MODIFYING PC1D TO MODEL SPONTANEOUS AND PIEZOELECTRIC POLARIZATION IN III-V NITRIDE SOLAR CELLS

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ABSTRACT: Spontaneous and piezoelectric polarization present in the wurtzite group III-nitrides (AlN, GaN, InN and their alloys) influence the optical and electrical properties of these materials and thus, have significant consequences on solar cell design. First, the theoretical model of polarization implemented into the source code of PC1D is discussed. Polarization is introduced into PC1D as induced-surface/interface charges at the initialization of the solving routine. Simulations of InGaN solar cell test structures indicate an increase in efficiency by 38% due to an improved carrier collection efficiency caused by polarization-induced electric fields at the GaN/InGaN heterojunction. Scope for future enhancement of the III-nitride model includes optimizing radiative recombination for high band gap materials and optimizing the convergence routine of the program to handle abrupt changes in electric field and charge profiles.
Keywords: Fundamentals, III-V Semiconductors, Polarization

1 INTRODUCTION

The III-nitrides offer substantial potential to develop ultra-high efficiency solar cells due to their direct-band gap ranging from 0.65eV (InN) to 6.2eV (AlN) [1, 2]. The InGaN material system offers a wide range of direct band gaps that spans the bulk of the solar spectrum. Additional advantages of this material system include low effective mass of electrons and holes, high mobilities, high peak and saturation velocities [3], high absorption coefficients and radiation tolerance. These features not only enable InGaN to be exploited for large-stack tandems, but they can also be explored for applications such as quantum-dots and intermediate-bands for third generation photovoltaics.

A unique feature of the III-nitrides is strong polarization and piezoelectric effects [4, 5]. It has been theoretically calculated and confirmed experimentally [6] that the III-nitrides are highly polar molecules due to the non-centrosymmetry of charge in the wurtzite structure and large ionicity of the covalent bonds. Spontaneous and piezoelectric polarization present in the wurtzite III-nitrides influence the optical and electrical properties of these materials and thus, have significant consequence on solar cell design. Polarization in the III-nitrides induce sheet charges and electric fields with reported values as high as 1MV/cm [6]. Polarization can be used constructively in solar cell design to enhance carrier collection, reducing ohmic resistances and bending bands to reduce surface recombination. Conversely, polarization can also generate electric fields and energy spikes in the bands detrimental for carrier collection and potential wells that can act as recombination centers. Thus, it becomes imperative to consider polarization effects while designing III-nitride solar cells.

Due to the unavailability of a suitable solar cell modeling program with polarization simulation capabilities, an polarization sub-routine is incorporated into PC1D [7]. This paper first discusses the theory of polarization in the III-nitrides as incorporated into the source code of PC1D. The program is then used to simulate InGaN solar cell test structures to study the implications of polarization on device performance.

2 MODELING POLARIZATION IN III-V NITRIDES

Polarization affects the semiconductor via the following equation [8]:

$$D = \epsilon_o \epsilon_r E + P \qquad \text{--- (1)}$$

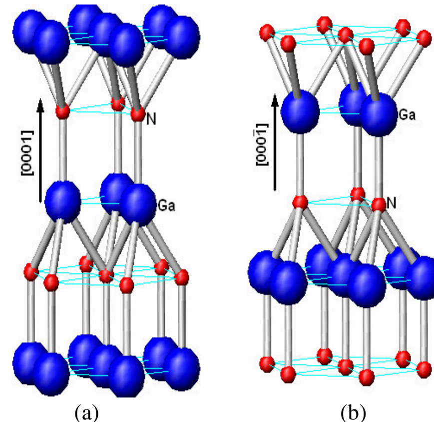
where, D = Electric flux density (C/m^2),
E = Electric field (V/m),
P = Net Polarization (C/m^2),
ϵ_o = vacuum permittivity,
ϵ_r = relative permittivity

The net polarization is composed of two parts: (1) spontaneous, which is intrinsic to a material, and (2) piezoelectric, which is strain-induced.

$$P = P_{SP} + P_{PZ} \qquad \text{--- (2)}$$

where, P = Net Polarization (C/m^2),
P_{SP} = Spontaneous Polarization (C/m^2),
P_{PZ} = Piezoelectric Polarization (C/m^2)

The orientation of spontaneous and piezoelectric polarization is determined by the polarity of the III-nitride material. In general, the wurtzite III-nitride crystal exhibits two opposite sequences of atomic layering in the



(a) (b)

Figure 1: (a) Ga-face, and (b) N-face GaN.

c-direction resulting in either a cation-face or anion face epitaxy. Figure 1 shows a GaN crystal where (a) is cation-faced (Ga-face) and (b) is anion-faced (N-face).

