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Theoretical analysis of strategies for improving p-type conductivity in wurtzite III-nitride devices for high-power opto- and microelectronic applications

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Achieving high p-type conductivity is one of the most significant bottlenecks to the efficient operation of wurtzite III-N based optoelectronic and microelectronic devices. Through judicious volumetric redistribution of fixed negative polarization charge, compositionally graded layers may be exploited to achieve nearly flat valence band profiles free from electrostatic barriers to hole injection into the active region. This may potentially ameliorate problems associated with poor p-type conductivity and inefficient hole transport that complicates the design of DUV laser diodes and light emitting diodes.

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1 Introduction Wurtzite III-nitride alloys exhibit a range of direct bandgap energies conducive to diverse optoelectronic applications from the infrared to the deep ultraviolet (DUV) extremes of the optical spectrum. The realization of DUV devices in particular has been impeded by a number of materials and processing issues [1, 2], none of which are considered to be fundamental in nature with the possible exception of the apparent high electrical activation energy of the most efficient p-type dopant, magnesium [3]. Whether or not the effective activation energy of Mg is symptomatic of an auto-compensation between Mg incorporated indiscriminately among cation and anion sites, both the growth of high-conductivity p-type material suitable for most DUV applications as well as effective Ohmic contacting thereto have heretofore proven elusive.

Several authors have advocated strategies for leveraging intrinsic material properties of the wurtzite III-nitrides to realize high-conductivity wide-bandgap p-type material, and pursued them with varying degrees of success (see, e.g. [2] and references therein). One such strategy for overcoming the high activation energy of Mg involves exploitation of the substantial band edge discontinuities across III-nitride heterointerfaces for the modulation doping of short period superlattice (SPSL) layers [3]. More recently, compositional grading of strained epitaxial layers has been suggested by some authors as a means to achieve high free hole concentrations, both with and without the actual presence of p-type dopant species, and both with and without appeal to field-induced ionization of acceptors [4-10].

In this article, we explore the efficacy of various compositional grading strategies to achieve high-conductivity p-type material, through application of state-of-the-art numerical device simulation. A critical assessment of the ability to exploit volumetrically redistributed polarization charge in a meaningful way for device applications is given, with particular focus on the distinctions between equilibrium and non-equilibrium, depleted and quasi-neutral material, doped and undoped material, and metal- vs. N-face growth. We apply this understanding to suggest a strategy for achieving efficient hole injection for DUV

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light-emitting devices, and demonstrate proof of concept through rigorous numerical simulation.

2 Results and discussion

Much of the recent research into LDs and LEDs operating within the visible and UV spectra has focused on techniques for improving the conductivity of p-type layers, hole injection efficiency and electrical confinement of carriers inside the active region. Strategies for enhancing free hole concentration or reducing the activation energy of Mg dopants have received particularly intense attention (see, e.g. [2] and references therein). One such strategy, known as “polarization doping”, has been proposed for improving the electrical activation of Mg in compositionally graded AlGaN layers through the ionization of dopant atoms by means of the macroscopic electric fields induced by polarization charge [4-10]. What is certain, however, is that in lieu of abrupt heterointerfaces, compositional grading can volumetrically redistribute an interfacial polarization charge, making it energetically favorable for free holes in adjacent material to drift or diffuse into the compositionally graded region. It is important to critically assess the ability to exploit volumetrically redistributed polarization charge in a meaningful way for UV light-emitting devices.

2.1 Equilibrium and non-equilibrium

In a compositionally graded layer, the bandgap energy may increase or decrease along the growth direction. Based on the particular choice of grading, the sign of the redistributed polarization charge may be either positive or negative. On the basis of an equilibrium energy band diagram alone, one may easily draw premature conclusions concerning the efficacy of graded p-type layers to block the leakage of electrons from the active region, and the degree to which these layers block (or facilitate) the flow of holes into the active region. The energy band diagram of a given epitaxial layer structure may look considerably different under non-equilibrium conditions in strong forward bias than it does at zero bias – a condition which is underappreciated and in fact exacerbated by low p-type conductivity in quasi-neutral material. It is therefore critical for devices exploiting graded p-type layers to be designed in consideration of the band diagram under far-from-equilibrium conditions.

Moreover, although thermodynamics can provide information about the free hole density in equilibrium, it cannot provide information about how long it takes to establish this equilibrium. Indeed, despite claims to the contrary, compositionally graded layers are not intrinsically conductive, and unless a compositionally graded region is immediately adjacent to a conductive p-type layer capable of injecting free holes into the graded layer at a rate sufficient to support the high current densities required of light emitting devices, the use of compositionally graded layers is not generally efficacious, and the electrical resistance introduced into the series path can be dramatically counterproductive.

