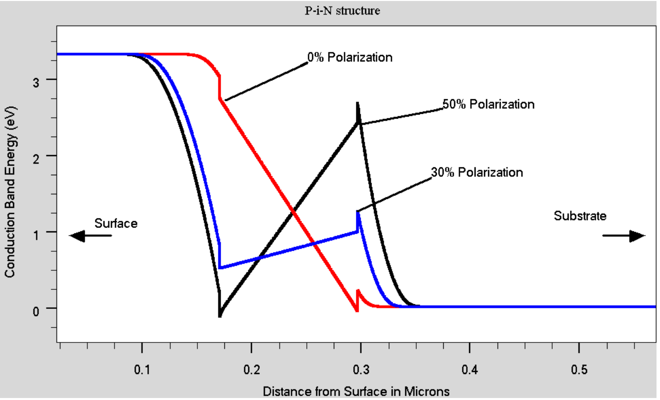

Fig. 1. Typical conduction band for a P-i-N solar cell device (0% polarization) along with photocurrent inhibiting energy band diagrams arising from polarization effects (30% and 50% shown). This and all simulations performed on Silvaco TCAD software [15].

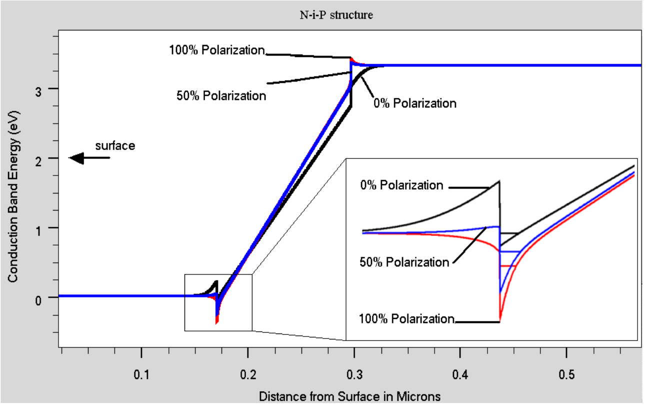

Fig. 2. Conduction band for a N-i-P solar cell device (0%, 50% and 100% polarization shown). Inset shows how the barrier at the GaN/InGaN interface is reduced and the quantum well on the InGaN side is deepened.

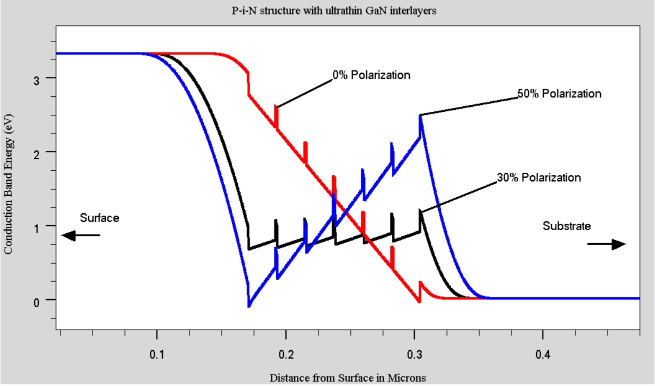

Fig. 3. Typical conduction band for a P-i-N solar cell device with ultrathin GaN layers (0%, 30% and 50% polarization shown).

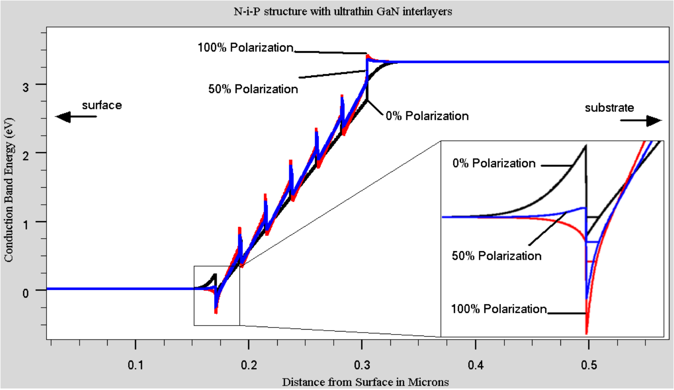

Fig. 4. Typical conduction band for a N-i-P solar cell device with ultrathin GaN layers added (0%, 50% and 100% polarization shown). Inset shows how the barrier at the GaN/InGaN interface is reduced and the quantum well on the InGaN side is deepened.

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