The direction of spontaneous polarization in the III-nitrides is from the nitrogen atom to the closest metal atom, i.e. along the $\pm$c-axis as shown in Figure 2, which is also the typical direction of epitaxial growth in MBE or MOCVD. The direction of piezoelectric polarization is dependent on the polarity of the material as well as on the strain. Spontaneous and piezoelectric polarizations are parallel and add to each other when planar strain (perpendicular to c-axis) is tensile and are anti-parallel when planar strain is compressive.

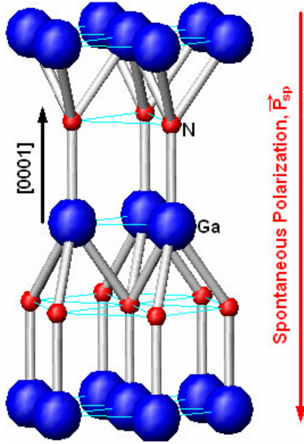


Figure 2: Direction of spontaneous polarization in Ga-face GaN.

Spontaneous polarization values can be theoretically calculated, established experimentally, or can be determined for ternary compounds by interpolating the values of the constituent binary compounds using an appropriate bowing factor as indicated in Equation 3 [4]:

$$P_{sp}^{ABN}(x) = P_{sp}^{AN}(x) + P_{sp}^{BN}(1-x) + bx(1-x) \quad \text{--- (3)}$$

In a perfectly pseudomorphic growth, the epilayer undergoes strain and assumes the lattice constant of its substrate. If the lattice constant 'a' of the epilayer is a_e and lattice constant of the substrate is a_s, then assuming a pseudomorphic epitaxial growth where the lattice constant of the substrate does not change, the strain in the epitaxial layer along the a-plane, ε, is given by:

$$\varepsilon = \frac{a_s - a_e}{a_e} \quad \text{--- (4)}$$

However, in practical scenarios, the epitaxy may not be pseudomorphic and there would be relaxation in the epitaxial layers. In that case, the epilayer at the interface would assume a lattice constant somewhere between its own original value and that of the substrate depending on the degree of relaxation. Thus, the calculation of piezoelectric polarization requires an additional strain relaxation model at the interfaces of active epitaxial layers of the solar cell. If the new strained lattice constant of GaN at the interface is a'_e, then the strain at this interface along the a-plane is given as:

$$\varepsilon_x = \frac{a'_e - a_e}{a_e} = \frac{a_s - a_e}{a_e}(1-R) \quad \text{--- (5)}$$

where, R = Relaxation Factor, $0 < R < 1$

For an ideal pseudomorphic case ($a'_e = a_s$) R = 0, while for a completely relaxed epilayer, R = 1, and strain at the interface is zero ($\varepsilon_x = 0$). This relaxation factor can be determined experimentally. The resultant strain in GaN at the interface in z-direction is given by:

$$\varepsilon_z = -2\left(\frac{C_{13}}{C_{33}}\right)\varepsilon_x \quad \text{--- (6)}$$

There is also a gradual exponential strain-relaxation profile along the thickness of the epitaxial layer, which determines the piezoelectric polarization within the bulk of the material. The strain decays exponentially along the thickness of the epitaxial material with respect to the z-direction at a rate corresponding to the Strain Relaxation Constant (RC). This RC is specific to the material as well as the conditions under which it was grown.

$$\varepsilon_z(z) = \varepsilon_{z,z=0}\, e^{-\frac{z}{RC}} \quad \text{--- (7)}$$

where,

$\varepsilon_z(z)$ = strain in GaN in the z-direction as a function of distance (z) from the interface,

$\varepsilon_{z,z=0}$ = strain in GaN in the z-direction at the interface,

RC = strain Relaxation Constant, µm

Figure 3 shows the strain relaxation profile of a GaN epilayer on AlN along the c-direction, where (a) the epitaxy is pseudomorphic, i.e. there is no relaxation at the interface, and (b) the epitaxial GaN relaxes by 95% at the AlN interface.