2.2 Quasi-neutral and depleted material

The activation energy of p-type dopant atoms (Mg) is very high in the wide bandgap III-N materials. The situation worsens as the bandgap increases. As a result, only a small fraction of the Mg atoms are ionized when the material is quasi-neutral. To the contrary, 100% of the Mg atoms are ionized in depleted material. Consequentially, the equilibrium band diagram may exhibit very small depletion widths, as well as flat and smooth spatial variation in the quasi-neutral materials. Under non-equilibrium conditions, significant voltage may be dropped across p-type quasi-neutral materials because of low p-type conductivity. This may promote spill-over current under non-equilibrium conditions. Equilibrium energy band diagrams do not generally hint at such deleterious behavior.

2.3 Doped and undoped material

The sign and magnitude of the net interfacial polarization charge of an $Al_xGa_{1-x}N/Al_yGa_{1-y}N$ interface (or any III-N/III-N interfaces) depends on several factors, including growth axis, metal-face vs. N-face growth, difference between mole fraction x and y and their relative significance [11]. It is obvious that a large mole fraction contrast will increase the magnitude of the net interfacial polarization charge, but it is the sign of the difference between x and y which determines the sign of the polarization charge. For the case of metal-face growth, if we assume that a layer of $Al_xGa_{1-x}N$ is grown on top of $Al_yGa_{1-y}N$, the net interfacial polarization charge will be positive if $x > y$ and vice versa. The opposite is true for N-face growth. The sign of the redistributed polarization charge in a compositionally graded region may therefore be chosen to oppose that of the bound charges associated with dopant atoms, or to reinforce them. In cases where the magnitude of the redistributed polarization charge exceeds the charge of electrically active dopant atoms in that layer, even the location of the p-n junction itself may be shifted.

2.4 Metal- and N-face growth

Judiciously chosen compositional grading, as an alternative to abrupt heterointerfaces, can volumetrically redistribute sufficient negative polarization charge to make it energetically favorable for free holes in adjacent material to enter into the compositionally graded region, thereby creating a high free hole density irrespective of whether Mg atoms are electrically active – but only if there exists a high density of free holes in adjacent material in the first place. Both N-face [4-6, 10] and the conventional metal-face [7-9] growth can, at least in principle, benefit from compositional grading, producing a flat and smooth valence band profile right up to the edge of the active region to ensure superlative hole injection efficiency. If N-face growth is adopted, one must not only ensure good crystalline quality of the epitaxial layers, but also make Ohmic contact to a wide bandgap p-type layer [9] at the top. Technical challenges associated with making Ohmic con-

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tact to wide bandgap p-type material suggest the alternative approach.

2.5 Heavy doping and thick EBLs

Inverse tapered p-waveguide layers, with c-axis and metal-face growth may be very useful for DUV LDs and LEDs to solve the problems of hole injection and poor p-type conductivity. To illustrate this point, we have simulated a prototypical AlGaN based DUV edge-emitting LD structure. The details of our simulation model may be found in [1, 2, 12, 13]. The structure simulated here is similar to the ones presented in [1, 2] except the fact that it does not employ AlInN or polarization-charge-matched quaternaries. The epitaxial structure is based entirely on ternary AlGaN material and assumes realistic levels of chemical concentrations for Mg dopant atoms, and accounts for optical losses in both bulk p-type material and p-Ohmic metallization. Incomplete ionization of dopant atoms has been calculated using bandgap dependent activation energy.

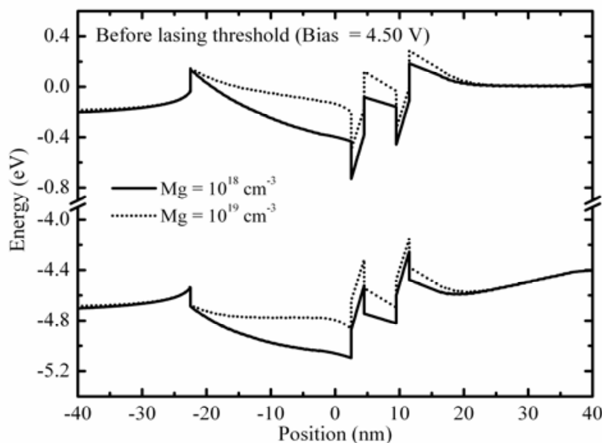

Figure 1 Heavy doping can partially mitigate unintentional polarization-induced hole blocking by the EBL

From the energy band diagram of Fig. 1, one may observe that a conventionally tapered EBL (in which the bandgap increases along the growth direction) acts as a large hole blocking layer primarily due to the unscreened polarization charge at the p-waveguide layer/EBL and spacer/QW interfaces. The substitutional dopant (Mg) concentration of the spacer, EBL and p-waveguide layer is taken to be 10^{18} cm^{-3}. (For the n-waveguide layer, the substitutional Si concentration is assumed to be 2×10^{18} cm^{-3}.) We point out that the prominence of this hole blocking layer will be artificially but only partially masked if 100% ionization of dopant atoms is assumed; however, this is not only incorrect, but also leads to a gross overestimate of hole injection efficiency.

