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Improvement of hole injection and electron overflow by a tapered AlGaN electron blocking layer in InGaN-based blue laser diodes

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We studied the influence of a tapered AlGaN electron blocking layer (EBL) with step-graded aluminum composition on hole injection and electron overflow effects in InGaN-based laser diodes (LDs) theoretically. Schrödinger-Poisson self-consistent method together with transfer matrix method was applied to calculate carrier distribution and transport properties for both electrons and holes in tapered EBL and conventional EBL. The results indicate that the new structure favors the tunneling of low energy holes from the p-side to the active region. Meanwhile, more uniform carrier distribution and better balance between electrons and holes are obtained for the tapered structure by proper modification of band diagrams. An advanced device simulation shows the elimination of electron overflow even at a current of 180 mA in the LD with tapered EBL. Decrease of threshold current density from 2.0 kA/cm² to 1.6 kA/cm² is benefited from the more uniform local gain profile. © 2012 American Institute of Physics. [doi:10.1063/1.3678197]

III-nitride laser diodes (LDs) have attracted much attention since 1990s because of their potential usage as violet, blue, and green coherent light sources.1 The blue-violet LDs have been introduced since 1990s because of their potential usage as violet, blue, and green coherent light sources. They are the key products for data storage, full-color printing, and projection. However, several obstacles still impede the high performance of LDs. First, the III-nitride LDs are suffering from low hole injection efficiency because of inefficient Mg-doping in wide band-gap nitrides.2 In addition, the leakage of electrons overflow can be troublesome due to the low mobility of the hole in p-type III-nitrides and the high threshold carrier density required for lasing.3 As a result, recombination of carriers outside of the active region reduces the quantum efficiency of lasers.

In the early research, a typical design of 20 nm Al0.2Ga0.8N electron blocking layer (EBL) was inserted between the active layer and the p-type layer of light emitters in order to improve the above mentioned problem. It was found that the polarization mismatch between the last quantum barrier (QB) of the multiple quantum wells (MQWs) and EBL would introduce a fixed charge at this interface and create a parasitic electron inversion layer.4 At the same time, the valence band offset at the interface would form a barrier to block the transport of holes.5 The results of this structure showed a non-uniform distribution of carriers leading to an absorbing quantum well.6 To overcome this interface polarization charge problem, Chen et al.7 proposed that when the aluminum and indium compositions in the AlInGaN EBL were appropriately designed, the built-in charge density at the interface between the InGaN barrier and the AlInGaN EBL could be reduced. Lee et al.8 pointed out that the multiple quantum barrier structure could be a replacement of conventional EBL as it could block electrons more effectively. Wang et al.9 has employed the Al/Ga ratio ramping technique to grow a graded Al composition EBL from 0% to 25% in light emitting diodes and achieved enhancement of hole transportation. Zhang et al.10 recently reported a tapered AlGaN EBL with step-graded Al content in their LD structure with lower threshold current density and higher slope efficiency. This topic is still under intensive investigation but little work has been done to demonstrate the influence of EBL on the transport properties for both electrons and holes or to discuss its effects with respect to device performance.

In this work, the tapered three-layer AlGaN EBL was investigated comprehensively to disclose its effects on the blocking ability for both electrons and holes. One dimensional Schrödinger-Poisson equation was solved numerically to study the band profile and carriers distribution of the whole LD structure under polarization. Then transfer matrix method combined with the band structure of EBL was applied to study carrier transport including the reflecting probability for electrons and transmitting probability for holes. An advanced device simulation was also executed to compare the continuous wave operation of the LD structure with tapered EBL to that of a reference LD with conventional EBL.

Our simulated LD structure is composed of a 3 µm Si-doped n-type GaN layer, a 0.1 µm Si-doped n-type In0.05Ga0.95N layer, a 0.5 µm Si-doped n-type Al0.08Ga0.92N cladding layer, a 0.09 µm Mg-doped p-type Al0.08Ga0.92N cladding layer, a MQWs active region, a 20 nm AlInGaN EBL, a 0.1 µm Mg-doped p-type GaN waveguide layer, a 0.3 µm Mg-doped p-type Al0.08Ga0.92N cladding layer, and a 0.09 µm Mg-doped p-type GaN layer. The MQWs consist of three pairs of 3.5 nm In0.15Ga0.85N well layers and 7 nm In0.02Ga0.98N barrier layers where the thickness of both the first and last QB is 10 nm. For comparison, the EBL of the reference structure is a single Mg-doped Al0.18Ga0.82N layer, and that of the tapered EBL is formed by replacing the last 10 nm QB as a 5 nm p-type Mg-doped Al0.04Ga0.96N layer followed by

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another 5 nm p-type Mg-doped Al$_{0.09}$Ga$_{0.91}$N layer, while the single Al$_{0.18}$Ga$_{0.82}$N layer is left unchanged. The effective active region of the ridge geometry is 4 $\mu$m in width and the cavity is 550 $\mu$m in length. The reflectivities of both two end mirrors are set as 0.5. These two structures are shown in Fig. 1.

The self-consistent Schrödinger-Poisson equation was employed to calculate the band profile and carrier distribution of whole LD structure with different EBLs. In the simulation, built-in interface charges due to spontaneous and piezoelectric polarization were calculated by nonlinear formulas given by Bernardini et al., and the screening effect due to defects was set to be 25%. The band off-set ratio was determined to be 0.67:0.33. Other material parameters used in this simulation were adopted from the literature by Vurgaftman and Meyer. Then the band profile of EBL was taken from the whole structure to apply the transfer matrix method. For the calculation of carrier transport properties, the electron starts from the beginning of last QW and the hole starts from p-type waveguide layer.