The nonvanishing component of piezoelectric polarization caused by biaxial strain is along the c-axis, and is given by:

$$P_{pz} = \varepsilon_x e_{31} + \varepsilon_y e_{32} + \varepsilon_z e_{33} \quad \text{--- (8)}$$

where,

$\varepsilon_x, \varepsilon_y, \varepsilon_z$ are strain components in the x, y, z direction,

e_{31}, e_{32}, e_{33} are piezoelectric constants.

Sheet charge is formed due to the gradient in polarization and is quantified at heterointerfaces as the difference in net polarization (spontaneous + piezoelectric) of the two semiconductors. In general, the polarization induced charge density with a gradient of polarization in space is given by:

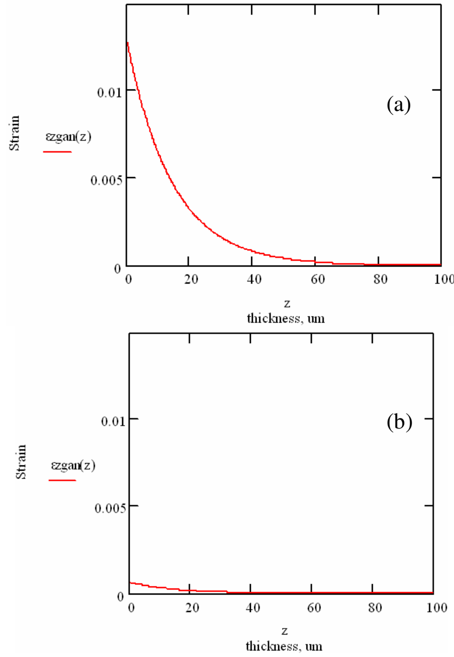


Figure 3: Strain relaxation profile of GaN on AlN template for (a) perfectly pseudomorphic epilayer, and (b) epilayer relaxed by 95%.

$$\sigma_P = -\nabla P \qquad \text{--- (9)}$$

By analogy, the fixed polarization charge density at the abrupt interface of a heterostructure is given by:

$$\sigma_P = P_{bottom} - P_{top} \qquad \text{--- (10)}$$

where, P_{bottom} = Polarization in bottom layer
P_{top} = Polarization in top layer

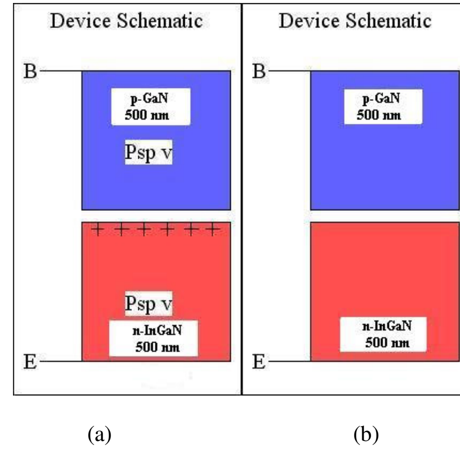
At the top and bottom of the device, P_{top} and P_{bottom} are considered to be that of air i.e. 0. The Polarization-induced sheet charge density, n_s, at the interface is then calculated by using the following equation:

$$n_s = \frac{\sigma_P}{e} \qquad \text{--- (11)}$$

This charge density causes an accumulation of carriers that influences the bands of that region and is used as the starting point for PC1D solving routine at that interface. If the sheet charge concentration at the interface is positive, it results in the formation of a 2-dimensional electron gas (2-DEG) as free electrons will tend to compensate the positive charge; similarly, a negative sheet charge concentration will result in the formation of a 2-dimensional hole gas (2-DHG). The polarization charges cause strong band bending, often causing doping inversion, and may act as a potential barrier or a trap decreasing the photogenerated current. Conversely, 2DEGs or 2DHGs can be constructively used to generate front/back surface fields to reduce surface recombination, while gradients in piezoelectric charge can be used to generate electric fields within the solar cell to enhance carrier collection.