One way to reduce the potential barrier for hole injection is to dope the p-type layers heavily. Figure 1 also shows the effect of heavy Mg doping on the energy band diagram. As expected, the barrier height of the hole blocking layer is reduced significantly. Both threshold current and voltage are lowered due to improved hole injection efficiency (results not shown here). Although heavy doping degrades carrier mobility [14-16], this effect alone does not exert a large influence on either threshold current or voltage. Instead, it is the energetic barrier to hole injection due to the valence band discontinuity at the p-waveguide layer/EBL interface with conventional tapering which is the dominant effect, limiting the mechanism for hole injection to mere thermionic emission. Making the EBL thicker does not solve the problem (see Fig. 2). Instead, it worsens the situation by offering a bigger hole blocking layer.

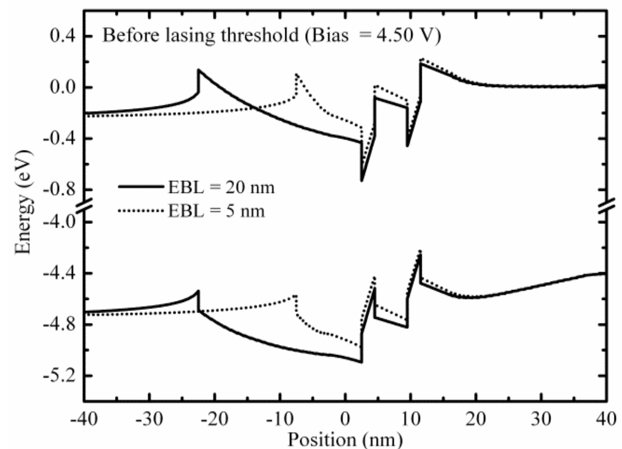

Figure 2 Thick EBL layers exacerbate polarization-induced potential barriers to hole injection.

2.6 Two-step tapered EBLs

The abrupt valence band discontinuity at the p-waveguide layer/EBL interface can be eliminated by using an EBL with two-step tapering. Specifically, the bottom half of the EBL may be tapered upwards such that its bandgap increases in the growth (c-axis, metal-face) direction (from $Al_{0.54}GaN$ to $Al_{0.60}GaN$) for efficient electron blocking. The upper half may be tapered downwards (inverse tapered) along the direction of growth (from $Al_{0.60}GaN$ to $Al_{0.48}GaN$) to eliminate abrupt valence band discontinuities. We have simulated the baseline epitaxial structure of Fig. 1 by replacing the conventionally tapered EBL with the proposed two-step tapered design, and the results are shown in Figs. 3 and 4. For meaningful comparison, the EBL thickness is held constant at 20 nm. Two-step tapering of the EBL yields a 46% reduction in threshold current and 76% improvement in slope efficiency (see Fig. 4). The band diagram of Fig. 3 clearly indicates that the two-step tapered EBL does not reduce the size of the potential barrier to hole injection, but halves its effective thickness and eliminates the abrupt valence band offset. The upper half provides a flat and smooth valence band by volumetrically redistributing negative polarization charge.

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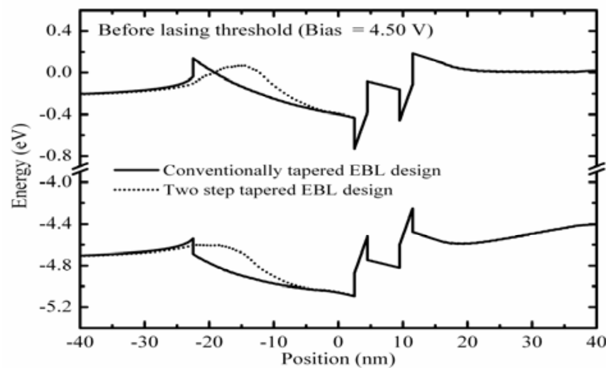

Figure 3 Two-step EBL tapering eliminates the abrupt valence band offset at the P-waveguide/EBL interface and reduces the effective thickness of the hole blocking layer.