The energy band profiles for reference and tapered structure at 60 mA are shown in Fig. 2. We can see from Fig. 2(a) that an unintentional suppression of conduction band edge is evident at the interface between the last QB and EBL. This dip is under electron quasi-Fermi level and thus electrons would accumulate at this edge. Consequently, holes from p-type material would be attracted to this edge and non-radiative recombination occurs, which is detrimental to the performance of light emitters. However, in Fig. 2(b), the conduction band offset at the interface is small due to the graded aluminum composition of tapered structure, and the strain-induced polarization charge would be spatially distributed. More importantly, p-type doping of the original QB will help to lower the electron quasi-Fermi level with respect to conduction band edge. Hence, the small dip lies high above the electron quasi-Fermi level. This optimization of energy band profile would have a considerable influence on the carrier distribution as shown in Fig. 3. For conventional EBL structure, the carrier distribution is far from uniform among the three QWs, especially for holes. In addition, electrons would gather at the band edge to form a parasitic electron inversion layer as depicted by the arrow in Fig. 3(a). However, the parasitic electron inversion layer disappears in a tapered structure as shown in Fig. 3(b). At the same time, the three layer tapered structure would lower the barrier for hole transport and p-type doping will increase hole population.

The tunneling probability of carriers in different EBLs with respect to carrier energy is summarized in Fig. 4. The positive energy corresponds to the electron transport while the negative energy corresponds to the hole transport. The transmitting probability of holes for tapered structure is larger than that of the reference EBL when hole energy is low (below 500 meV). As the hole energy increases, the
former is able to tunnel through the barrier much more easily. This result is reasonable since the tunneling of holes depends largely on the last barrier that is just above the InGaN well. The reflecting probability for electrons shows quasi-periodical behavior for the tapered structure, so it is not convenient to draw a direct conclusion whether the new structure is better than the reference one. However, as the conduction band offset between EBL and p-type GaN layer is mainly responsible for the electron blocking effect and both structures exhibit nearly the same barrier height, we would expect that the tapered structure would allow more holes to tunnel through while not deteriorating the effect of electron confinement.

In order to further investigate the influence of the above EBL structures on electron overflow effect in LDs, we performed advanced device simulation of the whole LDs with a commercial software package LASTIP. This software combines band structures and gain profiles with two dimensional waveguide, current overflow, and heat transport. Most parameters used here are the same as those adopted in transfer matrix method. Other band parameters of the materials can be found in Ref. 15. An empirical expression by Caughey-Thomas approximation is used to model the mobility of electrons and holes. A non-equilibrium quantum transport model is also implemented to describe the phenomenon that the carriers escape from the QWs before being thermalized with the local quasi-Fermi level. In Fig. 5, the vertical electron current density versus position is plotted for both structures at current density of 8.2 kA/cm². An escalation of electron leakage from QWs to the p-side is presented.
in the reference structure, which prevents carriers from stimulated emission. The reason for electron overflow can be well understood from Fig. 3(a): when carrier density overcomes threshold and becomes larger, the non-uniform distribution behavior of electrons is more obvious for the reference structure. However, for the tapered EBL structure, as the electron distribution is more uniform, the carrier density in each QW shows little difference and no current leakage is expected. This result provides firm evidence that the tapered EBL structure is also an efficient electron blocker.

As Piprek et al.\textsuperscript{6} has demonstrated, at current density close to threshold, with the non-uniform distribution of carriers among the three QWs, the n-side well would not reach transparency and it absorbs photons generated by the other two wells. The local gain profile of the reference structure is far from uniform as illustrated in Fig. 6: although the n-side well is not a parasitic well, its gain is about one order of magnitude smaller than that of the p-side well. Previous reports proposed using two QWs instead; however, the tapered EBL structure could be an alternative method to solve this problem.

Removal of this parasitic well gives more uniform local gain profile among different QWs. Thus, carriers would be effectively utilized for lasing because of less absorption and a large part of total current contributes to stimulated emission. At the same current injection level, for reference structure, photons generated in the p-side well would be absorbed in the n-side well; while for tapered structure, all three QWs reach transparency almost simultaneously. As a result, the tapered structure would achieve lasing early with smaller threshold current. As demonstrated in Fig. 7, the threshold current density is reduced from 2.0 kA/cm\textsuperscript{2} to 1.6 kA/cm\textsuperscript{2} by using the tapered EBL structure instead of the conventional EBL. The current-voltage characteristic is also shown in Fig. 7, and the slightly increased forward voltage of the tapered structure can be attributed to the higher Al content compared to conventional GaN barrier, thus increase the series resistance in the device.\textsuperscript{19} However, further optimization with polarization doped graded Al composition layer would reduce forward voltage and series resistance.\textsuperscript{20} Light output intensity at a maximum current injection level of 180 mA exhibits a 15% increase. It is noteworthy that use of tapered EBL only changes the optical confinement factor of fundamental waveguide mode slightly (less than 3%), from 3.01% to 3.09%. Therefore, the increased output power is mostly a result of better carrier confinement and uniform carrier distribution.

In conclusion, the effects of a tapered AlGaN EBL on the hole injection and electron overflow behaviors in InGaN-based laser diodes were investigated theoretically. Self-consistent Schrödinger-Poisson equation and transfer matrix method were employed to study the carrier distribution and transport properties. The results show that the tapered structure would eliminate the parasitic electron inversion layer and facilitate hole transport by letting more low energy holes tunnel through. Suppression of electron overflow was achieved as the vertical electron current decreases to almost zero at the p-side. Reduction of threshold current density from 2.0 kA/cm\textsuperscript{2} to 1.6 kA/cm\textsuperscript{2} and 15% increase of light output power were also obtained.

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