3 SIMULATION RESULTS AND DISCUSSION

The described model is incorporated in the source-code of PC1D. The simulation results of a test structure (Figure 4) are presented and discussed. The test structure is a Ga-face device with p-GaN on n-IngaN ([In] = 20%). The GaN and InGaN layers are each 500nm thick with a p-type carrier concentration of $5\times10^{17}cm^{-3}$ and n-type carrier concentration of $5\times10^{18}cm^{-3}$, respectively. The polarization parameters used in the model are described in Table 1.



(a) (b)

Figure 4: Schematic of simulated device (a) with, and (b) without polarization.

A 500nm GaN layer is mostly relaxed and thus, does not demonstrate any piezoelectric polarization. As a first step, to ensure convergence of PC1D with this new model, we only calculate the polarization charges at the interface of the GaN/InGaN layers ignoring the effects of surface charges. The gradient in spontaneous polarization between the two layers results in the formation of a 2DHG at the interface on the InGaN side (as it is the lower band gap material). An evident effect of polarization is the increase in short circuit current from $1.307mA/cm^2$ to $3.889mA/cm^2$ as shown in Figure 5.

Table 1: Polarization parameters used in PC1D simulation of InGaN solar cell.

	GaN	$In_{0.2}Ga_{0.8}N$
Band gap (eV)	3.4	2.64
Electron Affinity (eV)	4.1	4.56
Spontaneous Polarization (Cm^{-2})	-0.029	-0.032
Lattice Const, a (Å)	3.189	3.241
Lattice Const, c (Å)	5.186	5.262
Elastic Const, C_{13} (GPa)	105	103.5
Elastic Const, C_{33} (GPa)	395	375.75
Piezoelectric Const, e_{31} (Cm^{-2})	-0.33	-0.313
Piezoelectric Const, e_{33} (Cm^{-2})	0.65	0.617

This increase in short circuit current is attributed to the increase in electric field (Figure 6) caused by polarization at the GaN/InGaN interface. The

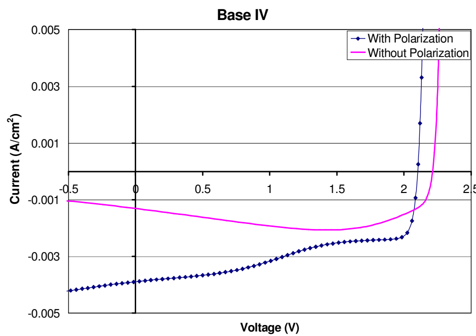


Figure 5: Base I-V curves of simulated devices with and without polarization.

polarization-induced 2DHG (2 $x10^{12}cm^{-2}$) increases the electric field from $2.745{\times}10^5$ V/cm to $4.17{\times}10^5$ V/cm, which in turn increases the collection efficiency. This effect is also supported by observation of an increase in the interface hole carrier density at the GaN/InGaN interface (Figure 7), and an increase in the depth of the triangular potential well in the valence band at the interface (Figure 8).

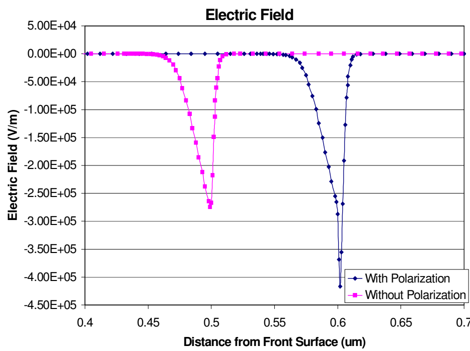


Figure 6: Spatial electric fields of devices with and without polarization. (Note: Graph with polarization shifted to right for clarity.)

The open circuit voltages for both the cases are comparable at around 2.2V. An increase in power is observed for the model with polarization at $4.615mW/cm^2$ compared to $3.343mW/cm^2$ for the model

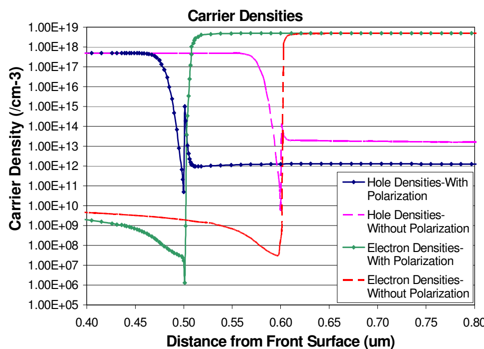


Figure 7: Spatial carrier density profile of simulated devices with and without polarization. (Note: Graph with polarization shifted to right for clarity.)

without polarization. This increase in power by 38% is primarily due to the enhancement in short-circuit current of the solar cell.