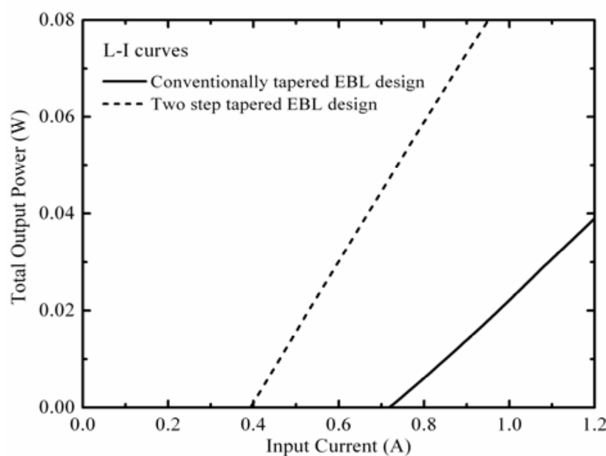

Figure 4 Comparison of L-I curves between conventionally tapered and two step tapered EBL designs. With two-step tapering, threshold current is reduced by 46% and slope efficiency is improved by 76%.

3 Conclusion

Compositionally graded layers have been investigated from multiple viewpoints. It may jeopardize efficient hole injection if not designed properly, paying special attention to several factors like growth direction, N-face growth or metal-face growth etc. Through volumetric redistribution of polarization charge, judiciously chosen compositional grading may be exploited to achieve smooth and slowly varying valence band profiles in quasi-neutral material. he concept has been applied to a DUV edge-emitting LD design and the performance improved significantly through the elimination of thermionic emission as the bottleneck to efficient hole injection, and the use of an inversely rather than conventionally tapered layer to electrostatically facilitate the supply of holes into the tapered layer from a highly conductive p-type layer above.

References

[1] M. M. Satter, H. J. Kim, Z. Lochner, J. H. Ryou, S. C. Shen, R. D. Dupuis, and P. D. Yoder, IEEE J. Quantum Electron. **48**, 703 (2012).
[2] M. M. Satter, Z. Lochner, J. H. Ryou, S. C. Shen, R. D. Dupuis, and P. D. Yoder, J. Lightwave Technol. **30**, 3017 (2012).
[3] B. Cheng, S. Choi, J.E. Northrup, Z. Yang, C. Knollenberg, M. Teepe, T. Wunderer, C. L. Chua, and N. M. Johnson, Appl. Phys. Lett. **102**, 231106 (2013).
[4] J. Simon, V. Protasenko, C. Lian, H. Xing, and D. Jena, Science **327**, 60 (2009).
[5] J. Piprek, Opt. Quantum Electron. **44**, 67 (2011).
[6] J. Verma, J. Simon, V. Protasenko, T. Kosel, H. Grace Xing, and D. Jena, Appl. Phys. Lett. **99**, 171104 (2011).
[7] S. Li, M. E. Ware, V. P. Kunets, M. Hawkridge, P. Minor, J. Wu, and G. J. Salamo, Phys. Status Solidi C **8**, 2182 (2011).
[8] L. Zhang, K. Ding, N. X. Liu, T. B. Wei, X. L. Ji, P. Ma, J. C. Yan, J. X. Wang, Y. P. Zeng, and J. M. Li, Appl. Phys. Lett. **98**, 101110 (2011).
[9] L. Zhang, K. Ding, J. C. Yan, J. X. Wang, Y. P. Zeng, T. B. Wei, Y. Y. Li, B. J. Sun, R. F. Duan, and J. M. Li, Appl. Phys. Lett. **97**, 062103 (2010).
[10] K. Dong, D. Chen, B. Liu, H. Lu, P. Chen, R. Zhang, and Y. Zheng, Appl. Phys. Lett. **100**, 073507 (2012).
[11] J. Piprek, Nitride Semiconductor Devices: Principles and Simulation (Wiley-VCH, Weinheim, 2007).
[12] M. M. Satter and P. D. Yoder, Opt. Quantum Electron. **42**, 747 (2011).
[13] M. M. Satter, Z. Lochner, J. H. Ryou, S. C. Shen, R. D. Dupuis, and P. D. Yoder, IEEE Photon. Technol. Lett. **25**, 313 (2013).
[14] P. Kozodoy, H. Xing, S. P. DenBaars, U. K. Mishra, A. Saxler, R. Perrin, S. Elhamri, and W. C. Mitchel, J. Appl. Phys. **87**, 1832 (2000).
[15] K. Kumakura, T. Makimoto, and N. Kobayashi, J. Appl. Phys. **93**, 3370 (2003).
[16] T. Katsuno, Y. Liu, D. Li, H. Miyake, K. Hiramatsu, T. Shibata, and M. Tanaka, Phys. Status Solidi C **3**, 1435 (2006).

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