The band spikes and carrier confinement at the band spikes introduces a bias-dependent recombination, which can be seen in the IV curves as deviations from a "conventional" shifted-diode IV curve.

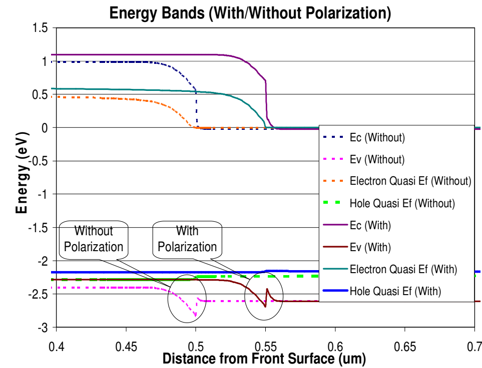


Figure 8: Spatial energy band diagrams of simulated devices with and without polarization. (Note: Graph with polarization shifted to right for clarity.)

4 CONCLUSION

The III-nitrides offer substantial potential to develop high-efficiency photovoltaics. Hence, it becomes imperative to develop a simulation program to accurately model polarization effects, which significantly affect the performance of the III-nitride solar cells. We present a detailed model for spontaneous and piezoelectric polarization and implement it in PC1D. Simulations of the GaN/InGaN test structure with polarization at the interface indicate an enhancement of the junction electric field causing an increase in short circuit current, and hence, efficiency by 38%. Future work involves optimizing radiative recombination for high band gaps in PC1D. It is also important to optimize the convergence routine of PC1D to handle abrupt charge and field profiles arising due to polarization in the device.

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REFERENCES

[1] O. Jani, I. Ferguson, C. Honsberg, S. Kurtz, "Design and characterization of GaN/InGaN solar cells," Accepted for publication in Appl. Phys. Lett.

[2] O. Jani, C. Honsberg, Y. Huang, J. O. Song, I. Ferguson, G. Namkoong, E. Trybus, A. Doolittle, S. Kurtz, *Design, Growth, Fabrication and Characterization of High-Band Gap InGaN/GaN Solar Cells,* Proc. of the IEEE 4th World Conference on Photovoltaic Energy Conversion, Waikoloa, Hawaii, May 7-12, 2006.s

[3] Y. Nanishi, Y. Saito and T. Yamaguchi, "R-F Molecular Beam Epitaxy Growth and Properties of

InN and Related Alloys", Jpn. J. Appl. Phys., 42 (2003), p. 2549.

[4] F. Bernardini, and V. Fiorentini, "Nonlinear Macroscopic Polarization in III-V Nitride Alloys", Phys. Rev. B, 64 (2001), p. 085207/1.

[5] V. Fiorentini F. Bernardini, "Spontaneous versus Piezoelectric Polarization in III-V Nitrides: Conceptual Aspects and Practical Consequences", Phys. Stat. Sol. B, 216 (1999), p. 391.

[6] O. Ambacher, J. Smart, J. R. Shealy, N. G. Weimann, K. Chu, M. Murphy,W. J. Schaff, L. F. Eastman, R. Dimitrov, L. Wittmer, M. Stutzmann, W.Rieger, and J. Hilsnbeck, "Two-dimensional electron gases induced by spontaneous and piezoelectric polarization charges in N- and Ga-face AlGaN/GaN heterostructures," J. Appl. Phys. 85 (1999), p. 3222.

[7] P. A. Basore and D. A. Clugston, PC1d Version 5.9, Sydney, Australia: Univ. New South Wales, 2003.

[8] J. C. Freeman, "*Basic equations for the modeling of Gallium Nitride (GaN) High Electron Mobility Transistors (HEMT),*" NASA/TM – 2003-211983